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OAK RIDGE NATIONAL LABORATORY

MARTIN MARIETTA

Engineering Physics and Mathematics Division Progress Report for Period Ending March 31, 1991

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ENGINEERING PHYSICS AND MATHEMATICS DIVISION PROGRESS REPORT FOR PERIOD ENDING MARCH 31, 1991

R. C. Ward, Director

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ORNL-6582	**Period Ending August 31, 1989**

Progress reports for research in the Mathematical Sciences prior to 1984 are as follows:

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ORNL-4514	**Period Ending December 31, 1969**
ORNL-4661	**Period Ending December 31, 1970**
ORNL-4761	**Period Ending December 31, 1971**
ORNL-4851	**Period Ending December 31, 1972**
ORNL-4989	**Period Ending June 30, 1974**
UCCND/CSD-18	**Period Ending June 30, 1975**
ORNL/CSD-13	**Period Ending June 30, 1976**
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ORNL/CSD-82	**Period Ending June 30, 1981**
ORNL/CSD-105	**Period Ending June 30, 1982**
ORNL/CSD-118	**Period Ending June 30, 1983**

PREFACE

The primary purpose of this report is to provide an archival record of the activities of the Engineering Physics and Mathematics Division during the period September 1, 1989 through March 31, 1991. Earlier reports in this series are identified on the previous pages, along with the progress reports describing ORNL's research on the mathematical sciences prior to 1984 when those activities moved into the division.

As in previous reports, our research is described through abstracts of journal articles, technical reports, and presentations. Summary lists of publications and presentations, staff additions and departures, scientific and professional activities of division staff, and technical conferences organized and sponsored by the division are included as appendices.

Some nontechnical events during the reporting period are worth noting. Fred Maienschein, who had been the Director of the Engineering Physics and Mathematics Division and its preceding divisions since 1966, retired on December 31, 1990. His excellent leadership and guidance will be sorely missed. The division organization chart, as of September 1, 1991, is included at the back of the report.

The Department of Energy sent a Tiger Team to ORNL to audit the Laboratory's environmental, safety, health, and management practices. The audit started on October 22, 1990, and concluded six weeks later. Division management and staff spent a considerable amount of time preparing for the visit, and fortunately, no significant problems were found in our division. With the emphasis on these issues continuing to increase, Cloyd O. Beasley, Jr., has been named Operations Manager with primary responsibility for overseeing the division's operations with respect to environmental, safety and health compliance.

Despite the time spent on environmental and safety issues, many important research accomplishments were attained and are briefly described in the pages that follow. The report is organized following the division of our research among four sections and information centers.

Mathematical Sciences. Increased emphasis in the mathematical sciences have been given to those research activities designed to help scientists solve computational grand challenges; that is, fundamental problems in science or engineering, whose solution would be enabled by the application of high-performance computing systems and algorithms. The Advanced Computing Laboratory took delivery in January, 1990, of the first Intel iPSC/860, which, at the time, was the world's most powerful multicomputer. High-performance algorithms and software tools have been developed so that most application codes exhibit sustained performance greater than 2 gigaflops on the Intel. Staff researchers have won two prestigious awards for their research: the 1990 Gordon Bell Award for Price/Performance and the 1990 IBM Supercomputing Competition in Computer Sciences.

Nuclear Data Measurement and Evaluation. The U.S. Evaluated Nuclear Data File, Version VI (ENDF/B-VI) was released in 1990, and our staff provided about 60% of the nuclear data measurement and evaluation work in the files. ORELA (the Oak Ridge Electron Linear Accelerator) remains as the prime nuclear data facility in the world and continues to attract a host of researchers from the United States and foreign countries. Researchers from the University of Vienna and ORNL staff collaborated to complete experiments on ORELA that made the first meaningful nonzero measurement of the electric polarizability of the neutron.

Intelligent Systems. The CESAR laboratory continues to add to its experimental capabilities. In addition to the mobile robot prototypes, HERMIES-IIB and HERMIES III, a new experimental platform based on VLSI fuzzy logic processor has been developed. A new Cognitive Engineering Research Laboratory equipped with eye-gaze test instruments is now available to support our human factors research. Increased emphasis has been given to the application of our research on neural nets and expert systems, specifically to pattern recognition problems in biophysics and molecular biology. Using software developed by our staff, researchers around the world can send their gene data via internet networks to one of our computers and have it analyzed and returned within a few seconds, all automatically.

Nuclear Analysis and Shielding. Shielding analysis, both experimental and computational, continues to be performed for important nuclear-related activities around the world. The Tower Shielding Facility, shut down due to DOE-wide reactor safety concerns, restarted in January 1990, allowing the joint U.S.–Japan reactor shielding program, JASPER, to resume in August of that year. Our computational capabilities continue to improve by upgrading our codes with new methods and experimenting with new computing technology. Our growing high-energy physics work now includes collaborations with the various detector systems vying for approval for use with the Superconducting Supercollider.

Engineering Physics Information Center. The Radiation Shielding Information Center continues to provide radiation transport software and related documentation and evaluation as a service to the nuclear industry. With the increased emphasis on the environment and safety, usage of this service has greatly increased over the reporting period. A new effort began in 1990 provides shielding analysis and documentation support for the Y-12 Plant radioactive material container and shipment program

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Section 1

MATHEMATICAL SCIENCES

1.0. INTRODUCTION

R. F. Sincovec

The Mathematical Sciences Section has three main objectives: to perform research in computer science, mathematics, and statistics germane to the solution of national energy problems; to collaborate and consult with other scientists and engineers on such problems especially with respect to the computer science and mathematical aspects of the problems; and to maintain expertise in advanced and leading-edge computer science and mathematical technologies with particular attention to technologies related to advanced large-scale parallel scientific computing.

The research program in computer science is focused on the development of algorithms for efficiently solving important basic computational problems of science and engineering, especially matrix computations, on advanced computer architecture, and on software tools that aid in this development. Recent highlights of the algorithmic research include the development and analysis of new serial and parallel algorithms for the ordering, symbolic factorization, and numerical factorization of sparse matrix problems, the development and analysis of parallel algorithms for computing eigenvalues of both symmetric and nonsymmetric tridiagonal systems, an investigation into the influence of matrix ordering on preconditioners for conjugate gradient methods, and the development of fast techniques for generating optimal piecewise polynomial models to histogram data. In the area of software tools, we have continued to develop and maintain PICL, a portable instrumented communication library, ParaGraph, a graphical display system for visualizing the performance of parallel programs, and PVM, a software package that allows the utilization of a heterogeneous network of parallel and serial computers as a single computational resource. These tools have recently proven crucial in the development of efficient parallel codes for global climate modeling and calculating the electronic structure of high temperature superconductors. We have also begun development of a new tool, hence, that supports the creation, compilation, execution, debugging, and analysis of parallel programs for a heterogeneous group of computers.

Research in mathematics during the reporting period emphasized the mathematical modeling of environmental problems using vector and parallel supercomputers. Particular accomplishments are effective parallel algorithms for global climate modeling, hypersingular boundary integral equation methods for groundwater flow, and comprehensive modeling of bioremediation processes. Recent highlights of our mathematics research and collaboration have been the development of parallel algorithms for the Legendre, Fourier, and spectral transforms used in many climate models; the implementation of fast methods for parallel computation of Lepton-pair production resulting from heavy ion collisions; and the development of symbolic computation techniques for evaluating hypersingular integrals which enables this method to be applied to a wide range of problems.

In statistics, our basic research focus has continued to be in the area of computational statistics and biostatistics. Some of the highlights include the development of an algorithm for use by computational scientists in the design and analysis of computer experiments and the use of derivatives in surface prediction for computer models, the development of a mathematical model that predicts hematopoietic response and associated probability of mortality during the following exposure to ionizing radiation, the development of new statistical methods for testing for mutagenicity and the development of an algorithm for finding a small set of the best models from a very large number (typically thousands) of possible hierarchical models. A new effort in the analysis of nonlinear dynamical systems involved collaboration between the Engineering Physics and Mathematics Division, Instrumentation and Controls Division and Engineering Technology Division. The work was recognized by Martin Marietta Energy Systems in the form of a technical achievement award. Our applied, or collaborative, research has involved our statisticians with work in most of the ORNL divisions and major organizations in Martin Marietta Energy Systems. Examples that illustrate the diversity of this collaborative research are quality control methods for detecting outliers in large data sets, life testing of irradiated materials, and the development of transfer functions between time series to determine water quality. Work has continued with the Y-12 Maintenance and Utilities Division on the development and establishment of a reliability centered maintenance (RCM) program. Defining sampling and methodological schemes for environmental restoration programs are becoming a large source of consulting activities.

The computational resources of the Mathematical Sciences Section are concentrated in the Advanced Computing Laboratory (ACL), which consists of a number of experimental multiprocessor systems and the infrastructure required to support the use of these computers. The ACL is also supported by the Computer Science Department of the University of Tennessee (UT). Our Intel iPSC/2 has been replaced by a much more powerful iPSC/860. The iPSC/860, which has 128 processors, each with 8 MBytes of local memory, and is capable of sustained performance in excess of 2 Gigaflops, is currently being used on some of ORNL's "grand challenge" problems. The iPSC/2, which was traded-in when the iPSC/860 was acquired, has been donated by Intel to the UT Computer Science Department and is, therefore, still accessible to ACL users. Other multiprocessors in the ACL are an Ncube/4 with 16 processors, a Cogent XTM containing 18 T800 transputers, and a 12-processor Sequent Balance. The ACL infrastructure consists of a DEC VAX 11/785 and numerous Sun and IBM workstations on a local area network with various compute, network, file, and print servers. A dedicated T1 communications link connects the ACL with the UT Computer Science Department to facilitate their access to our computers and to provide ORNL a connection to SURAnet, the southeastern regional network of NSFnet.

COMPUTER SCIENCE

General Parallel Computing

1.1

SOLVING COMPUTATIONAL GRAND CHALLENGES USING A NETWORK OF HETEROGENEOUS SUPERCOMPUTERS

A. Beguelin* J. Dongarra A. Geist R. Manchek* V. S. Sunderam†

[Abstract of paper presented at the 5th SIAM Conference on Parallel Processing for Scientific Computing, Houston, TX, March 25–27, 1991; Proc. p. A32 (1991)]

This paper describes simple experiments connecting a Cray XMP, an Intel iPSC/860, and a Thinking Machine CM2 together over a high speed network to form a much larger virtual computer. It also describes our experience with running a Computational Grand Challenge on a Cray XMP and an iPSC/860 combination. The purpose of the experiments is to demonstrate the power and flexibility of the PVM (Parallel Virtual Machine) system to allow programmers to exploit a diverse collection of the most powerful computers available to solve Grand Challenge problems.

Research sponsored by the Applied Mathematical Sciences Research Program, U.S. DOE Office of Energy Research.

*University of Tennessee, Knoxville, TN.

†Emory University, Atlanta, GA.

1.2

PERFORMANCE OF THE INTEL iPSC/860 HYPERCUBE

T. H. Dunigan

(Abstract of ORNL/TM-11491, June 1990)

The performance of the Intel iPSC/860 hypercube is contrasted with earlier hypercubes from Intel and Ncube. Computation and communication performance for a number of low-level benchmarks are presented for the Intel iPSC/1 hypercube, the Ncube hypercube, the Intel iPSC/2 hypercube, and the new Intel iPSC/860 hypercube. Performance of the concurrent file system of the iPSC/860 hypercube is also reported.

Research sponsored by Applied Mathematical Sciences Research Program, U.S. DOE Office of Energy Research.

1.3

HYPERCUBE CLOCK SYNCHRONIZATION

T. H. Dunigan

(Abstract of ORNL/TM-11744, March 1991)

Algorithms for synchronizing the times and frequencies of the clocks of Intel and Ncube hypercube multiprocessors are presented. Bounds for the error in estimating clock offsets and frequencies are formulated in terms of the clock read error and message transmission time. Clock and communication performance of the Ncube and Intel hypercubes are analyzed, and performance of the synchronization algorithms is presented.

Research sponsored by Applied Mathematical Sciences Research Program, U.S. DOE Office of Energy Research.

1.4

MODELING HIGH-TEMPERATURE SUPERCONDUCTORS AND RANDOM ALLOYS ON THE INTEL iPSC/i860

G. A. Geist B. W. Peyton
W. A. Shelton* G. M. Stocks*

[Abstract of paper presented at the Fifth Distributed Memory Computing Conference, Charleston, SC, April 8-12, 1990; Proc. Vol. 1, pp. 504-512 (1990)]

Oak Ridge National Laboratory has embarked on several computational Grand Challenges, which require the close cooperation of physicists, mathematicians, and computer scientists. One of these projects is the determination of the material properties of alloys from first principles and, in particular, the electronic structure of high-temperature superconductors.

The physical basis for high Tc superconductivity is not well understood. The design of materials with higher critical temperatures and the ability to carry higher current densities can be greatly facilitated by the modeling and detailed study of the electronic structure of existing superconductors.

While the present focus of the project is on superconductivity, the approach is general enough to permit study of other properties of metallic alloys such as strength and magnetic properties.

This paper describes the progress to date on this project. We include a description of a self-consistent KKR-CPA method, parallelization of the model, and the incorporation of a dynamic load balancing scheme into the algorithm. We also describe the development and performance of a consolidated KKR-CPA code capable of running on CRAYs, workstations, and several parallel computers without source code modification.

Performance of this code on the Intel iPSC/860 is also compared to a CRAY2, CRAYYMP, and several workstations. The code runs at over 1.6 Gflops on a 128 processor iPSC/860. Finally, some density of state calculations of two perovskite superconductors are given.

Research sponsored by Applied Mathematical Sciences Research Program, U.S. DOE Office of Energy Research.

*Metals and Ceramics Division.

1.5

ORNL RESEARCHERS DEVELOP NEW CODE FOR COMPUTATIONAL STUDIES OF SUPERCONDUCTORS

G. A. Geist

[Abstract of *SIAM News* **23(4)** (1990)]

Researchers at Oak Ridge National Laboratory (ORNL) and their colleagues have developed a computer program for calculating the electronic structure of alloys from first principles. The present version of the code executes at over 1.5 Gflops on a Cray YMP8 and over 1.6 Gflops on the Intel iPSC/860 while performing computational experiments on perovskite superconductors.

Research sponsored by Applied Mathematical Sciences Research Program, U.S. DOE Office of Energy Research.

1.6

PICL: A PORTABLE INSTRUMENTED COMMUNICATION LIBRARY – C REFERENCE MANUAL

G. A. Geist M. T. Heath
B. W. Peyton P. H. Worley

(Abstract of ORNL/TM-11130, July 1990)

PICL is a subroutine library that can be used to develop parallel programs that are portable across several distributed memory multiprocessors. The library provides portable syntax for the key communication primitives and related system calls required to program these machines. It also provides portable routines to perform certain widely-used, high-level communication operations, such as global broadcast and global sum. Finally, the library provides an execution tracing facility that can be used to monitor performance or to aid in debugging.

This report is the PICL reference manual for C programmers. It contains full descriptions of all PICL routines as well as explanations on how to use the routines to write a parallel program. A short users' guide to PICL containing examples of how to use it is available as a separate report.

Research sponsored by Applied Mathematical Sciences Research Program, U.S. DOE Office of Energy Research.

1.7

A USERS' GUIDE TO PICL: A PORTABLE INSTRUMENTED COMMUNICATION LIBRARY

G. A. Geist M. T. Heath
B. W. Peyton P. H. Worley

(Abstract of ORNL/TM-11616, October 1990)

This report is the PICL user's guide. It contains an overview of PICL and how it is used. Examples in C and Fortran are included.

PICL is a subroutine library that can be used to develop parallel programs that are portable across several distributed-memory multiprocessors. PICL provides a portable syntax for key communication primitives and related system calls. It also provides portable routines to perform certain widely-used, high-level communication operations, such as global broadcast and global summation. Finally, PICL provides execution tracing that can be used to monitor performance or to aid in debugging.

Research sponsored by Applied Mathematical Sciences Research Program, U S. DOE Office of Energy Research.

1.8

EARLY EXPERIENCE WITH THE INTEL iPSC/860 AT OAK RIDGE NATIONAL LABORATORY

M. T. Heath G. A. Geist
J. B. Drake

[Abstract of *Int. J. Supercomput. Appl.* **5(2)**, 10 (1991); also ORNL/TM-11655, September 1990]

This report summarizes the early experience in using the Intel iPSC/860 parallel supercomputer at Oak Ridge National Laboratory. The hardware and software are described in some detail, and the machine's performance is studied using both simple computational kernels and a number of complete applications programs.

Research sponsored by the Applied Mathematical Sciences Research Program, U.S. DOE Office of Energy Research.

1.9

SYNTHETIC MODELS OF DISTRIBUTED MEMORY PARALLEL PROGRAMS

D. A. Poplawski*

(Abstract of ORNL/TM-11634, September 1990)

This paper deals with the construction and use of simple synthetic programs that model the behavior of more complex, real parallel programs. Synthetic programs can be used in many ways: to construct an easily ported suite of benchmark programs, to experiment with alternate parallel implementations of a program without actually writing them, and to predict the behavior and performance of an algorithm on a new or hypothetical machine. Synthetic programs are constructed easily from scratch, from existing programs, and can even be constructed using nothing but information obtained from traces of the real program's execution.

Research sponsored by the Applied Mathematical Sciences Research Program, U.S. DOE Office of Energy Research.

*Michigan Technological University, Houghton, MI.

1.10

PVM: A FRAMEWORK FOR PARALLEL DISTRIBUTED COMPUTING

V. S. Sunderam*

(Abstract of ORNL/TM-11375, October 1989)

The PVM system is a programming environment for the development and execution of large concurrent or parallel applications that consist of many interacting, but relatively independent, components. It is intended to operate on a collection of heterogeneous computing elements interconnected by one or more networks. The participating processors may be scalar machines, multiprocessors, or special-purpose computers, enabling application components to execute on the architecture most appropriate to the algorithm. PVM provides a straightforward and general interface that permits the description of various types of algorithms (and their interactions), while the underlying infrastructure permits the execution of applications on a virtual computing environment

that supports multiple parallel computation models. PVM contains facilities for concurrent, sequential, or conditional execution of application components, is portable to a variety of architectures, and supports failure detection (and certain forms of recovery) at the process and processor levels.

Research sponsored by Applied Mathematical Sciences Research Program, U.S. DOE Office of Energy Research.

*Emory University, Atlanta, GA.

1.11

PIECEWISE LINEAR MODELS OF PROCESSOR UTILIZATION

M. D. Vose*

(Abstract of ORNL/TM-11566, June 1990)

This paper is part of a larger research effort to characterize the performance of parallel programs on distributed memory multiprocessors. We consider modeling processor utilization data by continuous piecewise linear approximations. We describe interactive tools for the identification of underlying trends and for the suppression of superfluous detail in processor utilization graphs.

Research sponsored by the Applied Mathematical Sciences Research Program, U.S. DOE Office of Energy Research.

*University of Tennessee, Knoxville, TN.

1.12

PERFORMANCE CHARACTERIZATION RESEARCH AT OAK RIDGE NATIONAL LABORATORY

P. H. Worley M. T. Heath

[Abstract of paper presented at the Fourth SIAM Conference on Parallel Processing for Scientific Computing, Chicago, IL, December 11–13, 1989; Proc. pp. 431–436 (1990)]

Research in performance characterization at Oak Ridge National Laboratory is focused on providing tools for analyzing and modeling the behavior of parallel algorithms on parallel architectures. The ultimate goal is to attain a deeper understanding of the complex interaction between parallel algorithms and architectures in order to improve performance on existing architectures and to predict performance as an aid to designing new architectures. In this paper, we describe our approach and the current status of the research.

Research sponsored by Applied Mathematical Sciences Research Program, U.S. DOE Office of Energy Research.

1.13

THE EFFECT OF TIME CONSTRAINTS ON SCALED SPEED-UP

P. H. Worley

[Abstract of *SIAM J. Sci. Stat. Comput.* **11(5)**, 838 (1990)]

Gustafson, Montry, and Benner introduced the concept of scaled speedup to characterize the capabilities of distributed-memory multiprocessors. They argued that, for a fixed-size problem, the behavior of the speedup of an algorithm as a function of the number of processors, the *speedup curve*, can be too pessimistic a measure of a multiprocessor architecture. Instead, they measured the speedup of algorithms when the size of the corresponding problem grew with the number of processors. They referred to the resulting function as the *scaled speedup curve*.

The scaled speedup curve is a function of how the size of the problem is allowed to grow. In this paper, it is demonstrated that allowing the size of a problem to grow to fill the available memory can produce dramatically different results from allowing the size of a problem to grow subject to satisfying an upper bound on the execution time. In particular, if a constraint on the execution time is enforced, then the scaled speedup curve is often very similar to the speedup curve for a fixed-size problem. It is shown that no more than 50 processors can be used efficiently for some common problems in scientific computation when using the current generation of distributed-memory multiprocessors. For other problems, it is shown that the scaled speedup curve indicates that massively parallel computers will be useful even if the execution time is constrained. In all of the cases examined, a meaningful interpretation of the scaled speedup curve depends on a constraint on the execution time.

Research sponsored by Applied Mathematical Sciences Research Program, U.S. DOE Office of Energy Research.

1.14

THE EFFECT OF MULTIPROCESSOR RADIUS ON SCALING

P. H. Worley

(Abstract of ORNL/TM-11579, June 1990)

In earlier work, it was established that, for a large class of linear partial differential equations (PDEs), increasing the problem size necessarily increases the execution time, independent of the algorithm and the number of processors used to solve the problem. In this paper, the analysis is extended to take into account the effect of the radius of the multiprocessor interconnection network on the growth in the execution time.

Define $r(p)$ to be the minimum radius over all subsets of p processors in a multiprocessor. An information-theoretic analysis is used to show that $r(p)$ determines a lower bound on the communication cost of a parallel algorithm, and that this in turn determines a lower bound on the parallel execution time. Assume that $r(p) \geq \beta \cdot p^{\gamma} - \mu$ for positive constants β, γ, and μ for a given multiprocessor. For example, this type of lower bound on $r(p)$ holds for a multiprocessor whose interconnection topology is a k-dimensional array. It is then established that, for the given class of PDEs, the time spent on interprocessor communication will be the dominant constraint on the performance of optimal algorithms when the problem and the multiprocessor are large. Moreover, as the problem and the multiprocessor increase in size, it is shown that the asymptotic increase in the parallel execution time will be determined by the communication cost and not by the computational requirements. The restriction to linear PDEs is not necessary, and similar results can be obtained for many problems in scientific computation.

Research sponsored by Applied Mathematical Sciences Research Program, U.S. DOE Office of Energy Research.

1.15

MODELING HISTORGRAM DATA WITH PIECEWISE POLYNOMIALS

P. H. Worley

(Abstract of ORNL/TM-11637, August 1990)

As part of a research project on the performance characterization of parallel programs, piecewise polynomials are used to model histogram data that represents the processor utilization curve. In this paper an algorithm is described that generates a discontinuous piecewise polynomial model in time proportional to the amount of data.

Research sponsored by the Applied Mathematical Sciences Research Program, U.S. DOE Office of Energy Research.

Dense Matrix Computations

1.16

COMPUTING THE EIGENVALUES AND EIGENVECTORS OF A GENERAL MATRIX BY REDUCTION TO GENERAL TRIDIAGONAL FORM

J. J. Dongarra G. A. Geist
C. H. Romine

(Abstract of ORNL/TM-11669, September 1990)

This paper describes programs to reduce a nonsymmetric matrix to tridiagonal form, compute the eigenvalues of the tridiagonal matrix, improve the accuracy of an eigenvalue, and compute the corresponding eigenvector.

Research sponsored by Applied Mathematical Sciences Research Program, U.S. DOE Office of Energy Research.

1.17

PARALLEL TRIDIAGONALIZATION OF A GENERAL MATRIX USING DISTRIBUTED-MEMORY MULTIPROCESSORS

G. A. Geist

[Abstract of paper presented at the Fourth SIAM Conference on Parallel Processing for Scientific Computing, Chicago, IL, December 11-13, 1989; Proc. pp. 29–35 (1990)]

Recently there has been a renewed interest in finding reliable methods for reducing general matrices to tridiagonal form. We have developed a serial reduction algorithm that appears to be very reliable in practice by incorporating an optimal pivot search and two recovery schemes. In this paper we describe a parallel version of our algorithm.

The algorithm was developed as one step in the process of finding eigenvalues of nonsymmetric matrices. Our original parallel eigenvalue routines reduced the matrix to Hesenberg form and then applied QR iteration, but the performance of the QR iteration was disappointing. Our new parallel algorithm reduces the matrix to tridiagonal form and then applies LR iteration. Using an iPSC/2, we compare the performance of the new parallel algorithm with our previous parallel algorithm and show that the new algorithm is nearly an order of magnitude faster, allowing us to solve much larger problems than previously attempted.

Research sponsored by Applied Mathematical Sciences Research Program, U.S. DOE Office of Energy Research.

1.18

THE IBM SYSTEM/6000 AND LINEAR ALGEBRA OPERATIONS

J. J. Dongarra P. Mays*
G. Radicati di Brozolo†

(Abstract of ORNL/TM-11768, January 1991)

This paper discusses the IBM RISC System/6000 workstation and a set of experiments with blocked algorithms commonly used in solving problems in numerical linear algebra. We describe the performance of these algorithms and discuss the techniques used in achieving high performance on such an architecture.

Research sponsored by Applied Mathematical Sciences Research Program, U.S. DOE Office of Energy Research; by the Computer Science Department of the University of Tennessee, Knoxville, TN; by IBM; and by the National Science Foundation Science and Technology Center Cooperative Agreement.

*Numerical Algorithms Group Ltd., United Kingdom.

†IBM European Center for Scientific and Engineering Computing, Roma, Italy.

1.19

NUMERICAL CONSIDERATIONS IN COMPUTING INVARIANT SUBSPACES

J. J. Dongarra S. Hammarling*
J. H. Wilkinson†

(Abstract of ORNL/TM-11704, November 1990)

This paper describes two methods for computing the invariant subspace of a matrix. The first involves using transformations to interchange the eigenvalues; the second involves direct computation of the vectors.

Research sponsored by Applied Mathematical Sciences Research Program, U.S. DOE Office of Energy Research and by the Science Alliance, University of Tennessee, Knoxville, TN.

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†Deceased.

1.20

FORTRAN SUBROUTINES FOR COMPUTING THE EIGENVALUES AND EIGENVECTORS OF A GENERAL MATRIX BY REDUCTION TO GENERAL TRIDIAGONAL FORM

J. J. Dongarra G. A. Geist
C. H. Romine

[Abstract of *ACM TOMS Journal* (in press)]

This paper describes programs to reduce a nonsymmetric matrix to tridiagonal form, compute the eigenvalues of the tridiagonal matrix, improve the accuracy of an eigenvalue, and compute the corresponding eigenvector.

Research sponsored by Applied Mathematical Sciences Research Program, U.S. DOE Office of Energy Research.

Sparse Matrix Computations

1.21

A COMPUTE-AHEAD IMPLEMENTATION OF THE FAN-IN SPARSE DISTRIBUTED FACTORIZATION SCHEME

C. Ashcraft* S. C. Eisenstat†
J. W. H. Liu‡ B. W. Peyton
A. H. Sherman†

[Abstract of ORNL/TM-11496, August 1990; also paper presented at the 4th Canadian Supercomputing Symposium, Montreal, Canada, June 4-6, 1990; Proc. pp. 351-361 (1990)]

In this report, we consider a compute-ahead computational technique in the distributed factorization of large sparse matrices using the fan-in parallel scheme. Experimental results on an Intel iPSC/2 hypercube are provided to demonstrate the relevance and effectiveness of this technique. Fortran source code is also included in an appendix.

Research sponsored by the Office of Naval Research; by the National Science Foundation; by the Natural Sciences and Engineering Research Council of Canada; and by the Applied Mathematical Sciences Research Program, U.S. DOE Office of Energy Research.

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1.22

AN AUTOMATIC ORDERING METHOD FOR INCOMPLETE FACTORIZATION ITERATIVE SOLVERS

E. F. D'Azevedo P. A. Forsyth*
W. P. Tang*

(Abstract of paper presented at the Eleventh SPE Symposium on Reservoir Simulation, Anaheim, CA, February 17-20, 1991)

The minimum discarded fill (MDF) ordering strategy for incomplete factorization iterative solvers is developed. MDF ordering is demonstrated for several model non-symmetric problems, as well as a waterflooding simulation which uses an unstructured grid. The model problems show a three to five fold decrease in the number of iterations compared to natural orderings. Greater than twofold improvement was observed for the waterflooding simulation.

Research sponsored by the Natural Sciences and Engineering Research Council of Canada; by the Information Technology Research Centre; and by the Applied Mathematical Sciences Research Program, U.S. DOE Office of Energy Research.

*University of Waterloo, Waterloo, Ontario, Canada.

1.23

ORDERING METHODS FOR PRECONDITIONED CONJUGATE GRADIENT METHODS APPLIED TO UNSTRUCTURED GRID PROBLEMS

E. F. D'Azevedo P. A. Forsyth* Wei-Pai Tang*

[Abstract of *SIAM J. on Matrix Analysis and Applications* (in press); also paper presented at the Copper Mountain Conference on Iterative Methods, Copper Mountain, CO, April 1–5, 1990; Proc. (1990)]

It is well known that the ordering of the unknowns can have a significant effect on the convergence of Preconditioned Conjugate Gradient (PCG) methods. There has been considerable experimental work on the effects of ordering for finite difference problems. In many cases, good results have been obtained with preconditioners based on diagonal, spiral, red/black reduced system orderings or some others. The reduced system approach gives generally rapid convergence. There has been comparatively less work on the effect of ordering for finite element problems on unstructured meshes. In this paper, we develop an ordering technique for unstructured grid problems. At any stage of the partial elimination, the next pivot node is selected so as to minimize the norm of the discarded-fill matrix. Numerical results are given for model problems and for problems arising in groundwater contamination. Computations are reported for two-dimensional triangular grids, and for three-dimensional tetrahedral grids. The examples show that ordering is important even if a reduced system (based on a generalized red/black ordering) method is used.

Research sponsored by the Natural Sciences and Engineering Research Council of Canada; by the Information Technology Research Centre; and by the Applied Mathematical Sciences Research Program, U.S. DOE Office of Energy Research.

*University of Waterloo, Waterloo, Ontario, Canada.

1.24

TASK SCHEDULING FOR PARALLEL SPARSE CHOLESKY FACTORIZATION

G. A. Geist E. Ng

[Abstract of *International Journal of Parallel Programming* 18(4), 291 (1989)]

This paper presents a solution to the problem of partitioning the work for sparse matrix factorization to individual processors on a multiprocessor system. The proposed task assignment strategy is based on the structure of the elimination tree associated with the given sparse matrix. The goal of the task scheduling strategy is to achieve load balancing and a high degree of concurrency among the processors while reducing the amount of processor-to-processor data communication, even for arbitrarily unbalanced elimination trees. This is important because popular fill-reducing ordering methods, such as the minimum degree algorithm, often produce unbalanced elimination trees. Results from the Intel iPSC/2 are presented for various finite-element problems using both nested dissection and minimum degree orderings.

Research sponsored by Applied Mathematical Sciences Research Program, U.S DOE Office of Energy Research.

1.25

PARALLEL IMPLEMENTATION OF A NONSYMMETRIC TRIDIAGONAL EIGENSOLVER

G. A. Geist E. R. Jessup

[Abstract of paper presented at the 5th SIAM Conference on Parallel Processing for Scientific Computing, Houston, TX, March 25–27, 1991; Proc. p. A4 (1991)]

In this paper, we investigate parallel solution of the nonsymmetric tridiagonal eigenproblem by the LR method, inverse iteration, and Rayleigh quotient iteration on a distributed-memory computer. We examine serial computation of eigenvalues followed by parallel computation of block- or wrap-distributed eigenvectors and parallel computation of eigenvalues using a block algorithm. We also consider pipelining the calculation of eigenvalues with the calculation of the eigenvectors. Experiments on an Intel iPSC/860, where

the communication to computation ratio is very large, show that serial eigenvalue computation with wrap-mapped eigenvector computation has the lowest execution time.

Research sponsored by the Applied Mathematical Sciences Research Program, U.S. DOE Office of Energy Research.

1.26

PARALLEL ALGORITHMS FOR SPARSE LINEAR SYSTEMS

M. T. Heath E. Ng
B. W. Peyton

[Abstract of *SIAM Review* **33(3)** (1991); also book chapter in *Parallel Algorithms for Matrix Computations*, pp. 83-124 (1990)]

In this paper we survey recent progress in the development of parallel algorithms for solving sparse linear systems on computer architectures having multiple processors. We focus our attention on direct methods for solving sparse symmetric positive definite systems, specifically by Cholesky factorization. We survey recent progress on parallel algorithms for all phases of the solution process, including ordering, symbolic factorization, numeric factorization, and triangular solution.

Research sponsored by Applied Mathematical Sciences Research Program, U S. DOE Office of Energy Research.

1.27

ON FINDING SUPERNODES FOR SPARSE MATRIX COMPUTATIONS

J. W. H. Liu* E. G. Ng
B. W. Peyton

[Abstract of *SIAM J. Matrix Anal. Appl.* (in press); also ORNL/TM-11563, June 1990]

A simple characterization of fundamental supernodes is given in terms of the row subtrees of sparse Cholesky factors in the elimination tree. Using this characterization, we present an efficient algorithm that determines the set of such supernodes in time proportional to the number of nonzeros and equations in the original matrix. Experimental results are included to demonstrate the use of this algorithm in the context of sparse supernodal symbolic factorization.

Research sponsored by Applied Mathematical Sciences Research Program, U.S. DOE Office of Energy Research and by the Department of Science, York University, North York, Ontario, Canada.

*York University, North York, Ontario, Canada.

1.28

A SCHEME FOR HANDLING RANK DEFICIENCY IN THE SOLUTION OF SPARSE LINEAR LEAST SQUARES PROBLEMS

E. Ng

[Abstract of *SIAM J. Sci. Stat. Comput.* **12(5)** (1991)]

Recently we have presented several schemes for computing sparse orthogonal factorizations using static data structures are large enough to store both the orthogonal transformations and upper triangular factor explicitly. Thus, multiple least squares problems with the same observation matrix can be solved easily. However, in order to make use of the static data structures, the orthogonal factorization is computed without column interchanges. In this article we develop an algorithm that makes use of the resulting factorization to solve rank-deficient least squares problems. The techniques used are similar to those employed by Bjorck.

Research sponsored by Applied Mathematical Sciences Research Program, U.S. DOE Office of Energy Research.

1.29

MODELING SPEEDUP IN PARALLEL SPARSE MATRIX FACTORIZATION

L. S. Ostrouchov* M. T. Heath
C. H. Romine

(Abstract of ORNL/TM-11786, December 1990)

This paper is an attempt to explain the observed performance of sparse matrix factorization algorithms on parallel computers. In particular, we examine whether the disappointing performance of these algorithms is due to insufficient parallelism in the problem or to the architectural characteristic of existing parallel computers. Through a series of theoretical models of increasing realism, we first determine upper and lower bounds on the speedup that can be expected in practice for this problem, and end with a parameterized model that is capable of reproducing the full range of behavior within these bounds, including the speedups actually observed in practice. This model suggests that the current limits on speedup in sparse factorization are due to poor communication performance of the present generation of parallel computer architectures rather than to a lack of parallelism in the problem.

Research sponsored by Applied Mathematical Sciences Research Program, U.S. DOE Office of Energy Research.

*University of Tennessee, Knoxville, TN.

1.30

AN IMPROVED METHOD FOR ONE-WAY DISSECTION WITH SINGULAR DIAGONAL BLOCKS

J. L. Barlow* U. B. Vemulapati*

(Abstract of ORNL/TM-11477, June 1990)

We consider matrices arising out of the one-way dissection method for solving large sparse systems of linear equations. The systems that we consider are those that may have singular diagonal blocks. Such systems arise in certain fluid flow problems.

Gunzberger and Nicholaides proposed a method for resolving the singularity in the diagonal blocks. This method uses the Moore-Penrose pseudoinverse. We propose two improvements to the Gunzberger-Nicholaides procedure: (1) The substitution of a weighted pseudoinverse for the Moore-Penrose pseudoinverse; (2) A more elegant implementation of the back substitution procedure. A stability analysis of both our procedure and the Gunzberger-Nicholaides procedure is given. Both our analysis and empirical tests show that our method has better numerical stability properties than the Gunzberger-Nicholaides procedure. We also implement our procedure on Intel iPSC/1 Hypercube. Our improvement to the back substitution method makes the natural parallelism in the problem easier to exploit.

Research sponsored by Applied Mathematical Sciences Research Program, U.S. DOE Office of Energy Research; by the National Science Foundation; by the Air Force Office of Scientific Research; and by the Office of Naval Research

*Penn State University, University Park, PA.

Differential Equations

1.31

ON OPTIMAL TRIANGULAR MESHES FOR MINIMIZING THE GRADIENT ERROR

E. F. D'Azevedo R. B. Simpson*

[Abstract of *Numerische Mathematik* (in press)]

Construction of optimal triangular meshes for controlling the errors in gradient estimation for piecewise linear interpolation of data functions in the plane is discussed. Using an appropriate linear coordinate transformation, rigorously optimal meshes for controlling the error in quadratic data functions are constructed. It is shown that the transformation can be generated as a curvilinear coordinate transformation for any C^3 data function with nonsingular Hessian matrix. Using this transformation, a construction of nearly optimal meshes for general data functions is described and the error equilibration properties of these meshes discussed. In particular, it is shown that equilibration of errors is not a sufficient condition for optimality. A comparison of meshes generated under several different criteria is made, and their equilibrating properties illustrated.

Research sponsored by the Natural Sciences and Engineering Research Council of Canada; by the Information Technology Research Centre; and by the Applied Mathematical Sciences Research Program, U.S. DOE Office of Energy Research.

*University of Waterloo, Waterloo, Ontario, Canada.

1.32

OPTIMAL TRIANGULAR MESH GENERATION BY COORDINATE TRANSFORMATION

E. F. D'Azevedo

[Abstract of *SIAM J. Sci. Stat. Comput.* **12(4)**, 755 (1991)]

This paper presents the motivation for and construction of coordinate transformations that generate optimally efficient meshes for linear interpolation. The coordinate transformations are derived from a result in differential geometry characterizing a "flat" space. The optimality results are demonstrated for some numerical example. Adaptive meshes produced by PLTMG are included for comparison. The paper concludes that coordinate transformation is a promising strategy for investigation into more complex optimal meshing problems in finite element analysis.

Research sponsored by the Natural Sciences and Engineering Research Council of Canada; by the Information Technology Research Centre; by the Applied Mathematical Sciences Research Program, U.S. DOE Office of Energy Research; and by the Department of Science, York University, North York, Ontario, Canada.

1.33

EXPERIMENTS WITH AN ORDINARY DIFFERENTIAL EQUATION SOLVER IN THE PARALLEL SOLUTION OF METHOD OF LINES PROBLEMS ON A SHARED MEMORY PARALLEL COMPUTER

D. K. Kahaner* **E. Ng**
W. E. Schiesser† **S. Thompson‡**

[Abstract of book chapter in *Recent Advances in Numerical Methods and Software for ODEs/DAEs/ PDEs* (in press); also *Journal of Computational and Applied Mathematics* (in press)]

We consider method of lines solutions of partial differential equations on shared-memory parallel computers. Solutions using the ordinary differential equation solver SDRIV3 (which is similar to the well-known LSODE solver) are considered. It is shown that portions of the solver may be implemented in parallel. In particular, formation of the Jacobian matrix and the linear algebra required to solve the corrector equations are natural candidates for parallel implementation since these portions dominate the cost of solving large systems of equations. A variant of Gaussian elimination is described which allows efficient parallel solution of systems of linear equations. An implementation of SDRIV3 which performs the Jacobian related calculations in parallel and which uses this variant of Gaussian elimination is described. The modified solver is used to solve a model hyperbolic fluid flow problem. Timing results, obtained using a Sequent Balance parallel computer, are given which demonstrate that substantial speed ups are possible. Extensions of the techniques to sparse problems are discussed and illustrated for a problem involving a humidification column which contacts air and water.

Research sponsored by Applied Mathematical Sciences Research Program, U.S. DOE Office of Energy Research.

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1.34

LIMITS ON PARALLELISM IN THE NUMERICAL SOLUTION OF LINEAR PARTIAL DIFFERENTIAL EQUATIONS

P. H. Worley

[Abstract of *SIAM J. Sci. Stat. Comput.* **12**(1), 1 (1991)]

The problem considered is that of approximating the solution of a linear scalar partial differential equation (PDE) at one or more locations in its domain. A lower bound on the amount of data required to satisfy a given error tolerance in the approximation is described. Using this bound, a lower bound on the execution time of parallel algorithms that approximate the solution is derived. The lower bound on the execution time has the form $\alpha \cdot f_{(+)} \cdot \log_2 \epsilon^{-1}$, where α is a problem-dependent constant, $f_{(+)}$ is a measure of the speed of floating point arithmetic, and ϵ is an upper bound on the error. Thus, when $\alpha > 0$, the execution time increases as ϵ decreases, independent of the number of processors, the interconnection topology, and the algorithm used. Lower bounds on the execution time are also given for the cases where the interconnection network or the number of processors is specified.

Recent research has established that it is often possible to use a large number of processors efficiently when calculating the numerical solution of a PDE if the problem is sufficiently large. In this paper, it is shown that increasing the size of such a problem will usually come at the cost of increasing the execution time. Two examples are described that verify this conclusion, an algorithm-independent analysis of an elliptic PDE and an analysis of a specific algorithm for the approximation of a hyperbolic PDE.

Research sponsored by Applied Mathematical Sciences Research Program, U.S. DOE Office of Energy Research.

1.35

PARALLELIZING THE SPECTRAL TRANSFORM METHOD - PART I

P. H. Worley J. B. Drake

(Abstract of ORNL/TM-11747, March 1991)

The spectral transform method is a standard numerical technique used to solve partial differential equations on the sphere in global climate modeling. In particular, it is used in CCM1 and CCM2, the Community Climate Models developed at the National Center for Atmospheric Research. This paper describes initial experiences in parallelizing a program that uses the spectral transform method to solve the nonlinear shallow water equations on the sphere, showing that an efficient implementation is possible on the Intel iPSC/860. The use of PICL, a portable instrumented communication library, and ParaGraph, a performance visualization tool, in tuning the implementation is also described.

The Legendre transform and the Fourier transform comprise the computational kernel of the spectral transform method. This paper is a case study of parallelizing the Legendre transform. For many problem sizes and numbers of processors, the spectral transform method can be parallelized efficiently by parallelizing only the Legendre transform. A subsequent paper will discuss parallelizing the Fourier transform as well.

Research sponsored by Atmospheric and Climate Research Division, U.S. DOE Office of Energy Research.

1.36

PARALLELIZING ACROSS TIME WHEN SOLVING TIME-DEPENDENT PDEs

P. H. Worley

[Abstract of paper presented at the 5th SIAM Conference on Parallel Processing for Scientific Computing, Houston, TX, March 25-27, 1991; Proc. p. A36 (1991)]

The standard numerical algorithms for solving time-dependent partial differential equations (PDEs) are inherently sequential in the time direciton. The speaker will describe a class of algorithms for the time-accurate solution of linear parabolic PDEs that can be parallelized in both time and space and have serial complexities that are proportional to the serial complexities of the best known algorithms. The speaker will also describe an algorithm with similar properties for the homogeneous wave equation in one space dimension. The existence of these algorithms disproves a conjecture made by the speaker in earlier work.

Research sponsored by the Applied Mathematical Sciences Research Program, U.S. DOE Office of Energy Research.

MATHEMATICS

Phase Change Problems

1.37

CASTING OF HgCdTe PART I: THERMOPHYSICAL PROPERTY VALUES

V. Alexiades

(Abstract of ORNL/TM-11734, March 1991)

Mercury-Cadmium-Telluride is a technologically important electronic material, used primarily as an infrared-detector. In such applications, large crystals of uniform concentration are desirable, which is difficult to achieve when the crystal is grown under gravity. Modeling and numerical simulation can help us gain insight, in the interpretation of experiments, and in designing future earth-bound and microgravity experiments.

In this report we present a compilation of the relevant thermophysical properties of the pseudo-binary $(HgTe)_{1-\chi}(CdTe)_{\chi}$, as functions of composition, χ, and temperature, for both the solid and liquid phases, at the high temperatures ($\approx$600 – 100°C) relevant in the casting process. We compile those properties which are needed in our solidification model and numerical code presented in [1]. In addition to the liquidus and solidus curves of the phase diagram, these include: densities, heat capacities, partial enthalpies, thermal conductivities and solute diffusivities. They are presented in the form of formulas, easy to evaluate, obtained by curve-fitting available data.

Research sponsored by the Microgravity Science and Applications Division of NASA and by the Science Alliance, a Centers of Excellence Program of the State of Tennessee at the University of Tennessee, Knoxville, TN.

1.38

CASTING OF HgCdTe PART II: CONDUCTION-DIFFUSION MODEL AND ITS NUMERICAL IMPLEMENTATION

V. Alexiades

(Abstract of ORNL/TM-11753, March 1991)

HgCdTe is a technologically important electronic material for which large crystals of uniform composition are desirable. This is very difficult to achieve when the crystal is grown under gravity, so it is important to understand the details of the crystal growth process both qualitatively and quantitatively.

In this report we present the first stage of the effort towards a detailed macroscopic model of the casting process, and its numerical simulation: the basic coupled conduction-diffusion model of the solidification process with constitutional supercooling and its numerical implementation. A compilation of all the relevant thermophysical properties of the pseudo-binary $(HgTe)_{1-\chi}(CdTe)_{\chi}$, as functions of composition χ and temperature, is presented in Part I. Simulation experiments will be presented in Part III.

Research sponsored by the Microgravity Science and Applications Division of NASA and by the Science Alliance, a Centers of Excellence Program of the State of Tennessee at the University of Tennessee, Knoxville, TN.

1.39

MODELING CONVECTIVE MARANGONI FLOWS WITH VOID MOVEMENT IN THE PRESENCE OF SOLID-LIQUID PHASE CHANGE

J. B. Drake

(Abstract of ORNL-6516, January 1990)

This report describes a numerical method for solving heat conduction and fluid flow problems that involve phase changes. The complications arising from materials with different liquid and solid densities are discussed, and approximations are developed for Marangoni stress, curvature dependent pressure jumps and void movement. Applications to both 0-g and 1-g environments are discussed. The fluid flow algorithm is a variant of the projection method for incompressible liquids. A control volume method of discretization along with an appropriate formulation of the conservation laws for mass and momentum yield a weak form which applies throughout the computational region. In this form no fronts between liquid and solid or between liquid and void are explicitly tracked, though the position of the fronts is readily determined from the solution field variables. The discrete equations use an implicit Crank-Nicolson method. The non-linear implicit equations are solved using a Newton method with an Approximate Factorization method for the iterative solution of the Jacobian system.

Research sponsored by Applied Mathematical Sciences Research Program, U.S. DOE Office of Energy Research.

1.40

A WEAK FORMULATION FOR PHASE-CHANGE PROBLEMS WITH BULK MOVEMENT DUE TO UNEQUAL DENSITIES

V. Alexiades J. B. Drake

(Abstract of paper presented at the Free Boundary Problems: Theory and Applications CRM Conference, Montreal, Canada, June 13-22, 1990)

When the densities of solid and liquid are different, a change of phase induces a volume change, forcing movement of the bulk phases. Conservation of total energy across the interface leads to a modified Stefan Condition, which contains a term cubic in the interfacial speed. We present a weak formulation for the conservation of mass, momentum and energy and study numerically a 1-phase, 1-dimensional example.

Research sponsored by Applied Mathematical Sciences Research Program, U.S. DOE Office of Energy Research and by the Science Alliance, a Centers of Excellence Program of the State of Tennessee at the University of Tennessee, Knoxville, TN.

Environmental Mathematics

1.41

SUMMARY OF WORKSHOP ON MATHEMATICS AND ENVIRONMENTAL WASTE PROBLEMS

L. J. Gray

[Abstract of *SIAM News* **23(5)**, 2 (1990)]

A workshop on mathematics related to environmental waste problems was held at Oak Ridge National Laboratory (ORNL), July 23 and 24. Sponsored by the Mathematical Sciences Section, ORNL, the workshop was prompted by the costly soil and groundwater remediation required in the U.S., especially at the major Department of Energy facilities. The goal of the workshop was to establish a dialogue between applied mathematicians and environmental scientists/engineers working in this area, and consequently the program of twenty talks was approximately split between mathematical and "environmental" presentations.

A common theme from all of the talks was the difficulty in obtaining data: the environmental scientists needing data to accurately characterize a contaminated site, the mathematicians seeking data with which to verify that the models conform to reality. It was recognized that these problems can never fully be solved, as there are limits on our ability to define or even estimate all of the parameters in these complex systems. The models must therefore seek to identify the major physical effects, and attempt to incorporate these as well as possible.

The workshop hopefully provided a guide for further research on mathematical methods and computational models, aiming this work towards results that can be utilized in the field. One positive step in this qdirection coming out of the workshop is the beginning of a collaborative effort at ORNL to model and understand the soil vitrification process.

Research sponsored by the Applied Mathematical Sciences Research Program, U.S. DOE Office of Energy Research.

1.42

ON THE TREATMENT OF CORNERS IN THE BOUNDARY ELEMENT METHODS

L. J. Gray

[Abstract of *J. Computational Applied Mathematics* **32**, 369 (1990)]

A new technique for treating surface discontinuities within boundary element calculations is proposed. Multiple nodes are used to represent the geometry, and the necessary additional equations are obtained by differentiating the usual boundary element integral equation. In deriving expressions for the resulting singular integrals, it is found that constraints must be placed on the functional approximation at the discontinuity. An algorithm for incorporating these constraints is developed and numerical tests for an exactly solvable three-dimensional Laplace equation problem are presented.

Research sponsored by Applied Mathematical Sciences Research Program, U.S. DOE Office of Energy Research.

1.43

EVALUATION OF THE BOUNDARY STRESS TENSOR

E. D. Lutz* A. R. Ingraffea*
L. J. Gray

(Abstract of paper presented at the International Association for Boundary Element Methods, IABEM-90 Symposium, Rome, Italy, October 15-18, 1990)

As evidenced by the recent paper by Okada, Rajiyah, and Atluri (A Novel Displacement Gradient Boundary Element Method for Elastic Stress Analysis with High Accuracy, *Trans. ASME* **55**, 786-794, 1988), there is considerable interest in being able to compute the boundary stress field. A straightforward approach within a boundary integral formulation would be to calculate the stress by differentiating the displacement integral equation. While this works for an interior point, on the boundary it requires the evaluation of hypersingular integrals. These integrals have been difficult to handle, and the displacement gradient method proposed by Okada *et al.* is designed to avoid this situation.

Recent developments (Hypersingular Integrals in Boundary Element Fracture Analysis, *Int. J. Num. Meth. Engng.*, in press) have shown that the hypersingular integral can be analytically reduced to a form suitable for computation. Using these results, it will be demonstrated that an accurate boundary stress field can be computed in a direct manner. In comparison with the displacement gradient method, the principal advantage of this technique is efficiency: the construction and solution of a second boundary element system of equations is not required. Calculated stress fields for three dimensional problems, at both smooth and nonsmooth (i.e., corners and edges) boundary points, will be presented. The treatment of the hypersingular integral at a nonsmooth boundary point is considerably more complicated than for a smooth point, and this subject will be discussed in detail.

Research sponsored by the National Science Foundation and by the Applied Mathematical Sciences Research Program, U.S. DOE Office of Energy Research.

*Cornell University, Ithaca, NY.

1.44

HYPERSINGULAR INTEGRALS AND THE TWO DIMENSIONAL HELMHOLTZ EQUATION

L. J. Gray

(Abstract of paper presented at the Japan/USA Boundary Elements Symposium, Palo Alto, CA, June 5-7, 1990)

Hypersingular integral equations have proven to be a very effective tool in the boundary element analysis of regions containing cracks. In previous studies, the reduction of the singular terms to a computationally reasonable form has relied on the ability to analytically integrate the Green's function over a flat element. The purpose of this paper is to investigate the integration of a more complicated fundamental solution, that of the two dimensional Helmholtz equation, over a curved element. The Hankel functions are treated by integrating the singular part analytically, and the remainder numerically; this process should easily generalize to three dimensions and other Green's functions. However, the higher dimensional analogue of the procedure employed herein to treat the quadratic isoparametric element is not practical, and other techniques will be required.

Research sponsored by the Applied Mathematical Sciences Research Program, U.S. DOE Office of Energy Research.

Applied Mathematics

1.45

PARTICLE-IN-CELL PLASMA SIMULATION CODES ON THE CONNECTION MACHINE

D. W. Walker

[Abstract of *International Journal of Computing Systems in Engineering* (in press); also Symposium on Parallel Methods on Large Scale Structural Analysis and Physics Applications, Hampton, VA, February 5-6, 1991]

Methods for implementing three-dimensional, electromagnetic, relativistic PIC plasma simulation codes on the Connection Machine (CM-2) are discussed. The gather and scatter phases of the PIC algorithm involve indirect indexing of data, which results in a large amount of communication on the CM-2. Different data decompositions are described that seek to reduce the amount of communication while maintaining good load balance. These methods require the particles to be spatially sorted at the start of each time step, which introduces another form of overhead. The different methods are implemented in CM Fortran on the CM-2 and compared. It was found that the general router is slow in performing the communication in the gather and scatter steps, which precludes an efficient CM Fortran implementation. An alternative method that uses PARIS calls and the NEWS communication network to pipeline data along the axes of the VP set is suggested as a more efficient algorithm.

Research sponsored by Applied Mathematical Sciences Research Program, U.S. DOE Office of Energy Research.

1.46

CHAOTIC CHARACTERISTICS OF A COMPLEX GAS-SOLIDS FLOW

C. S. Daw* **W. F. Lawkins**
D. J. Downing **N. E. Clapp, Jr.**†

[Abstract of *Phys. Rev. A* **41(2)**, 1179 (1990)]

We interpret experimental pressure-drop measurements from a complex gas-solids flow system in terms of recently developed methods for chaotic time series analysis. The results strongly support the conjecture that the flow can be described by a low-dimensional strange attractor that changes as a key turbulence parameter is varied. The analysis methods also appear to permit clear separation of the chaotic and noise components in the signal.

Research sponsored by U.S. Department of Energy.

*Engineering Technology Division.

†Instrumentation and Controls Division.

1.47

STORAGE TANK DESIGN

L. J. Gray

[Abstract of *SIAM Review* 33, 271 (1991)]

The volume of water residing inside a tilted cylindrical pipe is computed.

Research sponsored by the Y-12 Engineering Division and U.S. Department of Energy.

1.48

SOFTWARE FOR THE NUMERICAL SOLUTION OF SYSTEMS OF FUNCTIONAL DIFFERENTIAL EQUATIONS WITH STATE DEPENDENT DELAYS

K. W. Neves* S. Thompson†

[Abstract of *Journal of Applied Numerical Mathematics* (in press)]

The theoretical basis for the numerical solution of a general class of functional differential equations is reviewed. A software package for the solution of differential equations with state dependent delays is discussed. The package uses continuously imbedded Runge-Kutta methods of Sarafyan. These methods are based on C^1 piecewise polynomial interpolants which are used to handle tasks associated with root finding and interpolation. In addition to providing a means to handle user-defined root finding requirements, they provide a means to locate automatically derivative discontinuities that arise in the solution of differential equations with delays. Examples are presented which demonstrate the manner in which the software takes into account the pertinent theoretical characteristics of functional differential equations.

Research sponsored by Applied Mathematical Sciences Research Program, U.S. DOE Office of Energy Research.

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1.49

STEPSIZE CONTROL FOR DELAY DIFFERENTIAL EQUATIONS USING CONTINUOUSLY IMBEDDED RUNGE-KUTTA METHODS OF SARAFYAN

S. Thompson*

[Abstract of *Journal of Computational and Applied Mathematics* 31, 267 (1990)]

The use of continuously imbedded Runge-Kutta-Sarafyan methods for the solution of ordinary differential equations with either time-dependent or state-dependent delays is discussed. It is shown how to get reliable solutions for such problems in a manner that does not require that the effect of the local approximation error be considered separately from the local integration error. It is also shown how to reliably handle derivative discontinuities that arise in the solution of differential equations with delays.

Research sponsored by Applied Mathematical Sciences Research Program, U.S. DOE Office of Energy Research.

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1.50

ELECTROPLATING CORNERS

L. J. Gray

[Abstract of paper presented at BETECH '90, University of Delaware, Newark, DE, July 10–12, 1990; Proc. *Computational Engineering with Boundary Elements*, Vol. 1, pp. 63–70, S. Grilli, C. A. Brebbia, and A. Cheng, Eds., Computational Mechanics (1990)]

A recently proposed method for treating boundary corners is applied to a problem of practical interest, the simulation of a three-dimensional electrochemical plating process. At an edge point on the cathode surface there are two unknown flux (normal derivative) values, and the hypersingular integral equation for the boundary derivatives is employed to complete the linear system of equations. The additional complications arising in electroplating are the presence of singular solutions at a reentrant corner, nonlinear boundary conditions, and the close proximity of two different edges. Results for a realistic problem geometry are reported.

Research sponsored by the Applied Mathematical Sciences Research Program, U.S. DOE Office of Energy Research.

1.51

OVERVIEW OF THE TOUCHSTONE GAMMA PROTOTYPE ACTIVITIES AT ORNL

R. E. Flanery

[Abstract of paper presented at the iSC East Coast User's Group Meeting, Reston, VA, March 15–16, 1990; Proc. Vol. 1, p. 27 (1990)]

The presentation is an overview of work at ORNL utilizing the 128 node iPSC/860 hypercube. It is derived from a paper currently being written by members of the Mathematical Sciences Section summarizing our initial findings on the iPSC/860 and the i860 chip.

The presentation covers:

- relevent aspects of the system software and architecture
- assembler coding of BLAS-like computations, LINPACK benchmarks w & w/o assembler codes, performance results compared to peak and other computers
- performance data and comparison to existing computers for a plasma flow project
- performance data and comparison to existing computers for a superconductivity project and
- performance data and comparison to existing computers for an atomic physics project

Research sponsored by Applied Mathematical Sciences Research Program, U.S. DOE Office of Energy Research.

1.52

OPTIMAL CONTROL OF A HEAT TRANSFER PROBLEM WITH CONVECTIVE BOUNDARY CONDITION

S. M. Lenhart D. G. Wilson*

[Abstract of *Journal of Optimization Theory and Applications* (in press); also paper presented at the Conference on Differential Equations and Mathematical Physics, University of Alabama, Birmingham, AL, March 15–20, 1990 and at the 29th IEEE Conference on Decision and Control Honolulu, HI, December 5–7, 1990; Proc. Vol. 1, pp. 142–143 (1990)]

We consider the problem of controlling the solution of the heat equation with the convective boundary condition taking the heat transfer coefficient as the control. We take as our cost functional the sum of the L^2 norms of the control and the difference between the temperature attained and the desired temperature. We establish the existence of solutions of the underlying initial boundary value problem and of an optimal control that minimizes the cost functional. We derive an optimality system by formally differentiating the cost functional with respect to the control and evaluating the result at an optimal control. We show how the solution depends in a differentiable way on the control using appropriate *a priori* estimates. We establish existence and uniqueness of the solution of the optimality system, and thus determine the unique optimal control in terms of the solution of the optimality system.

Research sponsored by Applied Mathematical Sciences Research Program, U.S. DOE Office of Energy Research.

*IBM, Kingston, NY.

1.53

A TWO-SIDED GAME FOR COMPETITIVE SYSTEMS WITH NONLOCAL INTERACTIONS

S. M. Lenhart V. Protopopescu
S. Stojanovic*

[Abstract of paper presented at the 29th IEEE Conference on Decision and Control, Honolulu, HI, December 5–7, 1990; Proc. Vol. 2, pp. 1030–1031 (1990)]

A two-sided game for the control of a stationary semilinear competitive system with autonomous sources is considered. Two basic situations can be envisaged in which the controls are the kernels of the nonlocal interaction terms and the source terms, respectively. In both cases, the saddle point (the optimal solution of the game) is characterized as a unique solution of the associated optimality system, which is solved by an iterative scheme.

Research sponsored by Applied Mathematical Sciences Research Program, U.S. DOE Office of Energy Research.

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1.54

VARIATIONAL APPROACH FOR COMPETITIVE SYSTEMS WITH OBSTACLES

S. M. Lenhart S. Stojanovic* V. Protopopescu

[Abstract of *Applied Mathematics and Computations* (in press)]

We prove existence and uniqueness results for competitive systems, consisting of two parabolic equations supplemented with positivity constraints. The coupling terms include local and nonlocal interaction terms. Monotone iteration schemes are used to obtain solutions in a variational approach. The solutions of the system are compared to the solution of a simplified ordinary differential system.

Research sponsored by U.S. Department of Energy.

*University of Cincinnati, Cincinnati, OH.

1.55

A MINIMAX PROBLEM FOR SEMILINEAR NONLOCAL COMPETITIVE SYSTEMS

S. M. Lenhart V. Protopopescu S. Stojanovic*

[Abstract of *Applied Mathematics & Optimization* (in press)]

A two-sided game for the control of a stationary semilinear competitive system with autonomous sources is considered. Two basic situations can be envisaged in which the controls are the kernels of the nonlocal interaction terms and the source terms, respectively. In both cases, the saddle point (the optimal solution of the game) is characterized as a unique solution of the associated optimality system, which is solved by an iterative scheme.

Research sponsored by U.S. DOE and Defense Advanced Research Projects Agency.

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1.56

ON THE USE OF ROOTFINDING ODE SOFTWARE FOR THE SOLUTION OF A COMMON PROBLEM IN NONLINEAR DYNAMICAL SYSTEMS

D. K. Kahaner* W. F. Lawkins S. Thompson†

[Abstract of *Journal of Computational and Applied Mathematics* **28**, 219 (1989)]

We discuss how rootfinding, which is built into some ODE software, can be used to generate Poincaré sections. An interactive program is also described.

Research sponsored by Applied Mathematical Sciences Research Program, U.S. DOE Office of Energy Research.

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1.57

CONTROL STRATEGIES FOR STABILIZING A ROTATING FLUID-MECHANICAL SYSTEM

W. F. Lawkins W. K. Sartory* S. Thompson† G. T. Gillies‡ R. C. Ritter‡

[Abstract of *Journal of Comp. Physics* (in press)]

A model for investigating strategies for controlling instabilities in a rotating fluid-mechanical system, where the fluid system is composed of two immiscible, incompressible fluids, is formulated. Two control strategies, one based on modern control theory and the other on direct numerical optimization of certain system parameters, are implemented in the model. The numerical approach and scientific software used to implement and solve the overall model are described and numerical results presented.

Research sponsored by the Applied Mathematical Sciences Research Program, U.S. DOE Office of Energy Research.

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‡University of Virginia, Charlottesville, VA.

STATISTICS

Design and Analysis of Computational Experiments

1.58

BAYESIAN PREDICTION OF DETERMINISTIC FUNCTIONS, WITH APPLICATIONS TO THE DESIGN AND ANALYSIS OF COMPUTER EXPERIMENTS

C. Currin* **T. J. Mitchell**
M. D. Morris **D. Ylvisaker†**

[Abstract of *Journal of the American Statistical Association* (in press)]

This article is concerned with prediction of a function $y(t)$ over a (multidimensional) domain T, given the function values at a set of "sites" $\{t_1, t_2, \ldots, t_n\}$, and with the "design,"i.e., selection of those sites. The motivating application is the design and analysis of computer experiments, where t determines the input to a computer model of a physical or behavioral system and $y(t)$ is a response that is part of the output or is calculated from it. Following a Bayesian formulation, prior uncertainty about the function y is expressed by means of a random function (stochastic process) Y, which is taken here to be a Gaussian process with stationary mean and variance. The posterior process, which is also Gaussian, is easily computed. Its mean can be used as the prediction function $\hat{y}(t)$, and its variance can be used as a measure of uncertainty about the prediction at each t. The method is driven primarily by the choice of correlation function $\mathrm{Corr}(Y_t, Y_s)$, which can be expressed as $R(t-s)$ for stationary processes. Emphasis is placed on linear and cubic correlation functions, which yield prediction functions that are, respectively, linear or cubic splines in every dimension. A posterior entropy criterion is adopted for design; this is fundamentally similar to the criterion of D-optimality that is used frequently in the design of regression experiments. A computational algorithm for finding entropy-optimal designs on multidimensional grids is described. Several examples are discussed, including a two-dimensional experiment on a computer model of a thermal energy storage device and a six-dimensional experiment on an integrated circuit simulator. Finally, some alternative approaches are discussed.

Research sponsored by Applied Mathematical Sciences Research Program, U.S. DOE Office of Energy Research.

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1.59

BAYESIAN APPROXIMATION OF SOLUTIONS TO LINEAR ORDINARY DIFFERENTIAL EQUATIONS

K. Herzog* **M. D. Morris**
T. J. Mitchell

(Abstract of ORNL/TM-11688, November 1990)

An approach to numerically solving linear ordinary differential equations, based on statistical Bayesian prediction, is described. Preliminary results on the details of choice of correlation parameters and experimental design are given, using first- and second-order example problems.

Research sponsored by Applied Mathematical Sciences Research Program, U.S. DOE Office of Energy Research.

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1.60

FACTORIAL SAMPLING PLANS FOR PRELIMINARY COMPUTATIONAL EXPERIMENTS

M. D. Morris

[Abstract of *Technometrics* 33, 161 (1991)]

A *computational model* is a representation of some physical system of interest, first expressed mathematically and then implemented in the form of a computer program; it may be viewed as a function of *inputs* which, when evaluated, produces *outputs.* In this paper, we are concerned with computational models which are deterministic, complicated enough so as to make classical mathematical analysis impractical, and which have a moderate to large number of inputs. We consider the problem of designing computational experiments to determine which inputs have important effects of an output. The proposed approach is based on classical sampling ideas, involves the use of one-factor-at-a-time experimental designs, and does not rely on assumptions such as the adequacy of a low-order polynomial as an approximation to the computational model, effect sparsity, or monotonicity of outputs with respect to inputs.

Research sponsored by Applied Mathematical Sciences Research Program, U.S. DOE Office of Energy Research.

1.61

SCREENING, PREDICTION, AND COMPUTER EXPERIMENTS

W. J. Welch* R. J. Buck†
J. Sacks† H. P. Wynn‡
T. J. Mitchell M. D. Morris

[Abstract of *Technometrics* (in press)]

Many scientific phenomena are now investigated by complex computer models or codes. Given the various input values, the code produces an output via a complex mathematical model. Often, there are many input factors, and an initial problem is to formulate a strategy to cope with this high dimensionality. We model the output of the computer code as the realization of a stochastic process. This provides a statistical basis, via the likelihood, for a stepwise algorithm to determine the important factors. We present an example where we find the six important variables amongst a 20-dimensional input, detect curvature and interactions, and produce a useful predictor with just 30 runs of the computer code. A second example applies these methods to the simulation of an electronic circuit.

Research sponsored by AT&T, NSF, NSA, and U.S. Department of Energy.

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Computational Distribution Theory

1.62

THE APPROXIMATE DISTRIBUTION OF FOUR MOMENT STATISTICS FROM TYPE III DISTRIBUTIONS

K. O. Bowman L. R. Shenton*

[Abstract of *Communications in Statistics-Theory and Methods A* 19(4), 1511 (1990)]

Taylor series in the sample size are set up for the first four moments of the standard deviation, skewness, kurtosis, and coefficient of variation, the populations being χ^2 (gamma, Pearson Type III). These moments being out of reach of purely mathematical development, the study proceeds along two independent lines. For the one, simulation methods are used, an attempt being made to fix a cycle length to ensure some stability – this cycle length is pivoted on the fourth moment of the kurtosis, an expression involving sixteenth powers of the basic χ^2-random variable. The second line of attack uses the Taylor moment series (which are taken out to at most sixty terms in the total derivatives). An algorithm is used to derive the expectation of a product of powers of elements which consists of non-central sample deviates; there are four of these involved in the kurtosis, three in the skewness, and two in the standard deviation. There is an added parameter for sample size. This expectation of products of powers of sample deviates generates a set of coefficients, each coefficient multiplied by a power of n^{-1}; the larger the moment product, the greater is the span of the powers of n^{-1}. If a final moment series is desired to include all contributions up to n^{-s}, then at least $2s$ terms will be required in the Taylor expansion; moreover the series turn out to be divergent, as far as can be judged by the behavior of the terms computed. At this point, since the series are not seen to be one-signed, and since divergence is not too chaotic (as fast as the triple factorial, say), rational fraction sequences are set up to dilute divergence (or accelerate apparent convergence); the approach is often successful but there are problems with small sample sizes and large skewness of the population sampled. Lastly, gross errors in relying on basic asymptotes are noted. The study brings out unusual confluences – computer oriented numerical analysis, distributional theory and approximation, and the power of rational fractions as divergency reducing tools.

Research sponsored by Applied Mathematical Sciences Research Program, U.S. DOE Office of Energy Research.

*University of Georgia, Athens, GA.

1.63

SOME EXACT EXPRESSIONS FOR FUNCTIONS OF SAMPLE MOMENTS

K. O. Bowman L. R. Shenton*

[Abstract of *Annals of the Institute of Statistical Mathematics* (in press)]

Exact expressions are given for the expectation of the sample coefficient of variation, particularly in uniform sampling; Frullani integrals studied by G. H. Hardy arise. A general expression is given for the moment generating function of the sample variance. The limitations of Fisher's symbolic formula for the characteristic function of sample moments (or more general statistics) are noted.

Research sponsored by Applied Mathematical Sciences Research Program, U.S. DOE Office of Energy Research.

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Research in General Statistical Methods

1.64

APPLICATIONS OF MIXTURES OF BINOMIAL DISTRIBUTIONS

K. O. Bowman M. A. Kastenbaum* L. R. Shenton†

[Abstract of *Biometrics* (in press)]

Mixtures of binomial distributions are considered in which the probability parameter p is taken to be a random variable. When the random variable is a Beta type, the mixture becomes a Skellam (1948) (negative hypergeometric) distribution. When the parameter is transformed to a continuous scale $(0,\infty)$, new mixtures arise, involving binomial expansions that may be expressed as Laplace transforms. Applications to mutation frequencies for the data of Skellam (1948) and Bender, et al. (1990) are given.

Research sponsored by the Center for Indoor Air Research and U.S. Department of Energy.

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1.65

MIXTURES OF BINOMIAL DISTRIBUTIONS

K. O. Bowman L. R. Shenton* M. A. Kastenbaum†

[Abstract of *IMS Bulletin* **19**, 607 (1990)]

Mixtures of binomial distributions arise from the basic probability by assuming the probability parameter ρ ($0< \rho < 1$) to vary according to some law; the negative hypergeometric arises when ρ has a beta density. The factorial moments have the simple form which is a Laplace transform. Thus, for example, if the function involves two parameters, then the first two sample factorial moments may be used to determine possible solutions. By replacing ρ by different functions, we have developed several other cases for mixtures of binomial distribution.

Research sponsored by U.S. Department of Energy and by the Center for Indoor Air Research.

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1.66

ON COUNTING THE NUMBER OF DATA PAIRS FOR SEMIVARIOGRAM ESTIMATION

M. D. Morris

[Abstract of *Mathematical Geology* (in press)]

In planning spatial sampling studies for the purpose of estimating the semivariogram, the number of data pairs separated by a given distance is often used as an index of the precision which can be expected from a given sampling design. Because spatial data are correlated, this can be an unreliable measure of the amount of information which can be expected from a given design. An alternative index, the "maximum equivalent uncorrelated pairs," is proposed as a measure which partially corrects for this correlation.

Research sponsored by Applied Mathematical Sciences Research Program, U.S. DOE Office of Energy Research.

1.67

A MODEL SEARCH PROCEDURE FOR HIERARCHICAL MODELS

G. Ostrouchov E. L. Frome

[Abstract of *Computational Statistics and Data Analysis* (in press)]

Large data sets cross-classified according to multiple factors are available in epidemiology and other disciplines. Their analysis often calls for finding a small set of best hierarchical log-linear models to serve as a basis for further analysis. This selection can be based on an Akaike information type statistic. Fitting all possible models

to find a best set is usually not feasible for as few as five factors (7581 possible models). By noting that the set of hierarchical models and their relationships can be represented by a graph, a graph traversal algorithm is developed that requires fitting a fraction of all models to find exactly a best subset of the models. The algorithm classifies as many models as possible on the basis of each fit. A data structure implementing the graph of model nodes keeps track of the information required by the algorithm.

Research sponsored by U.S. DOE Office of Health and Environmental Research; by the Applied Mathematical Sciences Research Program, U.S. DOE Office of Energy Research; and by the Center for Epidemiologic Research, Oak Ridge Associated Universities.

1.68

NONPARAMETRIC ANALYSES FOR TWO-LEVEL SINGLE-STRESS ACCELERATED LIFE TESTS

R. L. Schmoyer

[Abstract of *Technometrics* **33(2)**, 175 (1991)]

In accelerated life testing, information is sought about a process at normal stress levels by studying it at higher stress levels. Let $\Pr(t;x)$ be the probability of failure by time t of an item subjected to level x of a stress. In this article, I consider the nonparametric proportional hazards model. $\Pr(t;x)=1-e^{-g(x)h(t)}$, and the nonparametric accelerated failure time model, $\Pr(t;x)=F(g(x)t)$, where g and h are nonegative nondecreasing functions of x and t, respectively; F is an arbitrary distribution function; and g has sigmoid (S-shaped) curvature. I develop confidence bounds for low-stress long-time probabilities and quantiles. I also discuss a goodness-of-fit test of the proportional hazards model. The results, which are primarily for data at two levels of stress, accommodate simple right censoring.

Research sponsored by U.S. DOE Office of Health and Environmental Research.

1.69

ORDER-RESTRICTED GOODNESS-OF-FIT TESTS BASED ON SPACINGS

R. L. Schmoyer

[Abstract of *Communication in Statistics - Theory and Methods* **20(4)**, 1409 (1991)]

Goodness-of-fit tests are proposed for unimodal densities and U-shaped hazards. The tests are based on maximum product of spacings estimators, and incorporate unimodality of U-shapedness using order restrictions. A slightly improved "maximum violator" algorithm is given for computing the order-restricted estimates and test statistics. Modified spacings such as "k-spacings," which may actually increase power, ensure computational feasibility when sample sizes are large. Simulations demonstrate that the samples of size less than twenty, the use of order restrictions can increase power, even with modified spacings. The proposed methods can be used as approximations in cases of null hypotheses that are specified only up to unknown parameters that are estimated.

Research sponsored by U.S. Department of Energy and Oak Ridge Associated Universities.

1.70

COKRIGING TO ASSESS REGIONAL STREAM QUALITY IN THE SOUTHERN BLUE RIDGE PROVINCE

H. I. Jager* **M. J. Sale***
R. L. Schmoyer

[Abstract of *Water Resources Research* **26(7)**, 1401 (1990)]

Cokriging is used to predict stream chemistry at unsampled locations with the use of spatial and intervariable correlation. The technique is used in this study to predict the acid neutralizing capacity (ANC) of streams in the Southern Blue Ridge Province (SBRP). ANC measurements between pairs of streams surveyed in this region were found to be spatially correlated over distances up to around 40 km. Predictions were improved by including elevation in the analysis to represent the combined influence of elevational gradients in

climate, geology, soils, hydrology, and vegetation on stream ANC. The cokriging analysis identified specific stream reaches predicted to be most sensitive to acidification and located areas of high uncertainty. Stream ANC levels below 50 μeq/L were predicted for one-fifth of the upper nodes associated with digitized headwater reaches in the SBRP. The majority of these were located in hte higher elevations of the Great Smoky Mountains National Park, in the vicinity of Mount Mitchell, and in the Blue Ridge Mountains in southern North Carolina.

Research sponsored by U.S. Department of Energy.

*Environmental Sciences Division.

1.71

SHRINKING TECHNIQUES FOR ROBUST REGRESSION

R. L. Schmoyer S. F. Arnold*

[Abstract of *Contributions to Probability and Statistics, Essays in Honor of Ingram Olkin*, pp. 368–384, L. J. Gleser, M. D. Perlman, S. J. Press, and A. R. Sampson, Eds., Springer-Verlag, New York (1989)]

The asymptotic normality of robust estimators suggests that shrinking techniques previously considered for least squares regression are appropriate in robust regression as well. Moreover, the noisy nature of the data frequently encountered in robust regression problems makes the use of shrinking estimators particularly advantageous. Asymptotic and finite sample results and a short simulation demonstrate that shrinking techniques can indeed improve a robust estimator's performance.

Research sponsored by U.S. Department of Energy.

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1.72

PROBABILITY PROPORTIONAL TO SIZE (π ps) SAMPLING USING RANKS

T. Wright

[Abstract of *Communications in Statistics, Theory and Methods* 19(1), 347 (1990)]

There can be gains in estimation efficiency over equal probability sampling methods when one makes use of auxiliary information for probability proportional to size with replacement ($\pi pswr$) sampling methods. The usual method is simple to execute, but might lead to more than one appearance in the sample for any particular unit. When a suitable variable x is not available, one may know how to rank units reasonably well relative to the unknown y values before sample selection. When such ranking is possible, we introduce a simple and efficient sampling plan using the ranks as the unknown x measures of size. The proposed sampling plan is similar to, has the simplicity of, and has no greater sampling variance than with replacement sampling, but is without replacement.

Research sponsored by Applied Mathematical Sciences Research Program, U.S. DOE Office of Energy Research.

1.73

LAGRANGE'S IDENTITY REVEALS THE CORRELATION COEFFICIENT AND STRAIGHT LINE CONNECTION

T. Wright

[Abstract of *American Statistician* (in press)]

This note demonstrates for a wide audience that an elementary result, Lagrange's Identity, can be used to explicitly express the Pearson (Product-Moment) Correlation Coefficient so that its important properties are manifest.

Research sponsored by Applied Mathematical Sciences Research Program, U.S. DOE Office of Energy Research.

Applications of Statistical Methods

1.74

FATE OF VOLATILE AND SEMIVOLATILE ORGANIC CHEMICALS IN SOILS: ABIOTIC VERSUS BIOTIC LOSSES

T. A. Anderson* J. J. Beauchamp
B. T. Walton†

[Abstract of *Journal of Environmental Quality* 20(2), 420 (1991)]

Disappearance of 15 volatile and semivolatile organic compounds was determined in a mixture added to two different soil types, a Captina silt loam (Typic Fragiudult) and McLaurin sandy loam (Typic Paleudults), using experimental procedures to distinguish abiotic losses from biological degradation over a 7-d period. Losses due to volatilization were quantified and mass balances were calculated for each compound. Standard USEPA and National Institute of Occupational Health and Safety (NIOHS) methods were used for sample handling, storage, and analysis. The compounds (methyl ethyl ketone; tetahydrofuran; chlorobenzene; benzene; chloroform; carbon tetrachloride; *p*-xylene; 1,2-dichlorobenzene; *cis*-1,4-dichloro-2-butene; 1,2,3-trichloropropane; 2-chloronaphthalene; ethylene dibromide; hexachlorobenzene; nitrobenzene; and toluene) were applied to the soil in a mixture such that the concentration of each chemical was 100 mg/kg soil (dry wt.). The headspace of the soil samples and matched sterile (autoclaved) controls, which were incubated in the dark at 20°C in stoppered jars fitted with charcoal traps, was flushed daily to maintain aerobic conditions and to trap vapors. Apparent half-lives for the 15 organic compounds ranged from <2 to 11.3 d and showed good agreement with published values in the few instances where they were available. Rapid disappearance due to abiotic factors was observed for all chemicals during the 7-d period. Although short-term spike and recovery analyses yielded consistently reproducible recovery for all compounds, careful attempts to account for all losses, including the use of ^{14}C-toluene, were unsuccessful. Nonreversible sorption and preanalysis storage conditions were considered as contributors to this inability to achieve a mass balance. On the basis of these results, we strongly advise positive accounting for all test compounds and degradation products at the conclusion of studies involving volatile and semivolatile compounds.

Research sponsored by U.S. Department of Energy.

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†Environmental Sciences Division.

1.75

COMPARISON OF REGRESSION AND TIME-SERIES METHODS FOR SYNTHESIZING MISSING STREAMFLOW RECORDS

J. J. Beauchamp D. J. Downing
S. F. Railsback*

[Abstract of *Water Resources Bulletin* 25(5), 961 (1989)]

Regression and time-series techniques have been used to synthesize and predict the stream flow at the Foresta Bridge gage from information at the upstream Pohono Bridge gage on the Merced River near Yosemite National Park. Using the available data from two time periods (calendar year 1979 and water year 1986), we evaluated the two techniques in their ability to model the variation in the observed flows and in their ability to predict stream flow at the Foresta Bridge gage for the 1979 time period with data from the 1986 time period. Both techniques produced reasonably good estimates and forecasts of the flow at the downstream gage. However, the regression model was found to have a significant amount of autocorrelation in the residuals, which the time-series model was able to eliminate. The time-series technique presented can be of great assistance in arriving at reasonable estimates of flow in data sets that have large missing portions of data.

Research sponsored by U.S. Department of Energy.

*Environmental Sciences Division.

1.76

STATISTICAL QUALITY CONTROL TECHNOLOGY IN JAPAN

K. O. Bowman T. Hopp*
R. Kacker* R. Lundegard*

[Abstract of *Chance* (in press)]

From May 17 to June 1, 1989, a survey team organized by the National Institute of Standards and Technology, visited Japan to assess research and application of statistical quality control technology. The team explored the philosophy and conduct of total quality control (TQC) in Japanese industries, government laboratories, and national agencies. The philosophy and practice of TQC in Japan is quite different from that of the U.S. industries. Our findings are similar to the findings from "R&M 2000 Variability Reduction Process Trip to Japan," B. A. Johnson.

Research sponsored by U.S. Department of Energy and by the Office of Naval Research.

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1.77

PATTERNS OF FISH DISTRIBUTION IN RELATION TO LAKE/WATERSHED CHARACTERISTICS: REGRESSION ANALYSIS AND DIAGNOSTICS

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J. A. Shaakir-Ali† J. M. Coe†
J. P. Baker† E. P. Smith‡
J. Gallagher§

(Abstract of book chapter in *Adirondack Lakes Survey: An Interpretive Analysis of Fish Communities and Water Chemistry*, 1984–1987, published by Adirondack Lakes Survey Corporation)

The Adirondack Lake Survey Corporation (ALSC) surveyed 1469 lakes between 1984 and 1987. Of these, 1123 lakes had at least one species of fish, and 346 were fishless. Among the lakes having fish, the patterns of distribution varied widely. Information about many of the factors (environmental as well as enthropogenic) expected to account for this variation was collected during the survey. Our objectives at investigating this data set were to

- identify variables (lake and watershed characteristics) that may influence the distribution of selected fish species among Adirondack lakes, and
- examine general patterns of association between these candidate explanatory variables and fish species distributions.

Multiple logistic regression techniques were used to develop and test models for estimating the probability of fish presence/absence for brook trout, creek chub, and any fish species.

In addition to the usual maximum likelihood logistic regression results, we also applied collinearity and other associated diagnostics and variable selection procedure designed specifically for the logistic regression model in order to arrive at parsimonious models. For model evaluation, the data set was randomly divided into a model development subset and a verification subset. Several indices were calculated to compare the various models on both of these data sets. Logistic regression diagnostics were used to identify influential data points and the effect of these points on the derived model for the brook trout data. The removal of influential observations, as indicated by the logistic regression diagnostics, caused the estimated probability of brook trout being present to be more abrupt for a given change in the explanatory variables, indicating a more sharply focused model.

Research sponsored by U.S. Department of Energy.

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1.78

ESTIMATING CHARPY TRANSITION TEMPERATURE SHIFT USING WEIBULL ANALYSIS

D. J. Downing F. M. Haggag* R. K. Nanstad*

[Abstract of *Int. J. Pres. Ves. & Piping* **44**, 241 (1990)]

A primary consideration for operation of commercial nuclear light-water reactors is the fracture toughness of the reactor pressure vessel. One of the tests conducted for toughness determinations of the pressure vessel materials is the Charpy V-notch impact test. The tests are conducted over a range of test temperatures and the total impact energy required to break each specimen is determined and plotted vs test temperature. The impact energy values for a fixed temperature and radiation exposure are usually assumed to be Weibull distributed. This assumption was validated by a statistical selection process.

An important parameter in the evaluation of reactor vessel materials is termed the ductile-to-brittle transition temperature shift (ΔT_{41}) and is the temperature shift between the unirradiated and irradiated Charpy V-notch curves at the 41-J (30-ft-lb) energy level. The purpose of this paper is to introduce a methodology for estimating the ΔT_{41} value and to place limits on the error of estimation. This has been accomplished by assuming that the scale parameter in the Weibull distribution is a function of temperature (and neutron fluence for the irradiated Charpy V-notch data). An inverse regression technique is then used to solve for the temperature corresponding to an impact energy of 41 J. To obtain error bounds on this estimate, the parameters of the equation describing the scale parameter are resampled assuming a normal distribution and the inverse regression is repeated several times. This leads to several estimates of the temperature, and the variance of these values can be used to give bounds on the error of estimation.

Research sponsored by U.S. Department of Energy.

*Metals and Ceramics Division.

1.79

NONRESIDENTIAL BUILDINGS ENERGY CONSUMPTION SURVEY (NBECS): STUDY TO DEVELOP REGRESSION MODELS TO IMPUTE MISSING ELECTRICITY AND NATURAL GAS CONSUMPTION VALUES

D. M. Flanagan H. J. Tsao* R. L. Schmoyer J. M. MacDonald*

(Abstract of ORNL/TM-9421, October 1990)

Imputation procedures were designed for the 1983 Nonresidential Buildings Energy Consumption Survey (NBECS) of the Energy Information Administration (EIA) using 1979 NBECS data. The study included methodology development, data analysis, regression analyses, empirical evaluations of the regression models, and imputation procedures. Models considered were engineering models, stepwise regression, weighted regression, nonlinear regression, and log transformation regression. A method for determining the appropriateness of the imputation model for a particular set of independent variables is recommended.

Although this study was completed in 1985, this final version of the report is being issued due to continuing requests for information.

Research sponsored by U.S. DOE Office of Energy Markets and End Use, Energy End Use Division, Energy Information Administration.

*Energy Division.

1.80

POISSON REGRESSION ANALYSIS OF THE MORTALITY AMONG A COHORT OF WORLD WAR II NUCLEAR INDUSTRY WORKERS

E. L. Frome D. L. Cragle* R. McLain*

[Abstract of *Radiation Research* **123**, 138 (1990)]

A historical cohort mortality study was conducted among 28,008 white male employees who had worked for at least one month in Oak Ridge, Tennessee, during World War II. The workers were employed at two plants that were producing enriched uranium and a research and development laboratory. Vital status was ascertained through

1980 for 98.1% of the cohort members and death certificates were obtained for 96.8% of the 11,671 decedents. A modified version of the traditional standardized mortality ratio (SMR) analysis was used to compare the cause-specific mortality experience of the World War II workers with the U.S. white male population. An SMR and a trend statistic were computed for each cause-of-death category for the 30-year interval from 1950 to 1980. The SMR for all causes was 1.11, and there was a significant upward trend of 0.74% per year. The excess mortality was primarily due to lung cancer and diseases of the respiratory system. Poisson regression methods were used to evaluate the influence of duration of employment, facility of employment, socioeconomic status, birth year, period of follow-up, and radiation exposure on cause-specific mortality. Maximum likelihood estimates of the parameters in a main-effects model were obtained to describe the joint effects of these six factors on cause-specific mortality of the World War II workers. We show that these multivariate regression techniques provide a useful extension of conventional SMR analysis and illustrate their effective use in a large occupational cohort study.

Research sponsored by Applied Mathematical Sciences Research Program, U.S. DOE Office of Energy Research and Center for Epidemioilogic Studies, Oak Ridge Associated Universities, Oak Ridge, TN.

*Oak Ridge Associated Universities, Oak Ridge, TN.

1.81

MORTALITY AMONG WORKERS AT OAK RIDGE NATIONAL LABORATORY: EVIDENCE OF RADIATION EFFECTS IN FOLLOW-UP THROUGH 1984

S. Wing* C. M. Shy*
J. L. Wood* S. Wolfe*
D. L. Cragle[†] E. L. Frome

[Abstract of *JAMA* 265(11), 1397 (1991)]

White men hired at the Oak Ridge (Tenn) National Laboratory between 1943 and 1972 were followed up for vital status through 1984 (N=8318, 1524 deaths). Relatively low mortality compared with that in U.S. white men was observed for most causes of death, but leukemia mortality was elevated in the total cohort (63% higher, 28 deaths) and in workers who had at some time been monitored for internal radionuclide contamination (123% higher, 16 deaths). Median cumulative dose of external penetrating radiation was 1.4 mSv; 638 workers had cumulative doses above 50 mSv (5 rem). After accounting for age, birth cohort, a measure of socioeconomic status, and active worker status, external radiation with a 20-year exposure lag was related to all causes of death (2.68% increase per 10 mSv) primarily due to an association with cancer mortality (4.94% per 10 mSv). Studies of this population through 1977 did not find radiation-cancer mortality associations, and identical analyses using the shorter follow-up showed that associations with radiation did not appear until after 1977. The radiation-cancer dose response is 10 times higher than estimates from the follow-up of survivors of the bombings of Hiroshima and Nagasaki, Japan, but similar to one previous occupational study. Dose-response estimates are subject to uncertainties due to potential problems, including measurement of radiation doses and cancer outcomes. Longer-term follow-up of this and other populations with good measurement of protracted low-level exposures will be critical to evaluating the generalizability of the results reported herein.

Research sponsored by U.S. Department of Energy.

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1.82

ESTIMATING COMMERCIAL TRUCK VMT OF INTERSTATE MOTOR CARRIERS: DATA EVALUATION

P. S. Hu*   T. Wright
S.-P. Miaou†   D. J. Beal*
S. C. Davis*

(Abstract of ORNL/TM-11278, November 1989)

This memorandum summarizes the evaluation results of six data sources in terms of their ability to estimate the number of commercial trucks operating in interstate commerce and their vehicle miles of travel (VMT) by carrier type and by state. This is a more detailed report of the proceeding paper by P. S. Hu, T. Wright, and S. P. Miaou.

Research sponsored by U. S. Department of Energy.

*Energy Division.

†University of Tennessee, Knoxville, TN.

1.83

ESTIMATION OF COEFFICIENTS IN A MODEL OF RADIATION-INDUCED MYELOPIESIS FROM MORTALITY DATA FOR MICE FOLLOWING X-RAY EXPOSURE

M. D. Morris   T. D. Jones*
R. W. Young†

[Abstract of *Radiation Research* (in press)]

The rate coefficients in the model of cell kinetics and mortality introduced by Jones *et al.* are estimated using mortality data from several mouse experiments. Although the maximum likelihood estimates are non-unique, all estimates lead to greater cell survival than would be expected based on published CFU-S assays. The model predicts mortality accurately for a large variety of prompt, protracted, and fractionated irradiations with 250 kVp X-rays.

Research sponsored by the U.S. Department of Energy and Defense Nuclear Agency.

*Health and Safety Research Division.

†Defense Nuclear Agency, Washington, DC.

1.84

STATISTICAL ANALYSES OF FRACTURE TOUGHNESS RESULTS FOR TWO IRRADIATED HIGH-COPPER WELDS

R. K. Nanstad*   D. E. McCabe*
F. M. Haggag*   K. O. Bowman
D. J. Downing

(Abstract of paper presented at the 15th Symposium on Effects of Radiation on Materials, Nashville, TN, June 17–21, 1990)

The objectives of the Heavy-Section Steel Irradition Program Fifth Irradiation Series were to determine the effects of neutron irradiation on the transition temperature shift and the shape of the K_{Ic} curve described in Section XI of the *ASME Boiler and Pressure Vessel Code*. Two submerged-arc welds with copper contents of 0.23 and 0.31% were commercially fabricated in 215-mm-thick plates. Charpy V-notch (CVN) impact, tensile, drop-weight, and compact specimens up to 203.2 mm thick [1T, 2T, 4T, 6T, and 8T C(T)] were tested to provide a large data base for unirradiated material. Similar specimens with compacts up to 4T were irradiated at about 288°C to a mean fluence of about 1.5×10^{19} neutrons/cm^2 (>1 MeV) in the Oak Ridge Research Reactor. Both linear-elastic and elastic-plastic fracture mechanics methods were used to analyze all cleavage fracture results and local cleavage instabilities (pop-ins). Evaluation of the results showed that the cleavage fracture toughness, K_{Jc}, values determined at initial pop-ins fall within the same scatter band as K_{Ic} values from failed specimens; thus, they were included in the data base for analysis.

Research sponsored by U.S. Department of Energy.

*Metals and Ceramics Division.

1.85

COMPUTER COMMUNICATION: ELECTRONIC BULLETIN BOARDS

G. Ostrouchov

[Abstract of *Statistical Computing and Statistical Graphics Newsletter* 1(1), 14 (1990)]

This article gives a brief description of various electronic bulletin boards (sometimes known as mailing lists, news services, or electronic conferencing systems) that are potentially useful to statisticians.

Research sponsored by U.S. Department of Energy.

1.86

COMPUTER COMMUNICATION: SOFTWARE DISTRIBUTION LIBRARIES

G. Ostrouchov

[Abstract of *Statistical Computing and Statistical Graphics Newsletter* 1(2), 17 (1990)]

This article discusses software distribution libraries that are of potential interest to statisticians. Descriptions of Netlib and Statlib are included.

Research sponsored by U.S. Department of Energy.

1.87

COMPUTER COMMUNICATION: ANONYMOUS FTP

G. Ostrouchov

[Abstract of *Statistical Computing and Statistical Graphics Newsletter* 2(1), 15 (1991)]

FTP stands for file transfer protocol and allows the user to transfer files between two computer systems. Vast amounts of information are available via anonymous ftp. A brief description of anonymous ftp and its use is given.

Research sponsored by U.S. Department of Energy.

1.88

THE SOLUBILITY OF H, D, AND T IN $Pd_{(1-Z)}Ag_Z$ ALLOYS ($Z = 0$ to 1)

G. L. Powell* W. E. Lever R. Lasser†

[Abstract of *Zeitschrift für Physikalische Chemie Neue Folge* 163, 47 (1989)]

The equilibrium constants $K^{\infty} = X^2/P$, where P is the H_2 pressure in atms and X is the H-to-metal atom ratio, are reported for H and D dissolved in $Pd_{(1-Z)}Ag_Z$ alloys for nine alloy compositions over the range of Z=0 to 0.8. These determinations are bounded by the temperature extremes of 250 K to 1500 K and values of K^{∞} between 10^{-7} and 10. These results were pooled with those to T, for $Z < 0.3$ and with the upper temperature limited to 873 K, and for those for H in Ag above 650 K and described by an analytical model. The model indicated that the Einstein temperature increased from 800 K for Z=0 to 1350 K to Z=1.

Research sponsored by U.S. Department of Energy.

*Development Division, Y-12 Plant.

†Institut für Festkörperforschung, Federal Republic of Germany.

1.89

MOMENT INVARIANTS FOR AUTOMATED INSPECTION OF PRINTED MATERIAL

M. L. Simpson* R. L. Schmoyer
M. A. Hunt*

[Abstract of *Optical Engineering* 30(4), 424 (1991)]

The use of moment invariants for the detectoin of flaws in automated image processing inspection of printed graphic material is investigated. Prior work with moment invariants has concentrated on two-dimensional image pattern recognition. A major limitation in pattern recognition applications has been the segmentation of the image from its background. Automated image processing inspection of printed material does not suffer from this limitation because a standard image background exists. The potential for separating flawed and unflawed printed material using moment invariants is demonstrated with formal statistical experiments.

Research sponsored by U.S. Department of Energy.

*Instrumentation and Controls Division.

1.90

FEASIBILITY STUDY TO UPDATE ANNUALIZED COST OF LEAVING (ACOL) PROCEDURES AT THE NAVY PERSONNEL RESEARCH AND DEVELOPMENT CENTER (NPRDC)

D. Trumble* D. M. Flanagan

(Abstract of ORNL/TM-10613, December 1990)

Accurate forecasts of officer retention rates are required in order to shape correctly the size and internal structure of the Navy manpower force through accession, promotion, and related policies. This study, conducted in 1987 for the Navy Personnel Research and Development Center (NPRDC), reviews existing forecasting and simulation methodologies and suggests new methods to implement in the future in order to improve forecasts of naval officer retention rates. The study also considers alternative sources of data to capture civilian earnings opportunities in the models. Two major types of models – Annualized Cost of Leaving (ACOL) and Dynamic Retention (DR) – are discussed in detail with respect to the ability to model and evaluate manpower policies of interest to NPRDC staff. A variety of other techniques which should be considered during the estimation stage are also discussed.

Research sponsored by Navy Personnel Research and Development Center.

*Energy Division.

1.91

SOME STATISTICAL SAMPLING CONSIDERATIONS FOR THE NAVY RADON ASSESSMENT AND MITIGATION PROGRAM

T. Wright

(Abstract of DOE/HWP-96, March 1990)

This report pulls together several issues, problems, and questions with proposed statistical approaches that helped to guide the planning for the Navy Radon Assessment and Mitigation Program Implementation which took sample radon readings at all Navy and Marine Corps installations. Each section is in brief outline form.

Research sponsored by Naval Facilities Engineering Command, Department of the Navy, U.S. Department of Defense.

1.92

EXACT CONFIDENCE BOUNDS WHEN SAMPLING FROM SMALL FINITE UNIVERSES: AN EASY REFERENCE BASED ON THE HYPERGEOMETRIC DISTRIBUTION

T. Wright

[Abstract of book in *Lecture Notes in Statistics Series*, Vol. 66, Springer-Verlag, New York (1991)]

This volume provides a complete and elementary development with theory of the details for exact optimal upper and lower confidence bounds when sampling from small finite universes. An extensive and easy to use table is included with over eight different applications.

Research sponsored by Applied Mathematical Sciences Research Program, U.S. Department of Energy.

1.93

SELECTION OF FACTORS AFFECTING THE PRESENCE OF FISH IN ADIRONDACK LAKES: A CASE STUDY

J. J. Beauchamp S. W. Christensen*
E. P. Smith†

(Abstract of paper presented at the Second International Conference on Statistical Methods for the Environmental Sciences, Como, Italy, September 27-30, 1990)

One of the primary goals of the National Acid Precipitation Assessment Program is the development of fish response models that can be used to assess the effect of acidification on certain fish species. These models would be useful for predicting changes in fish species status as a result of changes in the water chemistry. In this paper, we present the results from the application of a derived logistic regression model, along with associated diagnostics, to estimate the probability of brook trout presence/absence as a function of given water chemistry variables and watershed characteristics. The data set used in this analysis consists of the Adirondack Lake Survey Corporation data collected on 1469 lakes during 1984-1987. Models fitted to different subsets of lakes, using candidate explanatory/predictor variables which were of particular interest, were developed and compared on the basis of coefficient consistency and predictive ability. In addition to the usual maximum likelihood logistic regression results, we also applied collinearity and other associated diagnostics and variable selection procedures designed specifically for the logistic regression model in order to arrive at parsimonious models. For model evaluation, the data set was randomly divided into a model development subset and a verification subset. Several indices were calculated to compare the various models on both of these data sets. There was a general consistency in the predictive performance of the resulting models, i.e., those models found to do a good job in predicting fish presence in the model development set were also found to be the better models when applied to the verification data. In addition, there was also general agreement with the estimated coefficients among the various models and also general agreement with expectation. The removal of influential observations, as indicated by the logistic regression diagnostics, caused the estimated probability of brook trout being present to be more abrupt for a given change in the explanatory variables, indicating a more sharply focused model.

Research sponsored by the Adirondack Lakes Survey Corporation; by the U.S. Environmental Protection Agency; and by U.S. Department of Energy.

*Environmental Sciences Division.

†Virginia Polytechnic Institute and State University, Blacksburg, VA.

1.94

A COMPARATIVE STUDY OF SIX DATA SOURCES' ABILITY FOR ESTIMATING INTERSTATE MOTOR CARRIER VMT

P. S. Hu* T. Wright
S.-P. Miaou†

[Abstract of paper presented at the American Statistical Association, Washington, DC, August 1989; Proc. pp. 29-34, (May 1990)]

Several Federal Government agencies require estimates of vehicle miles of travel (VMT) by interstate commercial trucks. These estimates are essential in determining accident exposure and accident rates for these trucks, and in determining highway investment needs and the allocation of highway costs. VMT estimates are currently based on various nationwide transportation surveys and/or data sources using various estimation procedures. Unfortunately, these data sources and estimation procedures do not provide consistent estimates. A summary of evaluation results of these data sources and estimation procedures are presented in this paper.

Research sponsored by U.S. Department of Energy.

*Energy Division.

†University of Tennessee, Knoxville, TN.

Computational Distribution Theory

1.95

A TUTORIAL ON SOME SAMPLING TECHNIQUES FOR MEASURING RADON LEVELS

T. Wright

[Abstract of paper presented at the SPECTRUM '90: Nuclear and Hazardous Waste Management International Topical Meeting, Knoxville, TN, September 30–October 4, 1990; Proc. pp. 419–421 (1990)]

This paper presents some exact methods for sampling from finite universes, which were useful in the Navy Radon Sampling Program. Specifically for a given universe size, theory is given for determination of minimum sample size n so that the probability is at least of selecting in the sample at least one unit with a specified attribute. Also background and theory are provided for construction of exact confidence bounds based on the hypergeometric probability distribution.

Research sponsored by U.S. Department of Energy and U.S. Naval Facilities Engineering Command.

1.96

A DECISION SUPPORT SYSTEM BASED ON STOCHASTIC COMPARISONS

V. R. R. Uppuluri

(Abstract of paper presented at the Workshop on Decision Support Methods for the Electric Power Industry, Boston, MA, May 29-31, 1990)

Suppose we have k objects and wish to rank them according to a characteristic. A judge compares these objects two at a time and indicates whether one object is better or worse or equal to another object. We analyze this data by log least squares procedure and the λ_{max} procedure suggested by Saaty. We show by examples, how one can incorporate the data from several judges to obtain a ranking of the objects. Finally, we consider the case when a judge compares the objects two at a time and indicates the probability that one object is better than another object, and show how one can get a ranking of the objects.

Research sponsored by U.S. Department of Energy.

1.97

METHOD FOR PRIORITIZATION OF FEDERAL FACILITIES REGARDING RADON LEVELS FROM STATISTICAL SAMPLES

H. W. Bertini* C. Dudney†
D. Wilson† T. Wright

[Abstract of paper presented at SPECTRUM '90: Nuclear and Hazardous Waste Management International Topical Meeting, Knoxville, TN, September 30–October 4, 1990; Proc. pp. 422–425 (1990)]

Although the current requirements of the Indoor Radon Abatement Act that pertain to federal facilities are only that federal agencies prepare study designs and take radon measurements from representative samples of federal buildings, it is expected that followup, detailed studies will be required in subsequent legislation. It is not likely that funds will be available to permit the detailed measurements of the radon levels in all federal buildings. It is likely, however, that some funds will be available to make those measurements in buildings or installations where the chances of finding high radon levels are the greatest. The method described in this paper addresses the need for the determination of those facilities that have the greatest chance of having high radon levels based on statistical samples taken from those facilities.

Research sponsored by the Applied Mathematical Sciences Research Program, U.S. DOE Office of Energy Research.

*Hazardous Waste Remedial Actions Program.

†Health and Safety Division.

Section 2

NUCLEAR DATA MEASUREMENT AND EVALUATION

2.0. INTRODUCTION

R. W. Peelle

In the Nuclear Data Section, measurements of neutron cross sections and related quantities are performed using the Oak Ridge Electron Linear Accelerator (ORELA). Most of the work is motivated by applications of nuclear physics, but difficult experiments are undertaken to provide fundamental physics results. In addition, complete neutron cross section evaluations are produced, and the theoretical model codes needed to aid in these evaluations are continually improved.

During 1990 the sixth version of the U.S. evaluated nuclear data file (ENDF/B-VI) was released worldwide. Relative to earlier versions, this file contains much-improved representations of many neutron cross sections and related quantities. Neutronics analysts and engineers will gradually use these data in preference to the outdated ones. Our group provided a large share of the data measurement and evaluation work to effect the improvements. These evaluated files are a principal conduit for the findings of the nuclear physics community to reach and thereby assist the larger society.

The ORELA pulsed neutron source is ideal (and the best available anywhere) for neutron resonance studies based on transmission, fission, radiative capture, and scattering angular distributions. During the past period we have continued to utilize this strength with the aid of SAMMY, the locally developed resonance analysis fitting program that allows a problem to be segmented using a Bayesian approach. Based in part on new high-resolution ORELA experiments, evaluated resonance parameters for iron and nickel isotopes, ^{59}Co, and for ^{235}U and ^{239}Pu were substantially improved. In several cases, including the important fissile nuclides, the new experimental data allowed the "resolved resonance region" to be extended in ENDF/B-VI evaluations. This extension allows users to reduce their reliance on the ambiguous "unresolved resonance region" statistical representation.

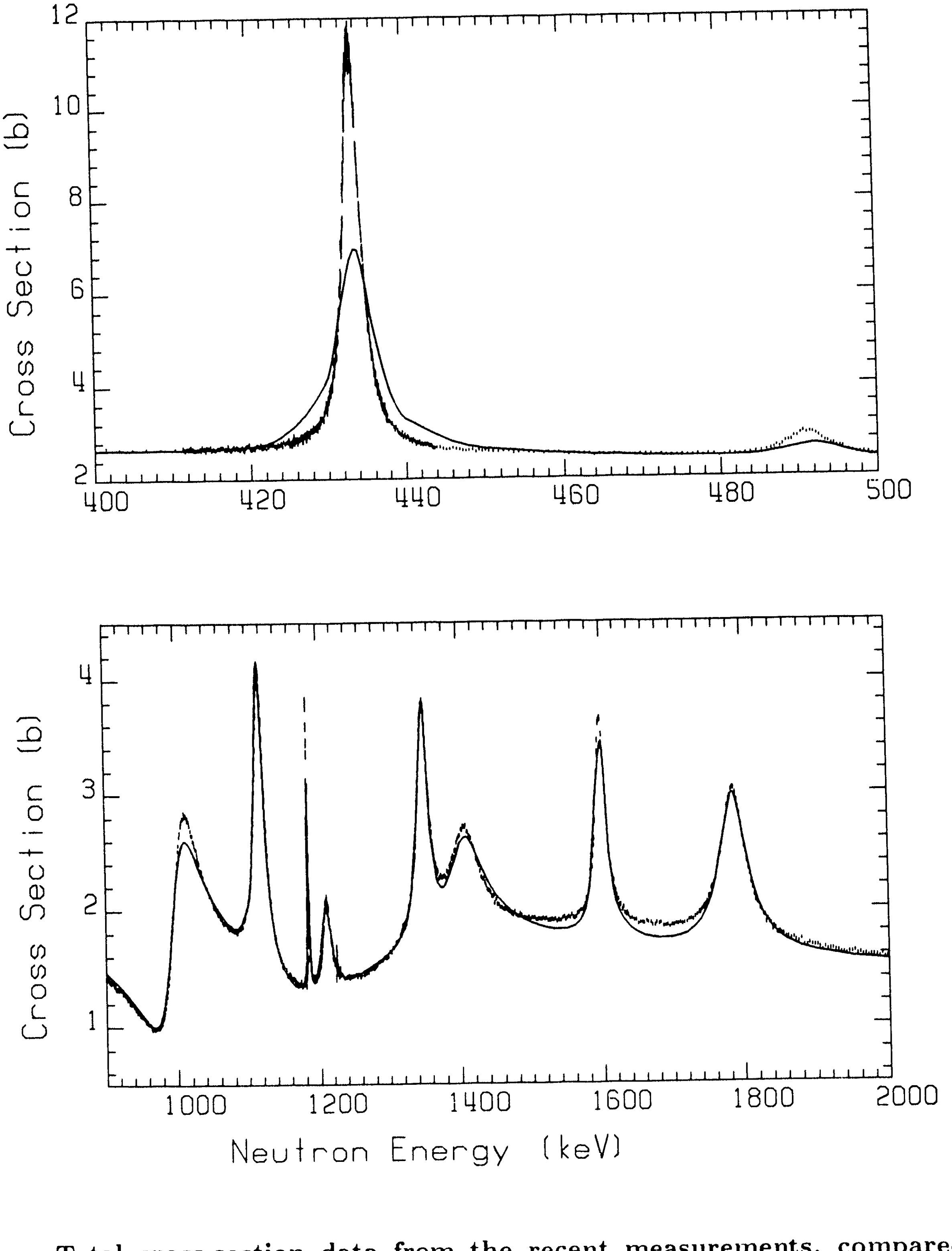
An interesting case is provided by the data recently obtained for nitrogen. During a reevaluation of this isotope at LANL for ENDF/B-VI, it was noted that the experimental data base was old and questionable, particularly for neutron energies less than 1 MeV. New transmission data on nitrogen gas were obtained over the neutron energy range from 0.5 eV to 50 MeV. The old data were found significantly in error in several energy ranges, as illustrated below. While most of our work is entirely supported by the Nuclear Physics program of the DOE Office of Energy Research, this particular effort was supported to a significant degree by the Defense Nuclear Agency because of its relevance to ongoing analyses of radiation effects due to the Hiroshima nuclear explosion. Recent recalculation of the neutron penetration for the 1000- to 1500-m range important to survivor analysis showed a reduced neutron dose but an underprediction of the neutron activation of cobalt in structural steel by a factor of 3. Since radiation doses permissible at accelerators as well as for applications of nuclear energy depend on the Hiroshima/Nagasaki experience, reductions of the estimated doses there have helped force reductions in radiation "tolerances." When the neutron transmission results can be supplemented by observations of resonance neutron scattering angular distributions and the results evaluated, new and better-founded neutron penetration analyses can be performed for the Hiroshima event.

The $^{10}B(n,\alpha)$ reaction is important because of the use of this nuclide in control rods, etc., and because the nearly (1/v) shape of its cross section below 0.1 MeV made it one of the earliest cross section standards. However, at incident neutron energies above about 0.1 MeV the measured data become discrepant and reaction theory cannot resolve the differences. An international effort has started to upgrade the experimental data for this nuclide. Experiments have so far been completed at ORELA on the $(n, \alpha\gamma)$ cross section and on the incident neutron energy dependence of the ratio between the alpha-particle groups to the ground and first excited states of ^{7}Li. Uncertainties are small enough to strongly influence future evaluation analyses.

A series of high-resolution measurements of photon spectra from interactions of MeV neutrons has been performed at ORELA, and final results have become available for ^{56}Fe. Data extend to about 40 MeV incident neutron energy, and show de-excitation gamma rays from inelastic scattering, (n, xn), and various yielding secondary charged particules. Observations have been made at an angle of 125 deg to the neutron beam to reduce angular distribution effects. These experiments were initiated on medium-A even-even structural material nuclides because the dominance of de-excitation via photon cascade through the first excited state allows a simple empirical approximation to the total inelastic scattering cross section. However, the results for more complex reactions such as (n, np) have proven to be as interesting. Many more data are required to guide the development and application of model codes in the region above 8 MeV.

Experiments in cooperation with scientists from the University of Vienna on the electric polarizability of the neutron were brought to a successful conclusion. Results were based on observations of the energy dependence of the non-resonant scattering of neutrons on ^{208}Pb to a precision of about 0.1%. This nuclide was chosen because of its simple resonance structure and the strong electric field just outside the nucleus. The polarizability was found to be $(1.20 \pm 0.25) \times 10^{-3}$ fm^3. This first meaningful non-zero measurement should be a useful constraint on quark theories of the neutron substructure. Experiments continue in order to check on the cross section shape at energies below a few electron volts using liquid lead samples to avoid solid state effects.

The scientific strength of the group has been significantly reduced by the retirement or transfer of several senior staff members. The surge in operating costs associated in part with increasingly complex environment, safety, and health procedures has also resulted in loss of staff, and has so far precluded hiring replacement scientists and engineers for the future. However, because of the phase of development of various projects, the publication rate is just beginning to decrease as it must if current conditions continue. The results being obtained are rewarding and valuable. There is no lack of interesting and useful projects for the future.



Total cross-section data from the recent measurements, compared with the ENDF/B-VI evaluation for ^{14}N. The evaluation was consistent with the then-existent data.

EXPERIMENTAL RESULTS AND THEIR ANALYSIS

2.1

NEUTRON AND GAMMA-RAY EMISSION CROSS SECTION MEASUREMENT PROGRAM AT ORELA

R. R. Spencer **J. K. Dickens**
D. C. Larson **N. W. Hill***
B. D. Rooney **J. H. Todd***

(Abstract of paper presented at the Fusion Data Meeting, Ohio University, Athens, OH, September 18–22, 1989)

Neutron and gamma-ray emission cross sections are required for calculations of neutron multiplication, tritium breeding, heating, shielding, and radiation damage. Measurements previously done at ORELA utilized a ring geometry and obtained data at one angle for incident neutron energies from 1–20 MeV. A new system has been developed to continue this measurement program, utilizing a new spectrometer designed to hold up to five NE-213 detectors in a conventional geometry. Data acquisition is done with a new IBM PS-2 based system designed as a replacement for the outdated ORELA data acquisition computers. The new system will be described, and preliminary results from a measurement of the neutron emission from iron will be shown.

Research sponsored by U.S. DOE Division of Nuclear Physics.

*Instrumentation and Controls Division.

2.2

MEASUREMENT OF THE ELECTRIC POLARIZABILITY OF THE NEUTRON

J. Schmiedmayer* **P. Riehs**†
J. A. Harvey **N. W. Hill**‡

[Abstract of *Phys. Rev. Letters* **66(8)**, 1015 (1991)]

The electric polarizability of the neutron was determined to be $\alpha_n = (1.20 \pm 0.15 \pm 0.20) \times 10^{-3}$ fm^3 from its characteristic influence on the energy dependence of the neutron ^{208}Pb scattering cross sections, as measured in a neutron time-of-flight transmission experiment at the Oak Ridge Electron Linear Accelerator pulsed neutron source.

Research sponsored by U.S. DOE Division of Nuclear Physics.

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‡Instrumentation and Controls Division.

2.3

MEASUREMENT OF THE $^{10}B(n,\alpha_0)/\ ^{10}B(n,\alpha\gamma)$ RATIO VERSUS NEUTRON ENERGY

L. W. Weston **J. H. Todd***

[Abstract of *Nucl. Sci. Eng.* (in press)]

The ratio of ground state transitions to excited state transitions following neutron absorption in ^{10}B has been measured for the neutron energy region from 20 to 1000 keV. Face-to-face silicon surface-barrier detectors were used to detect reactions and measure the total energy of the emitted alpha and Li particles. ORELA was used as a white neutron source and time-of-flight was used to determine the neutron energy. The ratio varied from 0.064 at the lowest energies to 0.72 at 920 keV. The present measurements tend to be smaller than the presently accepted values by 10 to 30% in the 100 to 600 keV energy region.

Research sponsored by U.S. DOE Division of Nuclear Physics.

*Instrumentation and Controls Division.

2.4

NEUTRON CAPTURE BY C-12 AT STELLAR TEMPERATURES

R. L. Macklin

[Abstract of *Astrophysical Journal* (in press)]

Prompt gamma-ray detector measurements with graphite samples were examined to establish their limit of sensitivity to weak resonances in the keV neutron energy range. For $kT = 30$ keV the cross section is estimated to be no larger than 14 μb. A lower limit of 3.2 μb is based on 1/v extrapolation of the measured thermal cross-section.

Research sponsored by U.S. DOE Division of Nuclear Physics.

2.5

TOTAL CROSS SECTION AND NEUTRON RESONANCE SPECTROSCOPY FOR n+^{40}Ar

R. R. Winters* **R. F. Carlton†**
C. H. Johnson‡ **N. W. Hill§**
M. R. Lacerna#

[Abstract of *Phys. Rev. C* **43(2)**, 492 (1991)

The neutron total cross section for ^{40}Ar has been measured over the incident neutron energy range 0.007 to 50 MeV. R-matrix analysis of the cross section from 0.007 to 1.52 MeV provides resonance parameters which provide a complete description of the neutron scattering functions for the $s_{1/2}$, $p_{1/2}$, and $p_{3/2}$ scattering channels and less nearly complete scattering functions for the $d_{3/2}$ and $d_{5/2}$ channels. The back-shifted Fermi gas model is used to model the level densities for s-, p-, and d-wave resonances.

Research sponsored by U.S. DOE Division of Nuclear Physics.

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2.6

CROSS SECTIONS FOR PRODUCTION OF 70 DISCRETE-ENERGY GAMMA RAYS CREATED BY NEUTRON INTERACTIONS WITH ^{56}Fe FOR E_n TO 40 MEV: TABULATED DATA

J. K. Dickens **J. H. Todd***
D. C. Larson

(Abstract of ORNL/TM-11671, September 1990)

Inelastic and nonelastic neutron interactions with ^{56}Fe have been studied for incident neutron energies between 0.8 and 41 MeV. An iron sample isotopically enriched in the mass 56 isotope was used. Gamma rays representing 70 transitions among levels in residual nuclei were identified, and production cross sections were deduced. The reactions studied were ^{56}Fe(n,n')^{56}Fe, ^{56}Fe(n,p)^{56}Mn, ^{56}Fe($n,2n$)^{55}Fe, ^{56}Fe($n,d + n,np$)^{55}Mn, ^{56}Fe($n,t + n,nd + n,2np$)^{54}Mn, ^{56}Fe(n,α)^{53}Cr, ^{56}Fe($n,n\alpha$)^{52}Cr, and ^{56}Fe($n,3n$)^{54}Fe. Values obtained for production cross sections as functions of incident neutron energy are presented in tabular form.

Research sponsored by U.S. DOE Division of Nuclear Physics.

*Instrumentation and Controls Division.

2.7

^{56}Fe RESONANCE PARAMETERS FOR NEUTRON ENERGIES UP TO 850 keV

C. M. Perey **F. G. Perey**
J. A. Harvey **N. W. Hill***
N. M. Larson†

(Abstract of ORNL/TM-11742, December 1990)

High-resolution neutron measurements for ^{56}Fe-enriched iron targets were made at the Oak Ridge Electron Linear Accelerator (ORELA) in transmission below 20 MeV and in differential elastic scattering below 5 MeV. Transmission measurements were also performed with a natural iron target below 160 keV. The transmission data were

analyzed from 5 to 850 keV with the multilevel R-matrix code SAMMY which uses Bayes' theorem for the fitting process. This code provides energies and neutron widths of the resonances inside the 5- to 850-keV energy region, as well as possible parameterization for resonances external to the analyzed region to describe the smooth cross section from a few eV to 850 keV. The resulting set of resonance parameters yields the accepted values for the thermal total and capture cross sections.

The differential elastic-scattering data at several scattering angles were compared to theoretical calculations from 40 to 850 keV using the R-matrix code RFUNC based on the Blatt-Biedenharn formalism. Various combinations of spin and parity were tried to predict cross sections for the well defined $\ell > 0$ resonances; comparison of these predictions with the data allowed us to determine the most likely spin and parity assignments for these resonances.

The mean values and standard deviations of the distributions of the radiation widths are 0.92 $\pm$ 0.41 eV for the s-wave resonances, 0.45 $\pm$ 0.23 eV for the p-wave and 0.75 $\pm$ 0.27 eV for the d-wave resonances. The correlation coefficient between the s-wave reduced neutron widths and radiation widths using the parameters of the 10 s-wave resonances below 300 keV is equal to 0.29 $\pm$ 0.15: a markedly smaller value than the ones found for other nuclides in this mass region.

Research sponsored by U.S. DOE Division of Nuclear Physics.

*Instrumentation and Controls Division.

†Computing and Telecommunications Division.

2.8

PRELIMINARY CROSS SECTIONS FOR GAMMA RAYS PRODUCED BY INTERACTION OF 1 TO 40 MeV NEUTRONS WITH ^{59}Co

T. E. Slusarchyk*

(Abstract of ORNL/TM-11404, October 1989)

Data for 46 distinct gamma rays previously obtained at the 20-meter station of the Oak Ridge Electron Linear Accelerator (ORELA) were studied to determine cross sections for 1.0–4.0 MeV neutron interactions with ^{59}Co. Data reduction methods and preliminary cross sections are given in this report.

Research sponsored by U.S. DOE Division of Nuclear Physics.

*U.S. Navy.

2.9

OBSERVATION OF PHONON SOFTENING AT THE SUPERCONDUCTING TRANSITION IN $Bi_2Sr_2CaCu_2O_8$

H. A. Mook* **M. Mostoller***
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[Abstract of *Phys. Rev. Letters* 65(21), 2712 (1990)]

Resonant neutron absorption spectroscopy has been used to determine the temperature dependence of the average kinetic energy $<E>$ of the Cu in $Bi_2Sr_2CaCu_2O_8$ for the directions along and perpendicular to the c axis. $<E>$ is directly related to the Cu phonon density of states and shows essentially normal behavior as a function of temperature for the c-axis direction. However, a sudden drop in $<E>$ is observed at the superconducting transition for the motions in the Cu-O planes.

Research sponsored by U.S. Department of Energy.

*Solid State Division.

†Instrumentation and Controls Division.

2.10

REICH-MOORE AND ADLER-ADLER REPRESENTATIONS OF THE U-235 CROSS SECTIONS IN THE RESOLVED RESONANCE REGION

G. de Saussure L. C. Leal*
R. B. Perez

[Abstract of paper presented at the International Conference on the Physics of Reactors: Operation, Design, and Computation, Marseille, France, April 23-27, 1990; Proc. Vol. 1, III:19-31 (1990)]

In the first part of this paper, a reevaluation of the low-energy neutron cross sections of ^{235}U is described. This reevaluation was motivated by the discrepancy between the measured and computed temperature coefficients of reactivity and is based on recent measurements of the fission cross section and of η in the thermal and subthermal neutron energy regions. In the second part of the paper, we discuss the conversion of the Reich-Moore resonance parameters, describing the neutron cross sections of ^{235}U in the resolved resonance region, into equivalent Adler-Adler resonance parameters and into equivalent momentum space multipole resonance parameters.

Research sponsored by U.S. DOE Office Division of Nuclear Physics.

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2.11

RESONANCE STRUCTURE IN THE FISSION OF (^{235}U + n)

M. S. Moore* L. C. Leal
G. de Saussure R. B. Perez
N. M. Larson†

[Abstract of *Nuclear Physics* A502, 443c (1989)

A new multilevel reduced R-matrix analysis of the neutron-induced resonance cross sections of ^{235}U has been carried out. We used as a constraint in the analysis the angular anisotropy measurements of Pattenden and Postma, obtaining a Bohr-channel (or J, K channel) representation of the resonances in a two-fission vector space for each spin state. Hambsch *et al.*, have reported definitive measurements of the mass- and kinetic-energy distributions of fission fragments of (^{235}U + n) in the resonance region and analyzed their results according to the fission-channel representation of Brosa *et al.*, extracting relative contributions of the two asymmetric and one symmetric Brosa fission channels. We have explored the connection between Bohr-channel and asymmetric Brosa-channel representations. The results suggest that a simple rotation of coordinates in channel space may be the only transformation required; the multilevel fit to the total and partial cross sections is invariant to such a transformation.

Research sponsored by U.S. DOE Division of Nuclear Physics.

*Los Alamos National Laboratory, Los Alamos, NM.

†Computing and Telecommunications Division.

2.12

AN R-MATRIX ANALYSIS OF THE ^{235}U NEUTRON INDUCED CROSS SECTIONS UP TO 500 eV

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R. B. Perez

(Abstract of *Nucl. Sci. Eng.* (in press)

A detailed evaluation of the R-matrix resonance parameters describing the interaction of neutrons with ^{235}U has been performed up to 500 eV using the most recent high-resolution measurements of the ^{235}U neutron cross sections. The availability of ^{235}U spin-separated neutron cross-section data, in conjunction with the use of the Δ_3-statistics of Metha and Dyson, has made possible a detailed study of the statistical distribution of the resonance parameters and their average values. The present R-matrix resonance parameters have been converted into equivalent sets of Adler-Adler parameters and multipole momentum space expansion parameters. Extensive validation of our evaluation has been performed by comparing self-shielded fission rates computed with our R-matrix parameters with the measurements of Czirr; a test of the ENDF/B unresolved resonance formalism for the calculation of ^{235}U self-shielding factors is also presented.

Research sponsored by U.S. DOE Division of Nuclear Physics.

*University of Tennessee, Knoxville, TN.

2.13

HIGH ENERGY RESOLUTION MEASUREMENT OF THE ^{238}U NEUTRON CAPTURE YIELD FROM 1 keV TO 100 keV

Roger L. Macklin* **R. B. Perez**
G. de Saussure **R. W. Ingle†**

[Abstract of *Annals of Nuclear Energy* (in press)]

The purpose of this work is the precise determination of the ^{238}U neutron capture yield (i.e., the probability of neutron capture) as a function of neutron energy with the highest available neutron energy resolution. The motivation for this undertaking arises from the central role played by the ^{238}U neutron capture process in the neutron balance of both thermal reactors and fast breeder reactors. The present measurement was performed using the Oak Ridge Electron Linear Accelerator (ORELA) facility.

The pulsed beam of neutrons from the ORELA facility is collimated on a sample of ^{238}U. The neutron capture rate in the sample is measured, as a function of neutron time-of-flight (TOF), by detecting the gamma rays from the $^{238}U(n,\gamma)^{239}U$ reaction with a large gamma-ray detector surrounding the ^{238}U sample. At each energy, the capture yield is proportional to the observed capture rate divided by the measured intensity of the neutron beam. The constant of proportionality (the normalization constant) is obtained from the ratio of theoretical to experimentally measured areas under small ^{238}U resonances where the resonance parameters have been determined from high-resolution ^{238}U transmission measurements. The cross section for the reaction $^{238}U(n,\gamma)^{239}U$ can be derived from the measured capture yield if one applies appropriate corrections for multiple scattering and resonance self-shielding.

Some 200 ^{238}U neutron resonances in the energy range from 250 eV to 10 keV have been observed which had not been detected in previous measurements.

Research sponsored by U.S. DOE Division of Nuclear Physics.

*University of Tennessee, Knoxville, TN.

†Instrumentation and Controls Division.

2.14

ANALYSIS OF BETA-RAY DATA IMPORTANT TO DECAY HEAT PREDICTIONS

J. K. Dickens

(Abstract of *Nucl. Sci. Eng.* (in press)

Recently obtained experimental total beta-ray spectra for 77 radionuclides created during fission of ^{235}U have been compared with predicted total beta-ray spectra based on beta-ray transition energies and intensities of individual components currently available in the Evaluated Nuclear Structure Data File (ENSDF). In addition, experimental average beta-ray energies, $< E_\beta >$, for 100 radionuclides are compared with evaluated/theoretical $< E_\beta >$ from four compilations, namely (a) a 1982 compilation by the author, (b) the current ENSDF (1989), (c) a compilation of the Japanese Nuclear Data Committee (1988), and (d) predictions using the microscopic theory of Klapdor and coworkers. No one of these evaluations/predictions is superior in reproducing the experimental data. A comparison of the experimental $< E_\beta >$ with the total available beta decay energies, Q_β, indicates that the approximation $< E_\beta > \approx Q_\beta/3$ somewhat overestimates $< E_\beta >$ on the average; however, the ratio $R = < E_\beta > / Q_\beta$ varies between 0.11 and 0.46, and there is no discernible trend in R vs Q_β or $< E_\beta >$, nor a discrenible difference for radionuclides having $T_{1/2} \leq 2$ sec compared with those having $T_{1/2} > 2$ sec. Lastly, the intensities of possible ground-state decay transitions were estimated for 47 radionuclides and compared with similar data in ENSDF. In 14 cases, a non-zero ENSDF value is supported by the experimental data, and in 8 cases a zero value in ENSDF is supported by the lack of experimental data suggesting a high-energy ground-state beta-ray transition. Of the remaining 25 radionuclides the experimental data for 9 cases suggests increases are needed in the ENSDF, and for 16 radionuclides the data indicate the need for smaller values of the ground-state transition intensities from those given in the ENSDF, being zero for 4 nuclides (^{80,81}Ga, ^{84}As, and ^{145}Cs).

Research sponsored by U.S. DOE Division of Nuclear Physics.

2.15

COMPARISONS OF EXPERIMENTAL BETA-RAY SPECTRA IMPORTANT TO DECAY HEAT PREDICTIONS WITH ENSDF EVALUATIONS

J. K. Dickens

(Abstract of ORNL/TM-11414, March 1990)

Graphical comparisons of recently obtained experimental beta-ray spectra with predicted beta-ray spectra based on the Evaluated Nuclear Structure Data File are exhibited for 77 fission products having masses 79–99 and 130–146 and lifetimes between 0.17 and 23650 sec. The comparisons range from very poor to excellent. For beta decay of 47 nuclides, estimates are made of ground-state transition intensities. For 14 cases the value in ENSDF gives results in very good agreement with the experimental data.

Research sponsored by U.S. DOE Division of Nuclear Physics.

2.16

COLD FUSION STUDIES PART 1: PRELIMINARY RESULTS FROM AN INVESTIGATION OF THE POSSIBILITY OF ELECTROCHEMICALLY INDUCED FUSION OF DEUTERIUM IN PALLADIUM AND TITANIUM CATHODES

D. M. Hembree, Jr. * **E. L. Fuller, Jr.†**
F. G. Perey **G. Mamantov‡**
L. A. Burchfield*

(Abstract of Y/DK-669, June 1990)

A series of experiments designed to detect the by-products expected from deuterium fusion occurring in the palladium and titanium cathodes of heavy water (D_2O) electrolysis cells is reported. The primary purpose of this account is to outline the integrated experimental design developed to test the cold fusion hypothesis and to report preliminary results that support continuing the investigation.

Apparent positive indicators of deuterium fusion were observed, but could not be repeated or proved to originate from the electrochemical cells. In one instance, two large increases in the neutron count rate, the largest of which exceeded the background by 27 standard deviations, were observed. In a separate experiment, one of the calorimetry cells appeared to be producing ~18% more power than the input value, but thermistor failure prevented an accurate recording of the event as a function of time. In general, the tritium levels in most cells followed the slow enrichment expected from the electrolysis of D_2O containing a small amount of tritium. However, after 576 hours of electrolysis, one cell developed a tritium concentration approximately seven times greater than the expected level.

Research sponsored by U.S. Department of Energy.

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†Metals and Ceramics Division.

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2.17

LACK OF EVIDENCE FOR COLD FUSION NEUTRONS IN A TITANIUM-DEUTERIUM EXPERIMENT

F. G. Perey **M. T. Naney***
J. G. Blencoe* **D. J. Wesolowski***

[Abstract of *Fusion Energy* (in press)]

In a previous paper we reported potentially significant results from a "cold fusion" experiment on a titanium-deuterium sample. A follow-up experiment with a much-improved neutron detection system has failed to indicate that neutrons were emitted from a similar Ti-D_2 sample.

Research sponsored by U.S. DOE Division of Nuclear Physics.

*Chemistry Division.

2.18

URR COMPUTER CODE: A CODE TO CALCULATE RESONANCE NEUTRON CROSS-SECTION PROBABILITY TABLES, BONDARENKO SELF-SHIELDING FACTORS, AND SELF-INDICATION RATIOS FOR FISSILE AND FERTILE NUCLIDES

L. C. Leal* **G. de Saussure**
R. B. Perez

(Abstract of ORNL/TM-11297/R1, February 1990)

The URR computer code has been developed to calculate cross-section probability tables, Bondarenko self-shielding factors, and self-indication ratios for fertile and fissile isotopes in the unresolved resonance region. Monte Carlo methods are utilized to select appropriate resonance parameters and to compute the cross sections at the desired reference energy.

The neutron cross sections are calculated by the single-level Breit-Wigner formalism with *s*-, *p*,- and *d*-wave contributions. The cross-section probability tables are constructed by sampling the Doppler broadened cross-sections.

The various self-shielding factors are computed numerically as Lebesgue integrals over the cross-section probability tables.

Research sponsored by U.S. DOE Division of Nuclear Physics.

*University of Tennessee, Knoxville, TN.

2.19

GASEOUS RADIONUCLIDE ACTIVITY IN THE BUILDING 6010 EXHAUST DETERMINED BY GAMMA-RAY ASSAY OF CRYOGENIC LIQUIFIED SAMPLES

J. K. Dickens

(Abstract of ORNL/TM-11738, January 1991)

Samples of gaseous components in the exhaust stack of Building 6010 at the Oak Ridge National Laboratory were obtained for two conditions, (a) the Oak Ridge Electron Linear Accelerator in a normal operating mode, and (b) the accelerator shut down. The decay of one radionuclide, ^{222}Rn, was observed equally in both measurements. The decay of three radionuclides, namely ^{11}C, ^{13}N, and ^{41}Ar, was observed during accelerator operation but not during shutdown. Gamma-ray assay measurements were obtained using a calibrated, high-resolution, Ge detector system. Background data were obtained to ascertain quantitatively the sample-independent contributions to the measurements. Data reduction utilized a combination of computer and manual methods. A complete analysis was carried out to determine the actual measured isotope radioactivity density (in pCi/ℓ) for the particular conditions existing at the time the samples were collected. Corrections were applied to these results to account for non-constant sample collection rates and for sample transfer losses. A complete report of all facets of the experiment is given.

Research sponsored by U.S. DOE Division of Nuclear Physics.

2.20

MAXWELLIAN CASCADE MODEL

R. L. Macklin

[Abstract of *Nucl. Instr. Meth. Phys. Res.* **A290**, 516 (1990); also ORNL/TM-11372, November 1989]

A model for gamma-ray cascade de-excitation of a nucleus derived from the Maxwellian energy distribution function while imposing energy conservation was investigated. Energy distributions and multiplicities and their averages were found over a range of nuclear temperatures and excitation energies appropriate to neutron capture. The model was compared to existing measurements for tantalum, a case where the level density was high and thus a good approximation to the model.

Research sponsored by U.S. DOE Division of Nuclear Physics.

2.21

A DATA ACQUISITION WORK STATION FOR ORELA

B. D. Rooney J. H. Todd*
R. R. Spencer L. W. Weston

(Abstract of ORNL/TM-11454, September 1990)

A new multiparameter data acquisition system has been developed and fabricated at the Oak Ridge Electron Linear Accelerator (ORELA) which utilizes an IBM PS/2 model 80 personal computer and data handler with a 2048 word buffer. The acquisition system can simultaneously acquire data from one, two, or three digitizers, multiplex up to four detectors, read and control up to 16 scalers, and output 32 D.C. logic signals which can be used to control external instrumentation. Software has been developed for the OS/2 operating system, supporting multiparameter data storage for up to three million channels with the capability of collecting data in a background mode, to make the computer available for other tasks while collecting data. The system also supports multiparameter biasing and can collect, crunch, and store data at rates as high as 30,000 events per second.

Research sponsored by U.S. DOE Energy Programs Division.

*Instrumentation and Controls Division.

NUCLEAR MODELING AND CROSS SECTION EVALUATION

2.22

STATUS OF THEORIES FOR CALCULATIONS OF PRODUCTION CROSS SECTIONS OF LONG-LIVED RADIONUCLIDES

C. Y. Fu

(Abstract of paper presented at the IAEA Consultants' Meeting on Cross Sections for the Generation of Long-Lived Radionuclides, Argonne, IL, September 13-14, 1989)

The theories discussed in this paper are confined to those currently being used or considered for the calculation of activation cross sections. The theories are the same regardless of whether the activation product is long lived or short lived. However, the cross sections for the generation of long-lived radionuclides are more difficult or expensive to measure, hence there are fewer data available and the requirement on the predictive capability of the theories used is more stringent.

Topics included in this paper are the optical model, gamma-ray strength function, total and exciton level-density theories, and the pre-compound model. In each subject, we describe the most commonly used theories first, followed by relatively new developments that are used in at least one model code or the promising theories that do not appear to require a large effort for incorporation into existing H-F codes.

Research sponsored by U.S. DOE Division of Nuclear Physics.

2.23

PAIRING INTERACTION EFFECTS IN EXCITON LEVEL DENSITIES

C. Y. Fu

(Abstract of paper presented at the NEANDC Specialists Meeting on Nuclear Level Densities, Bologna, Italy, November 15-17, 1989)

Pairing corrections in particle-hole (exciton) state-density formulas commonly used in precompound nuclear theories are, strictly speaking, dependent on the nuclear excitation energy U and the exciton number n. A general (but simple) formula for (U,n)-dependent pairing corrections has been derived, based on the BCS pairing equations

for constant single-particle spacing, for the exciton state-density formula for one kind of Fermion. It is shown that the constant-pairing-energy correction used in standard state-density formulas, such as Gilbert and Cameron, is a limiting case of the present (U,n)-dependent results. Spin cutoff factors with pairing effects are obtained in the same derivations, thereby defining the exciton level-density formula for applications in quantum mechanical precompound theories. Preliminary results from extending the pairing interaction effects to level-density formulas for two kinds of Fermions are summarized. The results show that the ratios in the exciton level densities in the one-Fermion and two-Fermion approaches depend on both U and n, thus likely leading to differences in calculated compound to precompound ratios. However, the changes in the spin cutoff factors in the two cases are rather small.

Research sponsored by U.S. DOE Division of Nuclear Physics.

2.24

PAIRING CORRECTIONS AND SPIN CUTOFF FACTORS IN EXCITON LEVEL DENSITIES FOR TWO KINDS OF FERMIONS

C. Y. Fu

(Abstract of *Nucl. Sci. Eng.* (in press)

Pairing corrections in particle-hole (exciton) state-density formulas used in precompound nuclear reaction theories are, strictly speaking, dependent on the nuclear excitation energy U and the exciton number n. A general formula for (U,n)-dependent pairing corrections has been derived in an earlier paper for the exciton state-density formula for one kind of Fermion. In the present paper, a similar derivation is made for two kinds of Fermions. In this formulation, it is assumed that neutrons and protons occupy different sets of single particle states. It is shown that the constant-pairing-energy correction used in standard state-density formulas, such as U_0 in Gilbert and Cameron, is a limiting case of the present general (U,n)-dependent results. Spin cutoff factors are calculated using the same pairing theory and parameterized into an explicit (U,n)-dependent function, thereby defining the exciton level-density formula for two kinds of Fermions. The results show that the ratios in the exciton level densities in the one-Fermion and two-Fermion approaches vary with both U and n, thus likely leading to differences in calculated compound to precompound ratios. However, the differences in the spin cutoff factors in the two cases are found to be rather small.

Research sponsored by U.S. DOE Division of Nuclear Physics.

2.25

COVARIANCES OF EVALUATED NUCLEAR DATA BASED UPON UNCERTAINTY INFORMATION OF EXPERIMENTAL DATA AND NUCLEAR MODELS

W. P. Poenitz* R. W. Peelle

[Abstract of paper presented at the IAEA Specialists' Meeting on Covariance Methods and Practices in the Field of Nuclear Data, Rome, Italy, November 17–19, 1986; Proc. INDC(NDS)-192/L, p. 72 (1988)]

A straightforward derivation is presented for the covariance matrix of evaluated cross sections based on the covariance matrix of the experimental data and propagation through nuclear model parameters.

Research sponsored by U.S. Department of Energy.

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2.26

DESCRIPTION OF EVALUATION FOR NATURAL CARBON PERFORMED FOR ENDF/B-VI

C. Y. Fu

(Abstract of ENDF-201, Summary Documentation compiled by Brookhaven National Laboratory, 1991)

An evaluation of data for neutron induced reactions on natural carbon was performed for ENDF/B-VI and is briefly described. The evaluation is based on R-Matrix fits to measured cross sections for $E_n < 5$ MeV, on least-squares adjustment of the ENDF/B-V data for new experimental information, including KERMA factors,

for E_n between 5 and 20 MeV, and on experimental data and theory from 20 to 32 MeV. Evaluated data are given for neutron induced reaction cross sections, angular and energy distributions of the secondary neutrons, and gamma-ray production cross sections and spectra. Uncertainty files are included for the File 3 cross sections. Resonances in ^{13}C below 2 MeV were added. Important improvements to ENDF/B-V were made for the (n,n'3α) cross sections. The upper incident energy was extended to 32 MeV, resulting in the addition of cross sections for many more reactions.

Research sponsored by U.S. DOE Division of Nuclear Physics.

*Computing and Telecommunications Division.

2.27

CALCULATED CROSS SECTIONS FOR NEUTRON INDUCED REACTIONS ON ^{19}F AND UNCERTAINTIES OF PARAMETERS

Z. X. Zhao* C. Y. Fu
D. C. Larson

(Abstract of ORNL/TM-11672, September 1990)

Nuclear model codes were used to calculate cross sections for neutron-induced reactions on ^{19}F for incident energies from 2 to 20 MeV. The model parameters in the codes were adjusted to best reproduce experimental data and are given in this report. The calculated results are compared to measured data and the evaluated values of ENDF/B-V. The covariance matrix for several of the most sensitive model parameters is given based on the scatter of measured data around the theoretical curves and the long-range correlation error of measured data. The results of these calculations form the basis for the new ENDF/B-VI fluorine evaluation.

Research sponsored by U.S. DOE Division of Nuclear Physics.

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2.28

ACCURATE CALCULATIONS OF NEUTRON KERMA AND DAMAGE FROM ENDF/B-VI EVALUATIONS FOR SILICON, CHRONIUM, IRON, AND NICKEL, AND COMPARISON WITH ENDF/B-V RESULTS

D. C. Larson D. M. Hetrick*
C. Y. Fu S. J. Epperson†
R. E. MacFarlane‡

(Abstract of paper presented at the Seventh ASTM-EURATOM Symposium on Reactor Dosimetry, Strasbourg, France, August 27–31, 1990)

For neutron radiation damage studies and KERMA calculations reliable cross-section data and associated spectral distributions are needed for outgoing charged particles, recoil nuclei, gamma rays and neutrons. If information available from the evaluated nuclear data files is incomplete, only approximate calculations can be made for the above quantities of interest. The severity of the approximation depends on the presence and quality of available cross-section data and spectral distributions. A fundamental point is the requirement of energy balance; no more (or less) energy can come out from a reaction in the form of particles and gamma rays than is carried into the reaction by the energy of the neutron plus the Q value ($E + Q$). Unfortunately, for many cross-section evaluations up through ENDF/B-V, energy conservation was only approximately achieved. This point was clearly made following preliminary release of ENDF/B-V, as a result of processing and data testing. A primary cause of this difficulty was the use of elemental evaluations, for which the Q value for a reaction is not well defined; only an average Q can be used.

Use of a sophisticated nuclear model code (TNG) to simultaneously reproduce experimental data in a global manner for all reactions at all incident energies has significantly improved the evaluated results. This method takes advantage of constraints imposed by the measured total cross section and results in smaller uncertainties in the final results than evaluation methods which use several unrelated codes to calculate the various partial cross sections.

Research sponsored by U.S. DOE Division of Nuclear Physics.

*Computing and Telecommunications Division.

2.29

DESCRIPTION OF EVALUATIONS FOR ^{50,52,53,54}Cr PERFORMED FOR ENDF/B-VI

D. M. Hetrick* **D. C. Larson**
N. M. Larson* **C. Y. Fu**

(Abstract of ENDF-201, Summary Documentation compiled by Brookhaven National Laboratory, 1991)

Isotopic evaluations for ^{50,52,53,54}Cr performed for ENDF/B-V' are briefly reviewed. The evaluations are based cn analysis of experimental data and results of model calculations which reproduce the experimental data. Evaluated data are provided for neutron induced reaction cross sections, angular and energy distributions, and for gamma-ray production cross sections associated with the reactions. File 6 formats are used to represent energy-angle correlated data and recoil spectra. Uncertainty files are included for all File 3 cross sections.

Research sponsored by U.S. DOE Division of Nuclear Physics.

*Computing and Telecommunications Division.

2.30

CHROMIUM AND NICKEL INELASTIC SCATTERING DISCREPANCIES

D. C. Larson

(Abstract of Contribution to *The INDC/NEANDC Joint Discrepancy File*, INDC(NDS)-235, compiled by B. H. Patrick and N. P. Kocherov, 1990)

The status of important data for the nickel and chromium isotopes is reviewed. No integral data are available. Differential data for incident energies up to 8 MeV exist for a number of isotopes, but differences often exceed quoted uncertainties. For the 8 to 14 MeV region important to fusion technologies, the data base is inadequate. For fast reactor applications, high resolution data in and just above the resonance region would remove the unphysical smooth cross sections from the evaluated files.

Research sponsored by U.S. Department of Energy.

2.31

GENERATION OF COVARIANCE FILES FOR THE ISOTOPES OF Cr, Fe, Ni, Cu, AND Pb IN ENDF/B-VI

D. M. Hetrick* **D. C. Larson**
C. Y. Fu

(Abstract of ORNL/TM-11763, February 1991)

The considerations that governed the development of the uncertainty files for the isotopes of Cr, Fe, Ni, Cu, and Pb in ENDF/B-VI are summarized. Four different approaches were used in providing the covariance information. Some examples are given which show the standard deviations as a function of incident energy and the corresponding correlation matrices.

Research sponsored by U.S. DOE Division of Nuclear Physics.

*Computing and Telecommunications Division.

2.32

DESCRIPTION OF EVALUATIONS FOR ^{54,56,57,58}Fe PERFORMED FOR ENDF/B-VI

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C. M. Perey F. G. Perey
N. M. Larson* D. C. Larson

(Abstract of ENDF-201, Summary Documentation compiled by Brookhaven National Laboratory, 1991)

Isotopic evaluations for ^{54,56,57,58}Fe performed for ENDF/B-VI are briefly reviewed. The evaluations are based on analysis of experimental data and results of model calculations which reproduce the experimental data, including data for the isotopes and the natural element. Evaluated data are given for neutron-induced reaction cross sections, angular and energy distributions of secondary particles, and gamma-ray production cross sections associated with the reactions. File 6 formats are used to represent energy-angle correlated data and recoil spectra. Uncertainty files are included for all File 3 cross sections. A detailed description of the evaluation is given for ^{56}Fe and results of calculations for the major reactions are used for evaluations of the minor isotopes, with particular attention paid to inelastic scattering to the low-lying levels in ^{57}Fe.

Research sponsored by U.S. DOE Division of Nuclear Physics.

*Computing and Telecommunications Division.

2.33

STATUS OF INTEGRAL AND DIFFERENTIAL CONSISTENCY FOR IRON INELASTIC SCATTERING

C. Y. Fu

(Abstract of Contribution to *The INDC/NEANDC Joint Discrepancy File*, INDC(NDS)-235, compiled by B. H. Patrick and N. P. Kocherov, 1990)

Upgrades since 1986 of evaluated (ENDF/B) files for neutron inelastic scattering in ^{56}Fe were based on known physical deficiencies and a series of integral experiments. The nature of these upgrades is reviewed. The upgrades are all included in the ENDF/B-VI evaluation.

Research sponsored by U.S. Department of Energy.

2.34

IMPROVEMENTS IN ENDF/B-VI IRON AND POSSIBLE IMPACTS ON PRESSURE VESSEL SURVEILLANCE DOSIMETRY

C. Y. Fu D. M. Hetrick*
C. M. Perey F. G. Perey
N. M. Larson* D. C. Larson

(Abstract of paper presented at the Seventh ASTM-EURATOM Symposium on Reactor Dosimetry, Strasbourg, France, August 27–31, 1990)

The ENDF/B-VI cross-section evaluations for the four iron isotopes are summarized, emphasizing the major improvements over ENDF/B-V. The evaluations were mostly based on a preliminary file generated in 1986 for natural iron that has been used for re-calculating several neutron-transport experiments, all of which showed improved agreement. These re-analyses, including those for pressure-vessel surveillance dosimetry, are also discussed.

Research sponsored by U.S. DOE Division of Nuclear Physics.

*Computing and Telecommunications Division.

2.35

TNG CALCULATION OF ^{60g}Co(n,p) AND ^{60m}Co(n,p) CROSS SECTIONS AND PROTON EMISSION SPECTRA FROM 1 TO 20 MeV

C. Y. Fu

[Abstract of a Contribution to *NEANDC Blind Intercomparison of Model Calculations* (1990)]

^{60g}Co(n,p) and ^{60m}Co(n,p) cross sections are needed for low-activation fusion material development. Since the targets are radioactive, there are no measured data. The NEANDC Working Group on Activation Cross Sections proposed at its 1989 Argonne Meeting a blind intercomparison of calculations for these cross sections as a first step in assessing uncertainties of calculated data which dominate all of the existing fusion activation libraries, some of which contain nearly 10,000 reactions. The calculation presented in this paper was performed with the TNG code developed at ORNL. A brief description of the computational

methods and parameters is given. The present calculated cross sections and proton-production spectra are presented in tables. A summary of the results of the intercomparison will be made by Dr. S. Cierjacks of Karlsruhe, Germany and Dr. C. Nordborg of the NEA Data Bank, Saclay, France, and will be presented at the Jülich Conference in May, 1991.

Research sponsored by U.S. DOE Division of Nuclear Physics.

2.36

DESCRIPTION OF EVALUATIONS FOR ^{58,60,61,62,64}Ni PERFORMED FOR ENDF/B-VI

D. C. Larson **C. M. Perey**
D. M. Hetrick* **C. Y. Fu**

(Abstract of ENDF-201, Summary Documentation compiled by Brookhaven National Laboratory, 1991)

Isotopic evaluations for ^{58,60,61,62,64}Ni performed for ENDF/B-VI are briefly reviewed. The evaluations are based on analysis of experimental data and results of model calculations which reproduce the experimental data. Evaluated data are given for neutron induced reaction cross sections, angular and energy distributions, and for gamma-ray production cross sections associated with the reactions. File 6 formats are used to represent energy-angle correlated data and recoil spectra. Uncertainty files are included for all File 3 cross sections.

Research sponsored by U.S. DOE Division of Nuclear Physics.

*Computing and Telecommunications Division.

2.37

DESCRIPTION OF EVALUATIONS FOR ^{63,65}Cu PERFORMED FOR ENDF/B-VI

D. M. Hetrick* **C. Y. Fu**
D. C. Larson

(Abstract of ENDF-201, Summary Documentation compiled by Brookhaven National Laboratory, 1991)

Isotopic evaluations for ^{63,65}Cu performed for ENDF/B-VI are briefly reviewed. The evaluations are based on analysis of experimental data and results of model calculations which reproduce the experimental data. Evaluated data are given for neutron-induced reaction cross sections, angular and energy distributions, and for gamma-ray production cross sections associated with the reactions. File 6 formats are used to represent energy-angle correlated data and recoil spectra. Uncertainty files are included fot all File 3 cross sections.

Research sponsored by U.S. DOE Division of Nuclear Physics

*Computing and Telecommunications Division.

2.38

DESCRIPTION OF EVALUATIONS FOR ^{206,207,208}Pb PERFORMED FOR ENDF/B-VI

C. Y. Fu **D. C. Larson**
N. M. Larson*

(Abstract of ENDF-201, Summary Documentation compiled by Brookhaven National Laboratory, 1991)

An evaluation of data for neutron induced reactions on ^{206,207,208}Pb was performed for ENDF/B-VI and is briefly described. The evaluation is based on experimental data guided by model calculations. Evaluated data are given for neutron induced reaction cross sections, angular and energy distributions of the secondary neutrons, recoil spectra, and gamma-ray production cross sections and spectra. File 6 formats are used to represent energy-angle correlated data for the outgoing neutrons. Uncertainty files are included for all File 3 cross sections. New data are available for (n,2n) cross sections and energy-angle correlated neutron emission spectra. Resonance parameters, absent from the previous evaluations,

have been added. Serious energy imbalance problems in ENDF/B-V have been completely removed by using isotopic evaluations, by using calculated gamma-ray production spectra instead of adopting experimental data directly, and by using the File 6 formats.

Research sponsored by U.S. DOE Division of Nuclear Physics.

*Computing and Telecommunications Division.

2.39

RESONANCE ANALYSIS AND EVALUATION OF THE ^{235}U NEUTRON INDUCED CROSS SECTIONS

L. C. Leal*

(Abstract of ORNL/TM-11547, June 1990; also Ph.D. Thesis, University of Tenessee, Knoxville, TN, April 1990)

Neutron cross sections of fissile nuclei are of considerable interest for the understanding of parameters such as resonance absorption, resonance escape probability, resonance self-shielding, and the dependence of the reactivity on temperature.

In the present study, new techniques for the evaluation of the ^{235}U neutron cross sections are described. The Reich-Moore formalism of the Bayesian computer code SAMMY was used to perform consistent R-matrix multilevel analyses of the selected neutron cross-section data. The Δ_3-statistics of Dyson and Mehta, along with high-resolution data and the spin-separated fission cross-section data, have provided the possibility of developing a new methodology for the analysis and evaluation of neutron-nucleus cross sections. The result of the analysis consists of a set of resonance parameters which describe the ^{235}U neutron cross sections up to 500 eV.

The set of resonance parameters obtained through a R-matrix analysis are expected to satisfy statistical properties which lead to information on the nuclear structure. The resonance parameters were tested and showed good agreement with the theory.

It is expected that the parameterization of the ^{235}U neutron cross sections obtained in this dissertation represents the current state of art in data as well as in theory and, therefore, can be of direct use in reactor calculations.

Research sponsored by U.S. DOE Division of Nuclear Physics

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2.40

STATUS OF THE ^{235}U, ^{239}Pu AND ^{241}Pu RESONANCE PARAMETERS

H. Derrien*   G. de Saussure

(Abstract of Contribution to *The INDC/NEANDC Joint Discrepancy File*, INDC(NDS)-235, compiled by B. H. Patrick and N. P. Kocherov, 1990)

The situation with the neutron resonance parameters for ^{235}U and the fissile plutonium isotopes is reviewed following the major improvements in experimental data, resonance analysis tools, and processing capabilities that occurred in the 1981–88 time period.

Research sponsored by U.S. Department of Energy.

*Centre d'Etudes Nucleaires de Cadarache, France.

2.41

R-MATRIX ANALYSIS OF ^{239}Pu NEUTRON CROSS SECTIONS IN THE ENERGY RANGE UP TO 1000 eV

H. Derrien*   G. de Saussure
R. B. Perez

[Abstract of *Nucl. Sci. Eng.* **106**, 434 (1990)]

The results of an R matrix analysis of the ^{239}Pu neutron cross sections up to 1000-eV neutron energy are reported. The analysis was performed with the multilevel multichannel Reich-Moore code SAMMY. The method of analysis is described, and the selection of experimental data is discussed. Some tabular and graphical comparisons between calculated and measured cross sections and transmissions are presented. The statistical properties of the resonance parameters are examined. The resonance parameters are proposed for the new evaluated data files ENDF/B-VI and JEF2.

Research sponsored by U.S. DOE Division of Nuclear Physics.

*Centre d'Etudes Nucleaires de Cadarache, France.

2.42

RESONANCE ANALYSIS OF THE ^{239}Pu NEUTRON CROSS SECTIONS IN THE ENERGY RANGE 300 to 2000 eV

H. Derrien* **G. de Saussure**

(Abstract of ORNL/TM-11490, June 1990)

A recent high-resolution measurement of the neutron fission cross section of ^{239}Pu has allowed the extension from 1 to 2 keV of a previously reported resonance analysis of the neutron cross sections, and an improvement of the previous analysis in the range 0.3 to 1 keV. Extensive tabular and graphical comparisons between results of measurements and calculations with the resonance parameters are given. The evaluation in ENDF-6 format is available at the nuclear data centers (NNDC at Brookhaven National Laboratory and NEADB at Saclay).

Research sponsored by U.S. DOE Division of Nuclear Physics.

*Retired from Centre d'Etudes Nucleaires de Cadarache, France.

2.43

R-MATRIX ANALYSIS OF THE ^{241}Pu NEUTRON CROSS SECTIONS IN THE THERMAL TO 300-eV ENERGY RANGE

H. Derrien* **G. de Saussure**

[Abstract of *Nucl. Sci. Eng.* **106**, 415 (1990)]

A description is given of the analysis of the ^{241}Pu neutron cross sections in the resolved resonance region at Oak Ridge National Laboratory using the multilevel, multichannel Reich-Moore code SAMMY. The resonance parameters were obtained in the 0- to 300-eV energy range. The statistical properties of the parameters are discussed. Tabulated and graphical comparisons between the experimental data and the calculated cross sections are given. The results are available in ENDF/B-V format and are proposed for the evaluated data libraries ENDF/B-VI and JEF2.

Research sponsored by U.S. DOE Division of Nuclear Physics.

*Centre d'Etudes Nucleaires de Cadarache, France.

2.44

REPORTS ON NUCLEAR DATA ACTIVITIES FOR THE DOE NUCLEAR DATA COMMITTEE

D. C. Larson

(Abstract of BNL-NCS-44362, p. 122, May 1990; and of BNL-NCS-46173, May 1991)

These reports were prepared for the DOE Nuclear Data Committee and cover work performed at ORNL since January 1989 in areas of nuclear data of relevance to the U.S. applied nuclear energy program. These reports were mostly generated through a review of abstracts of work completed to the point of being subjected to some form of publication in the open literature, formal ORNL reports, ORNL technical memoranda, progress reports, or presentations at technical conferences. As much as possible we have reproduced the complete abstracts of the original publications with only minor editing. In a few cases progress reports were written specifically for this publication. The editor has selected the materials to be included in these reports on the basis of perceived interest of DOE Nuclear Data Committee members and cannot claim completeness.

Research sponsored by U.S. DOE Division of Nuclear Physics.

Section 3

INTELLIGENT SYSTEMS

3.0. INTRODUCTION

R. C. Mann

Activities in the Intelligent Systems Section (ISS) concentrate on research in a broad spectrum of challenging areas ranging from intelligent interfaces between humans and complex systems to autonomous mobile robots, as well as biomedical applications of advanced pattern recognition systems. The section comprises the Autonomous Robotic Systems Group (ARSG) and the Cognitive Systems and Human Factors Group (CSHFG).

The Center for Engineering Systems Advanced Research (CESAR), sponsored since 1984 by the Engineering Sciences Program of the Department of Energy (DOE) Office of Basic Energy Sciences, represents the section's core long-term basic research program in intelligent machines. CESAR research includes studies in multiple cooperating robots, multi-sensor data analysis and fusion, control of mobile robots and manipulators, machine learning, and embedded high-performance computing. With support from the DOE Office of Nuclear Energy, the ISS has been performing applied robotics research, systems integration, and has provided overall coordination and management of a consortium of four university research groups (Florida, Michigan, Tennessee, Texas) in a program aimed at robotics for advanced nuclear power stations. The ISS also contributes unique expertise to the DOE Office of Nuclear Energy Advanced Controls Program for tasks related to cognitive modeling. Advanced intelligent machine and robotics technology development is also performed in the ISS for a large multi-laboratory program in robotics for environmental restoration and waste management funded by the DOE Office of Environmental Restoration and Waste Management. Non-DOE sponsors of research in the ISS include the Department of Defense and the Nuclear Regulatory Commission.

The section has outstanding facilities that support experimental research in autonomous and human-machine systems, as well as human performance experimental investigations. During this reporting period, the CESAR laboratory with its mobile robot prototypes (HERMIES-IIB, HERMIES-III, and a new experimental platform), and computer network, including hypercube concurrent processors, custom-made VLSI fuzzy logic processors, and scientific workstations, continued to be used as a collaborative research facility by numerous guest researchers and students from the United States and overseas (Japan, South Korea, France, Denmark, and Germany). A new Cognitive Engineering Research Laboratory was initiated with current primary focus on eye-gaze experiments to support cognitive modeling research.

Among the progress highlights during this reporting period are the following new developments: Significant improvements of machine learning algorithm performance were obtained through the introduction of random set representations. A hybrid architecture was introduced and investigated that combined neural network algorithms with knowledge-based systems for pattern recognition and other applications. A qualitative model of an expert's mental model of a complex system, such as a nuclear power plant, was developed and evaluated successfully. New efficient methods to effect rapid path planning for robots with non-holonomic mobility constraints were developed. Significant progress was made toward the solution of the important problem of controlling kinematically highly redundant systems, such as dextrous mobile robot manipulators. A new method was described to solve the problem of decoupling force and position control for two robot manipulators holding a common object. Unique VME-bus-compatible fuzzy logic inference boards that incorporate custom-designed VLSI chips were developed and successfully tested on-board a new mobile robot platform. Work in multi-sensor data analysis and fusion continued with the successful fusion of ultrasound distance data and 2-D robot vision data, and the use of laser range data in support of robot navigation. Concurrent computing for data processing in robotic systems continues to be a strong component of intelligent machine research in the ISS.

In collaboration with biophysicists and molecular biologists in the ORNL Biology Division, research in bioinformatics with initial focus on pattern recognition and parallel computing for DNA sequence analysis was started successfully with Laboratory Director's discretionary funds. The algorithms developed so far are being used by a growing number of researchers (through internet) to analyze rapidly growing genome data sets.

AUTONOMOUS MOBILE ROBOTS

3.1

ASYNCHRONOUS PRODUCTION SYSTEM FOR CONTROL OF AN AUTONOMOUS MOBILE ROBOT IN REAL TIME ENVIRONMENT

S. S. Iyengar* **A. Sabharwal***
F. G. Pin **C. R. Weisbin†**

[Abstract of *Journal of Applied Artificial Intelligence* (in press)]

Autonomous Robotic systems designed for hazardous environments require the development of onboard real-time knowledge-based systems capable of generating inference driven responses to asynchronous, external stimuli. Building such real-time expert systems involves the integration of traditional knowledge engineering methodologies with time-constrained response and control capabilities. To address such requirements, the Asynchronous Production System (APS), which is a rule-based inference engine capable of dynamic and rapid interaction with its environment, is presented. The APS uses a concurrent event driven execution mechanism and an external input data structure to facilitate monitoring and processing real-time asynchronous information. The enhanced conflict resolution strategies and rule interruptibility features of the APS execution mechanism allows the APS to make efficient use of the onboard system resources. The implementation of the APS involves the development of a shared-memory, multi-processor architecture operating in MIMD mode. This paper provides a description of the APS and then presents a prototype APS-based expert system developed to handle external emergencies for the HERMIES IIB (Hostile Environment Robotic Machine Intelligent Experiment Series) robot. The prototype expert system demonstrates the APS capabilities of handling multiple levels of emergencies and performing knowledge-based recovery after the asynchronous information is processed.

Research sponsored by U.S. DOE Office of Basic Energy Sciences.

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†Jet Propulsion Laboratory, Pasadena, CA.

3.2

A NEW APPROACH TO SOLVE THE KINEMATICS RESOLUTION OF A REDUNDANT ROBOT

P. F. R. Belmans **J.-C. Culioli***

(Abstract of ORNL/TM-11435, March 1990)

A classical redundancy resolution scheme for an m-degree of freedom robot involves the numerical or symbolic computation of the Moore-Penrose pseudo-inverse of the Jacobian matrix, which in turn leads to a least norm solution for the joint velocities. Since the Jacobian matrix may be ill-conditioned, the computation of the inverse may often turn out to be lengthy and/or inaccurate. In this paper, we propose an alternative method to find this least norm solution. Namely we modify the original underdetermined problem by transforming it into a set of determined new problems. We compute in parallel the solutions of these problems and find their least norm simplex combination. We prove that if the dimension of the task-space is n, we need only $(m - n + 1)$ such solutions. We also show that the approach can take into account obstacle avoidance and maximum of manipulability or any other type of analytical criterion. We apply the method to a planar redundant arm.

Research sponsored by U.S. DOE Office of Basic Energy Sciences.

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3.3

MULTI-CRITERIA POSITION AND CONFIGURATION OPTIMIZATION FOR REDUNDANT PLATFORM/ MANIPULATOR SYSTEMS

F. G. Pin **J.-C. Culioli***

[Abstract of paper presented at the IEEE International Workshop on Intelligent Robots and Systems, Tsuchiura, Ibaraki, Japan, July 3-6, 1990; Proc. 295-299 (1990)]

Mobile manipulators, i.e., manipulators mounted on mobile platforms, are attracting significant interest in the manufacturing, military, and public service communities, mainly because

they provide the potential for efficient accomplishment by a single autonomous system of complex missions involving sequences of widely varying tasks. An important characteristic of practical mobile manipulators is their particular kinematic redundancy created by the addition of the degrees of freedom of the platform to those of the manipulator. This redundancy, quite desirable for dexterous manipulation and transport functions in cluttered environments, allows the systems to be optimally positioned and configured for maximum performance when given stringent task requirements and/or system, environment and task constraints.

In the accomplishment of sequences of tasks, the resolution of the redundancy generally involves two steps: the global optimization of the motion and configuration of the system during execution of a task with given requirements and constraints, and the local optimization of the position and configuration of the system during task commutation when changes in both task requirement and constraints occur. This paper is concerned with the latter topic for redundant mobile manipulator systems performing sequences of tasks involving position, load force and displacement requirements. Criteria and optimization schemes for optimally positioning and configuring the platform and the manipulator with respect to obstacle avoidance, maneuverability, motion energy and maximum actuator torque are first developed. Emphasis is then placed on methods and problems involving multi-requirements and multicriteria optimization. Sample results of the methods for a system including a three-link manipulator mounted on a mobile platform are presented and discussed in terms of their use in conjunction with the global motion optimization schemes. Conclusions are drawn as to the applicability of the methods to the general problem of position and configuration optimization for redundant systems with combined mobility and manipulation capabilities.

Research sponsored by U.S. DOE Office of Basic Energy Sciences and the U.S. Army Advanced Technology Program.

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3.4

OPTIMAL POSITIONING OF REDUNDANT MANIPULATOR-PLATFORM SYSTEMS FOR MAXIMUM TASK EFFICIENCY

F. G. Pin J.-C. Culioli*

[Abstract of paper presented at the Third International Symposium on Robotics and Manufacturing, Vancouver, B.C., Canada, July 18–20, 1990; Proc. pp. 489–495 (1990)]

Mobile manipulators are attracting significant interest in the industrial, military and public service communities because of the potential they provide for increased efficiency in material handling and manipulation tasks. Corresponding interest has risen in the robotic research community since the combination and coordination of the mobility of an autonomous platform with the robotic motion of a manipulator introduce complex problems. This paper focuses on a subset of these problems, namely the utilization of the redundancy occurring in most mobile manipulators to optimize their initial positioning and configuration in the accomplishment of given tasks. Optimization schemes are developed for cases when force, position, and displacement constraints are applied at the end-effector. Various optimization criteria are investigated for optimizing the position of the platform and the configuration of the manipulator with respect to obstacle avoidance, maneuverability and several torque functions. Sample results are presented for a system involving a three-link manipulator on a mobile platform. The various optimization schemes are discussed and compared, and directions are outlined for further extensions of the methods to the general problem of optimal positioning and configuring of redundant robotic systems with combined mobility and manipulation capabilities.

Research sponsored by U.S. DOE Office of Basic Energy Sciences.

*Laboratoire d'Automatique, Fontainebleau, France.

3.5

OPTIMAL POSITIONING OF COMBINED MOBILE PLATFORM-MANIPULATOR SYSTEMS FOR MATERIAL HANDLING TASKS

F. G. Pin J.-C. Culioli*

[Abstract of *Robotic Systems* (in press)]

Mobile manipulators are attracting significant interest in the industrial, military, and public service communities because of the potential they provide for increased efficiency in material handling and manipulation tasks. Corresponding interest has arisen in the robotics research community since the combination and coordination of the mobility of an autonomous platform with the robotic motion of a manipulator introduce complex analytical problems. One such problem arises from the particular kinematic redundancy which characterizes practical mobile manipulators. This paper is concerned with the resolution of this redundancy, and in particular with its utilization to optimize the system's position and configuration during task commutations when changes occur in both task requirements and task constraints. Optimization schemes are developed for cases when load and position constraints are applied at the end-effector. Various optimization criteria are investigated for task requirements including obstacle avoidance, maneuverability and several torque functions. The problem of optimally positioning the platform for execution of a manipulation task requiring a given reach is also treated. Emphasis is then placed on optimization methods for problems involving multi-requirements and multi-criteria optimization. Sample results are presented for a system involving a three-link planar manipulator on a mobile platform. The various optimization schemes are discussed and compared, and several directions including global optimization, tunneling algorithms, and minimax optimization are outlined for further extensions of the methods to the general problem of motion planning and control of redundant robotic systems with combined mobility and manipulation capabilities.

Research sponsored by U.S. DOE Office of Basic Energy Sciences and by the Advanced Concept and Technology Program of the U.S. Army Material Command.

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3.6

TIME OPTIMAL TRAJECTORIES FOR A TWO WHEELED ROBOT

D. B. Reister

(Abstract of ORNL/TM-11510, May 1990)

Our objective is to move a two wheeled robot from one posture to the next in the minimum time in a planar environment without obstacles. We assume that the maximum acceleration on each wheel is bounded. We have used Pontryagin's Maximum Principle to find the optimal paths.

The optimal trajectories are bang-bang; at every point on the optimum path, the acceleration on each wheel is either at the upper limit or at the lower limit. We can use a coordinate transformation to move the initial posture to the origin. We can reach any point by a rotation followed by a translation. Adding a final rotation moves the robot to an arbitrary posture.

A switch point is a point at which the acceleration on one of the wheels changes sign. We can characterize a trajectory by the number of switch points. A path with a smaller number of switch points will have a higher average velocity and a longer distance traveled by the wheels. The path with the smallest number of switch points has two (one of each wheel). (For translation, both wheels accelerate from zero to the maximum velocity. After the switch point, both wheels decelerate to zero.) However, there are only two paths with two switch points: translation and rotation. Rotation followed by translation requires five switch points, while rotation, translation, rotation has eight switch points.

We have explored paths with three and four switch points. The paths with three switch points and initial rotation can reach any point faster than a rotation followed by a translation. Paths with three switch points and initial translation or paths with four switch points are useful if the final orientation is considerably different than the direction of travel.

Research sponsored by U.S. DOE Office of Basic Energy Sciences.

3.7

NAVIGATION OF CAR-LIKE MOBILE ROBOTS IN OBSTRUCTED ENVIRONMENTS USING CONVEX POLYGONAL CELLS

H. A. Vasseur F. G. Pin J. R. Taylor*

[Abstract of *Robotics and Autonomous Systems* (in press)]

Due to their kinematics, car-like mobile robots cannot follow an arbitrary path. Besides obstacle avoidance, the path planning problem for such platforms has to satisfy two additional constraints: a lower bounded radius of turn and a non-holonomic constraint. When the robot is not circular, precise maneuvering always implies working in the configuration space of the vehicle. Due to the complexity of representing this space, the planning of a path typically involves computer intensive methods, and rarely allows for real time applications.

In environments described with two-dimensional convex polygonal cells, we show that maneuvering can be completely handled with geometric reasoning. Within a convex cell, joining any two configurations of the vehicle only requires computation of maneuvers related to the beginning and the end of the trajectory. Just a few boundary configurations have to be checked to avoid collision. Because of the convexity of the cell, maneuvers related to the initial configuration and to the final configuration can be connected by a straight trajectory. This geometric reasoning approach allows not only precise calculation of the trajectories within the convex cells, but also extremely fast path planning computation since it avoids representation of the whole configuration space.

In general environments, a graph connecting adjacent convex cells is generated. To find a path between two distant configurations, the graph is searched to identify the cells that have to be traversed. Intermediate configurations are computed at the boundary of adjacent cells and the trajectory planning algorithm is applied to each set of consecutive configurations. Finally, the trajectories generated inside each cell are assembled to produce global collision free paths in complex environments.

Research sponsored by U.S. DOE Office of Engineering Research Program, Basic Energy Sciences.

*Y-12 Central Engineering Division.

3.8

MOTION PLANNING IN A DYNAMIC DOMAIN

K. Fujimura H. Samet*

[Abstract of paper presented at the 1990 IEEE International Conference on Robotics and Automation, Cincinnati, OH, May 13-18, 1990; Proc. pp. 324–330 (1990)]

Motion planning is studied in a time-varying environment. Each obstacle is a convex polygon that moves in a fixed direction at a constant speed. The robot is a convex polygon that is subject to a speed bound. A method is presented to determine whether or not there is a translational collision-free motion for a polygonal robot from an initial position to a final position, and to plan such a motion, if it exists. Our method makes use of the concepts of configuration spaces and accessibility. An algorithm is given for motion planning in such an environment and its time complexity is analyzed.

Research sponsored by U.S. DOE Office of Basic Energy Sciences.

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3.9

SAFE MOTION PLANNING FOR MOBILE AGENTS — A MODEL OF REACTIVE PLANNING FOR MULTIPLE MOBILE AGENTS

K. Fujimura

[Abstract of paper presented at the 1990 SPIE Symposium on Advances in Intelligent Systems, Mobile Robots V, Boston, MA, November 4-9, 1990; Proc. pp. 260–269 (1990)]

The problem of motion planning for multiple mobile agents is studied. Each planning agent independently plans its own action based on its map which contains a limited information about the environment. In an environment where more than one mobile agent interacts, the motions of the robots are uncertain and dynamic. A model for reactive agents is described and simulation results are presented to show their behavior patterns.

Research sponsored by U.S. DOE Office of Basic Energy Sciences.

3.10

AUTONOMOUS TRAJECTORY GENERATION FOR MOBILE ROBOTS WITH NON-HOLONOMIC AND STEERING ANGLE CONSTRAINTS

F. G. Pin H. A. Vasseur

[Abstract of paper presented at the IEEE International Workshop on Intelligent Motion Control, Istanbul, Turkey, August 20-22, 1990; Proc. pp. 295-299 (1990)]

This paper presents an approach to the trajectory planning of mobile platforms characterized by non-holonomic constraints and constraints on the steering angle and steering angle rate. The approach is based on geometric reasoning and provides deterministic trajectories for all pairs of initial and final configurations (position x,y and orientation Θ) of the robot. Furthermore, the method generates trajectories taking into account the forward and reverse mode of motion of the vehicle, or combination of these when complex maneuvering is involved or when the environment is obstructed with obstacles. The trajectory planning algorithm is described, and examples of trajectories generated for a variety of environmental conditions are presented. The generation of the trajectories only takes a few milliseconds of run time on a micro Vax, making the approach quite attractive for use as a real-time motion planner for teleoperated or sensor-based autonomous vehicles in complex environments.

Research sponsored by U.S. DOE Office of Basic Energy Sciences.

3.11

MOTION PLANNING FOR THE UNIVERSAL SELF-DEPLOYABLE CARGO HANDLER (USDCH)

S. F. Sousk* F. G. Pin
C. D. Crane†

[Abstract of paper presented at the U.S. Army Science Conference, Omni Hotel, Durham, NC, June 12-15, 1990; Proc. Vol. 3, pp. 369-382 (1990)]

Belvoir Research, Development and Engineering Center (Belvoir) is developing advanced material handling equipment for sustaining material requirements of Airland Battle-Future. In particular, Belvoir is developing a rough terrain forklift truck, the Universal Self-Deployable Cargo Handler (USDCH), that also is called ATLAS. USDCH program approach allows interaction between the operator and the automated controlling systems, while progressively adding robotics, artificial intelligence, and automated methods. Major challenges involve the development of methodologies to provide real-time operations in hostile field environments and to exploit human-machine synergism for maximum efficiency and reliability.

This paper reports on robotic motion planning for two major functions of the USDCH: platform mobility and motion of the material handling arm. Novel approaches were necessary to automate the basic motion of the platform and the arm. The algorithms for positioning the platform at a work area are presented and results showing optimum trajectories of the vehicle are given. These results show that the methodologies and algorithms developed are applicable to a wide class of vehicles. The kinematics governing the planning of the redundant arm motion are presented and strategies for controlling the arm in various cargo acquisition tasks are discussed. The methods are readily extendable to the more general problem of sensor-based motion planning in unknown and unstructured environments. Conclusions are drawn for applicability of the methods to a wide range of material handling vehicles.

Research sponsored by the U.S. Army, Fort Belvoir Research, Development, and Engineering Center and by the U.S. Department of Energy.

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†University of Florida, Gainesville, FL.

3.12

NAVIGATION USING RANGE IMAGES ON A MOBILE ROBOT

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J. J. Sorensen* N. O. S. Kirkeby*
J. P. Jones H. I. Christensen*

[Abstract of *Robotics and Autonomous Systems* (in press)]

We describe an integrated navigation system for an autonomous mobile robot using a laser range camera to obtain knowledge about the environment. The implemented system maintains a

2D world model (floor map) by integrating knowledge obtained from several range images acquired as the robot moves around in its attempt to find a path to the goal position. A path planner uses the floor map to generate collision-free paths consisting of sequences of configurations. Car-like kinematic constraints ensure smooth paths that can be sent directly to a wheel controller. The system was implemented on the HERMIES III robot, a vehicle with 3 degrees of freedom, and tested in both laboratory and simulated environments. These tests showed that a simple integration of the environment modeler and the path planner provides the robot with basic explorative and navigational capabilities. In particular, the system is capable of performing total re-planning in cases where the initial path to the goal point turns out to be blocked.

Research sponsored by U.S. DOE Office of Basic Energy Sciences and by the Office of Nuclear Energy.

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3.13

NAVIGATION AND LEARNING EXPERIMENTS BY AN AUTONOMOUS ROBOT

G. de Saussure C. R. Weisbin* P. F. Spelt

[Abstract of *Robotics and Computer-Integrated Manufacturing* 6(4), 295 (1989)]

Developing an autonomous mobile robot capable of navigation, surveillance and manipulation in complex and dynamic environments is a key research activity at CESAR, Oak Ridge National Laboratory's Center for Engineering Systems Advanced Research. The latest series of completed experiments was performed using the autonomous mobile robot HERMIES-IIB (Hostile Environment Robotic Machine Intelligence Experiment Series II-B).

Research sponsored by U.S. DOE Office of Basic Energy Sciences.

*Jet Propulsion Laboratory, Pasadena, CA.

3.14

ROSES, A ROBOT OPERATING SYSTEM EXPERT SCHEDULER: METHODOLOGICAL FRAMEWORK

E. C. Halbert* J. Barhen† P. C. Chen‡

(Abstract of ORNL/TM-9987, August 1990)

The optimal scheduling of tasks among which complex interrelationships (such as precedence constraints) may exit is essential for driving the new generation of concurrent supercomputers to their utmost performance. To address this need, the project ROSES (Robot Operating System Expert Scheduler) has been initiated at the Oak Ridge National Laboratory's Center for Engineering Systems Advanced Research. The project, its method for optimizing schedules, and its implementing computer code are each called ROSES. The problem of finding optimum schedules is explosive in complexity (i.e., NP-complete). By combining heuristic techniques, graph-theoretic algorithms, and sophisticated data structures, ROSES achieves near-optimal solutions in a highly efficient manner both with respect to computer time and memory-space. In this report, the description of the methodology is followed by an overview of the ROSES computer code, including detailed outlines of selected algorithms. In addition, this report describes an application of ROSES to schedule inverse dynamics computations for a robot manipulator.

Research sponsored by U.S. DOE Office of Basic Energy Sciences.

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3.15

A HARDWARE/SOFTWARE ENVIRCNMENT TO SUPPORT R&D IN INTELLIGENT MACHINES AND MOBILE ROBOTIC SYSTEMS

R. C. Mann

(Abstract of paper presented at the DARPA Workshop on Distributed Intelligent Control Systems, Pacifica, CA, July 17-19, 1990)

The Center for Engineering Systems Advanced Research (CESAR) serves as a focal point at the Oak Ridge National Laboratory (ORNL) for basic and applied research in intelligent machines. R&D at CESAR addresses issues related to autonomous systems, unstructured (i.e. incompletely known) operational environments, and multiple performing agents. Two mobile robot prototypes (HERMIES-IIB and HERMIES-III) are being used to test new developments in several robot component technologies.

This paper briefly introduces the computing environment at CESAR which includes three hypercube concurrent computers (two on-board the mobile robots), a graphics workstation, VAX, and multiple VME-based systems (several on-board the mobile robots). The current software environment at CESAR is intended to satisfy several goals, e.g.: code portability, re-usability in different experimental scenarios, modularity, concurrent computer hardware transparent to applications programmer, future support for multiple mobile robots, support human-machine interface modules, and support for integration of software from other, geographically disparate laboratories with different hardware set-ups.

Research sponsored by U.S. DOE Office of Basic Energy Sciences.

3.16

PROCEEDINGS OF THE 1989 CESAR/CEA WORKSHOP ON AUTONOMOUS MOBILE ROBOTS

K. S. Harber F. G. Pin

(Abstract of ORNL/TM-11518, March 1990)

The U.S. Department of Energy's (DOE) Center for Engineering Systems Advanced Research (CESAR) at the Oak Ridge National Laboratory (ORNL) and the Commissariat a l'Energie Atomique's (CEA) Office de Robotique et Productique (OREP) within the Directorat à la Valorization are working toward a long-term cooperative agreement and relationship in the area of Intelligent Systems Research (ISR). Specialist meetings and periodic workshops focussed on specific topics of ISR are among the planned cooperation activities. This report presents the proceedings of the first CESAR/CEA Workshop on Autonomous Mobile Robots which took place at ORNL on May 30, 31, and June 1, 1989.

The purpose of the workshop was to present and discuss methodologies and algorithms under development at the two facilities in the area of perception and navigation for autonomous mobile robots in unstructured environments. Experimental demonstration of the algorithms and comparison of some of their features were proposed to take place within the framework of a previously mutually agreed-upon demonstration scenario or "base-case." The base case scenario described in detail in Appendix A, involved autonomous navigation by the robot in an *a priori* unknown environment with dynamic obstacles, in order to reach a predetermined goal. From the intermediate goal location, the robot had to search for and locate a control panel, move toward it, and dock in front of the panel face. The CESAR demonstration was successfully accomplished using the HERMIES-IIB robot while subsets of the CEA demonstration performed using the ARES robot simulation and animation system were presented. The first session of the workshop focussed on these experimental demonstrations and on the needs and considerations for establishing "benchmarks" for testing autonomous robot control algorithms.

Research sponsored by U.S. DOE Office of Basic Energy Sciences and by the French Commissariat a l'Energie Atomique, Sacley, France.

3.17

UNIVERSITY PROGRAM IN ROBOTICS FOR ADVANCED REACTORS

F. J. Sweeney R. C. Gonzalez*
M. M. Trivedi* D. Tesar†
J. S. Tulenko‡ D. K. Wehe§

(Abstract of DOE/OR-884/R2, May 1990)

The U.S. Department of Energy has provided support to four universities and the Oak Ridge National Laboratory in order to pursue research leading to the development and deployment of advanced robotic systems capable of performing tasks that are hazardous to humans, that generate significant occupational radiation exposure, and/or whose execution times can be reduced if performed by an automated system. The goal is to develop a generation of advanced robotic systems capable of economically performing surveillance, maintenance, and repair tasks in nuclear facilities and other hazardous environments.

The program features a unique teaming arrangement among the Universities of Florida, Michigan, Tennessee, Texas, and the Oak Ridge National Laboratory, and their industrial partners, Odetics, Gulf State Utilities, Florida Power and Light Company, Remotec, and Telerobotics International. Each of the universities and ORNL have ongoing activities and corresponding facilities in areas of R&D related to robotics. This program is designed to take full advantage of a balance of these existing resources at the participating institutions.

Research sponsored by U.S. DOE Office of Technology Support Programs.

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INTELLIGENT SENSOR SYSTEMS

3.18

PERFORMANCE OF VISUAL AND ULTRASOUND SENSING BY AN AUTONOMOUS ROBOT

M. Beckerman D. L. Barnett*

(Abstract of ORNL/TM-11733, January 1991)

This paper presents results of an experimental study of the reliability of an autonomous mobile robot operating in an unstructured environment. Examined in the study are the principal components of the visual and ultrasound sensor systems used to guide navigation and manipulation tasks of the robot. Performance criteria are established with respect to the requirements of the integrated robotic system. Repeated measurements are done of the geometric and spatial quantities used for docking the robot at a mock-up control panel, and for locating control panel devices to be manipulated. The systematic and random components of the errors in the measured quantities are exhibited, their origins are identified, and means for their reduction are developed. We focus on refinements of visual area data using ultrasound range data, and on extraction of yaw by visual and by ultrasound methods. Monte Carlo methods are used to study the sensor fusion, and angle-dependence considerations are used to characterize the precision of the yaw measurements. Issues relating to sensor models and sensor fusion, viewed as essential strategic components of intelligent systems, are then discussed.

Research sponsored by U.S. DOE Office of Basic Energy Sciences.

*Computing and Telecommunications Division.

3.19

PERFORMANCE OF MULTIPLE TASKS BY AN AUTONOMOUS ROBOT USING VISUAL AND ULTRASOUND SENSING

M. Beckerman D. L. Barnett*
M. Dickens† C. R. Weisbin‡

[Abstract of paper presented at the Third International Symposium on Robotics and Manufacturing, Vancouver, B.C., Canada, July 18–20, 1990; Proc. Vol. 3, pp. 389–395 (1990)]

While there have been many successful mobile robot experiments, only a few papers have addressed issues pertaining to the range of applicability, or robustness, of robotic systems. The purpose of this paper is to report results of a series of benchmark experiments done to determine and quantify the robustness of an integrated hardware and software system of a mobile robot.

Research sponsored by U.S. DOE Office of Basic Energy Sciences.

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3.20

ULTRASOUND AND VISUAL SENSOR FEEDBACK AND FUSION

M. Beckerman D. L. Barnett*
S. M. Killough†

[Abstract of paper presented at the Japan-USA Symposium on Flexible Automation, Kyoto, Japan, July 9–11, 1990; Proc. pp. 1315-1319 (1990)]

The HERMIES-IIB mobile robot developed at Oak Ridge National Laboratory's (ORNL's) Center for Engineering Systems Advanced Research was designed to carry out autonomous sensing, navigation and manipulation tasks in an unstructured laboratory environment. In this paper we report on the use of sensor feedback and sensor fusion as a means of compensating for HERMIES-IIB sensor and mechanical errors, uncertainties and limitations.

Research sponsored by U.S. DOE Office of Basic Energy Sciences.

*Computing and Telecommunications Division.

†Instrumentation and Controls Division.

3.21

TREATMENT OF SYSTEMATIC ERRORS II: FUSION OF ULTRASOUND AND VISUAL SENSOR DATA

M. Beckerman L. A. Farkas*
S. E. Johnston†

[Abstract of ORNL/TM-11349, June 1990; also *IEEE Trans. on Robotics and Automation* (in press)]

In this work we present a methodology for the fusion of ultrasound and visual sensor data as acquired by a mobile robot. The objective of the methodology was the reduction of systematic errors which arise in the processing of the data in the individual sensor domains. In the initial processing of the ultrasound scan, rectilinear (Cartesian map) and polar (strings) data structures were built. In the initial processing of the CCD camera image, vertical edge segments were identified and labelled according to their connectivity. The systematic errors treated included ultrasound distortions in size, and visual ambiguities in discriminating depth discontinuities from intensity gradients generated by other details in the image. These systematic errors were first flagged by comparing the ultrasound strings and visual vertical edges to one another. The ranges, spatial orientation of the camera, and geometric information extracted from least-squares fits were then used in the fusion stage processing of the visual image. Vertical edge information was used in the subsequent fusion stage processing of the ultrasound data. By the end of this feedback-like fusion process the data structures in each sensor domain carried some information from the other domain. We had identified the vertical edges of interest, tagged them with range information, and removed the distortions from the Cartesian navigation maps.

Research sponsored by U.S. DOE Office of Basic Energy Sciences.

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3.22

ROBOT SELF-LOCATION IN UNKNOWN ENVIRONMENTS

E. R. Stuck*

(Abstract of ORNL/TM-11718, February 1991)

It is often necessary for robots to navigate in environments which are not known in advance. In this context, self-location is the problem of determining how far and in what direction motion has occurred. Because of wheel slippage and other errors, odometry cannot be depended upon to provide precise or accurate positional information. Triangulating from visual features can help make position estimation more accurate. This paper describes work that was done during a three-month student research internship at the Center for Engineering Systems Advanced Research (CESAR) of the Oak Ridge National Laboratory, exploring the problem of robot self-location in unknown environments. This work included the development and integration of a set of programs which present a partial solution to this self-location problem. These programs use a sequence of images which are acquired as the camera moves between positions with a motion which is known approximately. Visual features are extracted from the images and matched through time. Triangulation using these features then provides a rough estimate of the range of these features from the camera. Kalman filtering (not implemented) can then be used to integrate the information from odometry and vision to provide a better estimate of the position of the robot.

Research sponsored by U.S. DOE Office of Basic Energy Sciences.

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3.23

LASER RANGE CAMERA MODELING

K. Storjohann

(Abstract of ORNL/TM-11530, April 1990)

This paper describes an imaging model that was derived for use with a laser range camera (LRC) developed by the Advanced Intelligent Machines Division of Odetics. However, this model could be applied to any comparable imaging system. Both the derivation of the model and the determination of the LRC's intrinsic parameters are explained. For the purpose of evaluating the LRC's extrinsic parameters, i.e., its external orientation, a transformation of the LRC's imaging model into a standard camera's (SC) pinhole model is derived. By virtue of this transformation, the evaluation of the LRC's external orientation can be found by applying any SC calibration technique.

Research sponsored by U.S. DOE Office of Basic Energy Sciences.

3.24

ADAPTING SENSORY DATA FOR MULTIPLE ROBOTS PERFORMING SPILL CLEANUP

K. Storjohann E. Saltzen*

(Abstract of ORNL/TM-11661, September 1990)

This paper describes a possible method of converting a single performing robot algorithm into a multiple performing robot algorithm without the need to modify previously written codes. The algorithm to be converted involves spill detection and clean up by the HERMIES-III mobile robot. In order to achieve the goal of multiple performing robots with this algorithm, two steps are taken. First, the task is formally divided into two sub-tasks, spill detection and spill clean-up, the former of which is allocated to the added performing robot, HERMIES-IIB. Second, an inverse perspective mapping, is applied to the data acquired by the new performing robot (HERMIES-IIB), allowing the data to be processed by the previously written algorithm without re-writing the code.

Research sponsored by U.S. Department of Energy.

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3.25

REVOLUTIONS AND EXPERIMENTAL COMPUTER VISION

K. W. Bowyer*   J. P. Jones

[Abstract of *Graphics Models and Image Understanding* 53(1), 127 (1991)]

Jain and Binford note that computer vision has failed to develop the rich experimental tradition characteristic of mature empirical sciences. If the field is preparadigmatic, then this is not surprising. There is little motivation to invest a great deal of effort in determining the obscure but telling facts which elucidate a particular theory unless it is a paradigm for the field. But let us assume that computer vision is a mature discipline, and ask what would be the necessary characteristics of experimental computer vision if it were to exist, and why such a tradition has failed to develop.

Research sponsored by U.S. DOE Office of Basic Energy Sciences.

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3.26

ON THE DESIGN OF A CONCURRENT IMAGE ANALYSIS SYSTEM

J. P. Jones

[Abstract of paper presented at the Third International Symposium on Robotics and Manufacturing, Vancouver, B.C., Canada, July 18–20, 1990; Proc. pp. 205–210 (1990)]

Because programming parallel computers is challenging, their use has been limited. To make the technology more accessible it is necessary to develop programming environments which hide the details. An environment for image analysis on concurrent computers is described which provides fundamental services for parallelism. The system is organized in a tripartite abstraction hierarchy. The topmost level can be programmed as though it were an ordinary sequential computer. Distributed memory and message passing appear only at lower levels. An operational taxonomy consisting of mathematical transformations, memory management, domain decomposition, and input/output facilities for relevant data structures form the nucleus of the environment. A collection of applications are enumerated; advantages and drawbacks are discussed.

Research sponsored by U.S. DOE Office of Technology Support Programs and the Office of Basic Energy Sciences.

3.27

DESIGN AND IMPLEMENTATION OF TWO CONCURRENT MULTI-SENSOR INTEGRATION ALGORITHMS FOR MOBILE ROBOTS

J. P. Jones   M. Beckerman
R. C. Mann

[Abstract of paper presented at the SPIE Symposium on Advances in Intelligent Robotic Systems, Philadelphia, PA, November 5–8, 1989; Proc. Sensor Fusion II: Human and Machine Strategies, SPIE 1198, pp. 301–312, P. S. Schenker, Ed. (1990)]

Two multi-sensor integration algorithms useful in mobile robotics applications are reviewed. A minimal set of utilities are then developed which enable implementation of these algorithms on a distributed memory concurrent computer.

Research sponsored by U.S. DOE Office of Basic Energy Sciences.

3.28

AN INPUT/OUTPUT ALGORITHM FOR M-DIMENSIONAL RECTANGULAR DOMAIN DECOMPOSITIONS ON N-DIMENSIONAL HYPERCUBE MULTICOMPUTERS

H. Embrechts   J. P. Jones

[Abstract of paper presented at the Fifth Distributed Memory Computing Conference, Charleston, SC, April 8–12, 1990; Proc. Vol. 2, pp. 876–882 (1990)]

Hypercube-topology concurrent multicomputers owe at least part of their popularity to the fact that it is relatively simple to decompose rectangularly-shaped M-dimensional domains into subdomains and assign these subdomains to processors (PEs) in a manner which preserves the adjacencies of the subdomains. However, this decomposition involves some rearrangement of the data during input/output operations to (linear memory) data acquisition, display, or mass storage devices. We show that this rearrangement can be done efficiently, in parallel.

The main consequence of this algorithm is that M-dimensional data can be stored in a simple, general format and yet be communicated efficiently independent of the dimension of the hypercube or the number of these dimensions assigned to the dimensions of the domain. This algorithm is also relevant to applications with mixed domain decompositions, and to parallel mass storage media such as disk farms.

Research sponsored by U.S. DOE Advanced Technology Development, Office of Technology Support Programs, and by the Office of Basic Energy Sciences.

COOPERATING ROBOT MANIPULATORS

3.29

MODELING CLOSED CHAIN MOTION OF TWO MANIPULATORS HOLDING A RIGID OBJECT

A. J. Koivo* **M. A. Unseren**

[Abstract of *Mech. Mach. Theory* 25(4), 427 (1990)]

A dynamical model is developed for the closed chain motion of two N-joint manipulators holding a rigid object in a three-dimensional workspace. Holonomic constraints are developed and combined with the equations of motion of the manipulators and of the object to obtain the dynamical model of the entire system. The behavior of the generalized contact forces and their impact on the coupling among the individual components of the system in the model is investigated. The problem of solving the model for the forward and inverse dynamics is discussed.

Research sponsored by the U.S. Department of Energy.

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3.30

A RIGID BODY MODEL AND DECOUPLED CONTROL ARCHITECTURE FOR TWO MANIPULATORS HOLDING A COMPLEX OBJECT

M. A. Unseren

[Abstract of *Robotics and Autonomous Systems* (in press); also ORNL/TM-11752, January 1991]

A rigid body dynamical model and control architecture are developed for the closed chain motion of two manipulators holding an object containing a spherical joint in a three-dimensional workspace. The model is first developed in the joint space and then transformed to obtain reduced order equations of motion and a separate set of equations describing the behavior of the generalized contact forces. The problem of solving the model for the unknown variables is discussed. A new control architecture consisting of the sum of the outputs of a primary and secondary controller is suggested which, according to the model, decouples for force and position controlled degrees of freedom during motion of the system. The proposed composite controller enables the designer to develop independent, non-interacting control laws for the force and position control of the closed chain system.

Research sponsored by U.S. DOE Office of Engineering Research Program, Basic Energy Sciences.

3.31

RIGID BODY DYNAMICS AND DECOUPLED CONTROL ARCHITECTURE FOR TWO STRONGLY INTERACTING MANIPULATORS

M. A. Unseren

[Abstract of *Robotica* (in press)]

A rigid body dynamical model and control architecture are developed for the closed chain motion of two manipulators holding a rigid object in a three-dimensional workspace. The manipulators may have an equal or unequal number of joints and can be structurally different even in the equal joint case. Dynamic and kinematic constraints are determined and combined with the equations of motion of the manipulators to obtain a dynamical model of the entire system in the joint space. A functional relation for the generalized contact forces exerted on the shared load is developed and

included in the model. The problem of solving the joint space model for the unknown variables is discussed. This includes an original proof that the problem of solving the model for the generalized input forces applied to the joint actuators (i.e., computing the joint torques) is underspecified in nature. Since the order of the model is higher than the degrees of freedom of the closed chain, the system is transformed to obtain reduced order equations of motion and a separate set of equations describing the behavior of the generalized contact forces. The latter form of the model is a new result for the case of two manipulators holding a rigid object. The problem of solving the reduced order model for the unknown variables is also addressed. A new control architecture consisting of the sum of the outputs of a primary and secondary controller is suggested which, according to the model, decouples the force and position controlled degrees of freedom during motion of the system. The proposed composite controller enables the designer to develop independent, non-interacting control laws for the force and position control of the complex closed chain system.

Research sponsored by U.S. DOE Office of Engineering Research Program, Basic Energy Sciences and by the National Science Foundation.

3.32

ADAPTIVE OPTIMAL CONTROL OF UNCERTAIN NONLINEAR SYSTEMS: ON-LINE MICROPROCESSOR-BASED ALGORITHM TO CONTROL MECHANICAL MANIPULATORS

C. March-Leuba*   R. B. Perez

[Abstract of *Journal of Robotic Systems* (in press)]

This paper presents an adaptive optimal control algorithm for uncertain nonlinear systems. A variational technique based on Pontryagin's Maximum Principle is used to track the system's unknown terms and to calculate the optimal control. The reformulation of the variational technique as an Initial Value Problem allows this microprocessor-based algorithm to perform on-line model-updating and control. To validate the algorithm, a system representing a two-link mechanical manipulator is simulated. In the control model, the coupling and friction terms are unknown. The robot's task is to follow a prescribed trajectory and to pick up an unknown mass.

Research sponsored by U.S. DOE Office of Basic Energy Sciences.

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MACHINE LEARING

3.33

IMPLEMENTATION OF VALIANT'S LEARNABILITY THEORY USING RANDOM SETS

E. M. Oblow

(Abstract of ORNL/TM-11512, August 1990)

Valiant's theory of learnability is recast into random set terms and implemented in an efficient computer learning algorithm. A theoretical and empirical analysis is presented which improves the bounds on the number of examples needed to learn such sets. A general purpose algorithm using these bounds is then described. This algorithm is tested on the multiplexor problem analyzed by others as a benchmark for decision tree and genetic algorithms. Results for this problem show that a set-theoretic implementation of Valiant's theory is computationally competitive with these more established methods. Conclusions are drawn about potential further improvements in the efficiency of Valiant's approach.

Research sponsored by U.S. DOE Office of Basic Energy Sciences.

3.34

ROBOT LEARNING FROM DISTRIBUTED SENSORY SOURCES

F. G. Pin   P. F. R. Belmans
S. I. Hruska*   C. W. Steidley†
L. E. Parker

[Abstract of *Trans. Syst. Man & Cybern.* **21**(5) (1991)]

Much of the prior work on machine learning has focussed on highly cognitive-based inferencing. Recent attempts at implementing these techniques in the area of experimental robotics, how-

ever, have shown that learning by an autonomous robot through high-level cognitive function-based schemes is highly dependent upon and currently constrained by the sensor data interpretation capabilities of the robot perception systems. As a consequence, a vast amount of task-specific knowledge and environmental information has to be provided *a-priori* to the robot. On the other hand, since learning is an incremental process, much of the basic task and environmental knowledge can be efficiently acquired over time by the robot using less complex inferencing schemes coupled with appropriate sensory sources. This paper describes recent work in this direction following a multimodal learning approach in which distributed sensory sources are used to both trigger the observation of and perceive relevant learning instances in a human-robot synergistic framework. Three components of the incremental learning system for our CESARm advanced manipulator test-bed are presented which encompass the learning of object and work area characteristics through triggering of attention and rote learning, the learning of elemental manipulation tasks by observation of human actions, and the self-assessment of acquired skills and learned knowledge through task performance evaluation. Feasibility experiments with each of these three learning methodologies are presented and some sample results are discussed. These results indicate the feasibility for sensor-equipped robots to efficiently allocate perception resources and learn characteristics of their environments with no or minimal *a-priori* knowledge or inferencing capabilities. Due to their low inferencing complexity, the proposed methods are shown to be readily upscalable to increasingly larger environmental and perceptive domains. Their associated knowledge representation are shown to be fully compatible with added processing using more complex inferencing algorithms to support knowledge growth through incremental observation/inferencing strategies. The results of the implemented algorithms are also discussed in terms of possible enhancements to further increase the efficiency of the developed perception/learning coupled subsystems.

Research sponsored by U.S. DOE Office of Engineering Research Program, Basic Energy Sciences.

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3.35

MACHINE LEARNING TECHNIQUES FOR NATURAL RESOURCE DATA ANALYSIS

G. E. Liepins R. Goeltz* R. Rush*

[Abstract of *AI Applications* 4(3), 9 (1990)]

Three machine learning techniques, ABACUS, decision trees, and genetic algorithms are used to assist in the determination of relationships among lake acidification data. ABACUS is a quantitative discovery program that determines algebraic relationships among variables and has previously (re)discovered the conservation of momentum law (for example). Decision trees have been developed within the statistical literature, as well as the artificial intelligence (AI) literature, and have been applied to tasks such as disease diagnosis. Genetic algorithms are optimization and design techniques for difficult, poorly characterized, and ill-structured problems. They were used in this study as an alternate means to estimate the parameters of non-linear regression models.

Each of the techniques is briefly described. To provide a standard for comparison and regression, Spearman rank correlation test results are cited; acid rain appears to be the primary cause for lake acidity and forest blowdown appears to be a contributing factor. Findings from the application of the machine learning techniques are summarized. For the reasons delineated in the paper, ABACUS was unable to determine any structure. Both decision tree and genetic algorithm approaches confirmed that acid rain seemed to be the primary factor leading to lake acidification, with forest blowdown contributing.

Research sponsored by U.S. DOE Office of Environmental Analysis.

*Energy Division.

GENETIC ALGORITHMS

3.36

DECEPTIVENESS AND GENETIC ALGORITHM DYNAMICS

G. E. Liepins M. D. Vose*

[Abstract of paper presented at the Genetic Algorithms Theory Workshop, Bloomington, IN, July 16–18, 1990; Proc. of *Foundations of Genetic Algorithms*, G. Rawlins, Ed., Morgan Kauffman Publisher (1991)]

We address deceptiveness, one of at least four reasons genetic algorithms can fail to converge to function optima. We construct fully deceptive functions and other functions of intermediate deceptiveness. For the fully deceptive functions of our construction, we generate linear transformations that induce changes of representation to render the functions fully easy. We further model genetic algorithm selection and recombination as the interleaving of linear and quadratic operators. Spectral analysis of the underlying matrices allows us to draw preliminary conclusions about fixed points and their stability. We also obtain an explicit formula relating the nonuniform Walsh transform to the dynamics of genetic search.

Research sponsored by U.S. Department of Energy Director's Seed Money R&D.

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3.37

PUNCTUATED EQUILIBRIA IN GENETIC SEARCH

M. D. Vose* G. E. Liepins

[Abstract of *Complex Systems* (in press)]

We introduce a formalization of a simple genetic algorithm. Mathematically, two matrices F and M determine selection and recombination operators. Fixed points and their stability for these operators are investigated in terms of the eigenvalues of the associated matrices. We apply our results to one point crossover with mutation to illustrate how the interaction between the focusing operator (selection) and the dispersion operator (recombination) results in the punctuated equilibrium frequently observed in genetic search.

Research sponsored by U.S. Department of Energy and the National Science Foundation.

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3.38

A GENETIC ALGORITHM APPROACH TO MULTIPLE FAULT DIAGNOSIS

G. E. Liepins W. D. Potter *

[Abstract of book chapter in *Handbook of Genetic Algorithms*, Chapter 17, pp. 237–250, L. Davis, Ed., Van Nostrand Reinhold (1991)]

Oak Ridge National Laboratory has developed the Communication Alarm Processor Expert System (CAP) for the Bonneville Power Administration. CAP is a near real-time system that helps microwave communication system operators determine the causes of communication system problems. At present, the CAP system is only able to perform single fault diagnosis. A genetic algorithm approach is being developed to extend CAP's capabilities to multiple faults. Alternate approaches that were considered for multiple fault diagnosis are reviewed together with the reasons that the genetic algorithm approach was chosen. Genetic algorithms themselves support a variety of diagnostic problem formulations. These are compared and contrasted. The genetic algorithm modifications necessary to support the chosen approach are detailed. Selected test results are presented.

Research sponsored by the U.S. Department of Energy.

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MEAN FIELD ANNEALING

3.39

SIMULATED ANNEALING USING THE MEAN FIELD APPROXIMATION

G. Bilbro* R. C. Mann
T. K. Miller* W. E. Snyder*
D. E. Van den Bout* M. White*

[Abstract of book chapter in *Advances in Neural Information Processing Systems I*, pp. 91–98, Morgan-Kaufmann, San Mateo, CA (1989)]

Nearly optimal solutions to many combinatorial problems can be found using the simulated annealing algorithm. This paper extends the concept of simulated annealing from its original formulation as a Markov process to a new formulation based on mean field theory (MFT). The new formulation essentially replaces the discrete degrees of freedom in stochastic simulated annealing with their average values as computed by the mean field approximation. The net result is that equilibrium at a given temperature is achieved in 1–2 orders of magnitude fewer iterations with mean field annealing (MFA) as compared with the stochastic approach. A general framework for the MFA algorithm is derived, and its dynamics are analyzed for a generic combinatorial optimization problem: graph bipartitioning. Neural networks and binary image restoration are presented as further examples of MFA optimization. Further, analysis of the behavior of systems undergoing mean field annealing provides important clues about how to better control neural networks.

Research sponsored by U.S. DOE Office of Basic Energy Sciences and Office of Technology Support Programs and North Carolina State University.

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3.40

RESTORATION OF PIECEWISE CONSTANT IMAGES VIA MEAN FIELD ANNEALING

H. Hiriyannaiah* G. L. Bilbro*
W. E. Snyder* R. C. Mann

[Abstract of *Journal Opt. Soc. America-A* **6(12)**, 1901 (1989)]

An algorithm is described which removes the noise from images without blurring or other distortion of edges. The problem of noise removal is posed as a restoration of an uncorrupted image, given additive noise. The restoration problem is solved using a new minimization strategy called *Mean Field Annealing* (MFA). An *a-priori* statistical model of the image is chosen which drives the minimization toward solutions which are locally homogeneous. The MFA strategy is derived, and the resulting algorithm discussed. Applications of the algorithm to both synthetic and real images are presented.

Research sponsored by U.S. DOE Office of Basic Energy Sciences.

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3.41

MEAN FIELD APPROXIMATION MINIMIZES RELATIVE ENTROPY

G. L. Bilbro* W. E. Snyder†
R. C. Mann

[Abstract of *J. Opt. Soc. Am. A* **8(2)**, 290 (1991)]

In this paper, we derive the mean field approximation from the information-theoretic principle of *minimum relative entropy*. We previously derived the mean field approximation from minimizing Peierls' inequality for the Weiss free energy of statistical physics theory. Here we show that information theory leads to our earlier statistical mechanics procedure. As an example, we consider a problem in binary image restoration. We find mean field annealing compares favorably to the stochastic approach.

Research sponsored by U.S. DOE Office of Basic Energy Sciences.

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HYBRID AI ARCHITECTURES

3.42

HYBRID NEURAL NETWORK AND RULE-BASED PATTERN RECOGNITION SYSTEM CAPABLE OF SELF-MODIFICATION

**C. W. Glover M. Silliman*
M. Walker† N. S. V. Rao‡**

[Abstract of paper presented at the SPIE's Applications of Artificial Intelligence VIII Conference, Orlando, FL, April 17–19, 1990; Proc. Vol. 1, pp. 290–300, Mohan Trivedi, Ed. (1990)]

This paper describes a hydrid neural network and rule-based pattern recognition system architecture which is capable of self-modification or learning. The central research issue to be addressed for a self-modifying multiclassifier hybrid system such as the one to be discussed here is whether such a system can perform better than either of the two classifiers taken by themselves. The hybrid system employs a hierarchical architecture and can be interfaced with one or more sensors. Feature extraction routines operating on raw sensor data produce feature vectors which serve as inputs to neural networks. At the next level in the hierarchy are neural network classifiers which are trained to provide discrimination of the sensor data. Feature vectors are formed from a concatenation of processed information from the feature extraction routines and the neural network results. A rule-based classifier system uses the feature vectors to determine if certain expected environmental states, conditions, or objects are present in the sensors' current data stream. The rule-based system has been given an *a priori* set of models of certain expected environmental states, conditions, or objects. These models can be represented as a directed graph of features vectors. The rule-based system forms many candidate directed graphs of various combinations of incoming features vectors and uses a suitably chosen metric to measure the similarity between candidate and model directed graphs. The rule-based system must then decide if there is a match between one of the candidate graphs and a model graph. If a match is found then the rule-based system invokes a routine to setup and train a new neural network from the appropriate feature vector data to recognize when this model state is present in future sensor data streams. A different neural network is created for each model state found by the rule-based system. Both the new neural networks and rule-based systems receive all subsequent feature vector data streams, and each classifier, neural net and rule-based, provide estimates of whether a certain model state exist in the data. If the neural network finds that a model state is present and the rule-based system does not, then the rule-based system will alter its model of the state — the rule-based system learns from the neural net. If the neural network does not find that a model state is present and the rule-based system does, then the rule-based system will invoke a neural network retraining routine — the neural network learns from the rule-base. A second research issue is whether the self-modification of models can be controlled, such that models are only altered to reflect new information and not be destroyed completely.

Research sponsored by U.S. Department of Energy.

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3.43

HYBRID NEURAL NETWORK AND RULE-BASED PATTERN RECOGNITION SYSTEM CAPABLE OF SELF-MODIFICATION

**C. W. Glover M. Silliman*
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N. S. V. Rao‡**

[Abstract of paper presented at the 1990 Summer National AIChE Meeting, San Diego, CA, August 19–22, 1990; Proc. abstract 33d (1990)]

This paper describes a hybrid neural network and rule-based pattern recognition system architecture which is capable of self-modification or learning. The Hybrid System is arranged in a hierarchical architecture of multiple disparate classifiers that can be interfaced with one or more sensors. At the lowest level in the hierarchy, low-level classifiers transform sensor information into symbols where ultimately a rule-based system will supervise the fusion of this information. (Neural

networks are used as low-level classifiers in this research.)

A rule-based system sits at the highest level of the hierarchy, its goal is to estimate whether a given set of objects or conditions is present in the sensed environment. The estimate is produced by fusing the symbolic information from the lower layers in accordance with a given set of rules. Once the rule-based system decides an object is present, it creates and trains a neural network classifier to recognize the object using information from the lower-level classifiers. The goal of this neural network is to provide the rule-based system with a second opinion as to whether a given object is present or not.

In the Hybrid System the neural network and rule-based system operate collectively as high-level fusion centers which can learn from one another. In all subsequent sensor scans the neural network will receive information from the lower layers of classifiers and produce an output to the rule-based system which is proportional to the probability the object, it was trained to recognize, is present in the environment. If the rule-based system and neural network both indicate that an object is or is not present, then this conclusion is reinforced by the mutual agreement. If the rule-based system and neural network disagree then one must be modified. If the rule-based system finds that the object is present and the neural network does not, then the rule-based system will add the information to the neural network's original training set and retrain the network. The neural network incrementally learns from the rule-based system. If, one the other hand, the neural network finds the object is present and the rule-based system does not, then the rule-based system will update its database to reflect new information. Here the rule-based system has learned from the neural network.

The advantage of the Hybrid System is that it not only fuses information, it can adapt to a changing environment. The Hybrid System is currently being implemented on a parallel hypercube computer architecture for use on an autonomous mobile robot.

Research sponsored by U.S. Department of Energy.

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3.44

HYBRID INTELLIGENT PERCEPTION SYSTEM: INTELLIGENT PERCEPTION THROUGH COMBINING ARTIFICIAL NEURAL NETWORKS AND AN EXPERT SYSTEM

C. W. Glover P. F. Spelt

[Abstract of paper presented at the First Workshop on Neural Networks: Academic/Industrial/NASA/Defense, Auburn University, Auburn, AL, February 5–6, 1990; Proc. pp. 321–332 (1990)]

This paper presents a report of work-in-progress on a project to combine Artificial Neural Networks (ANNs) and Expert Systems (ESs) into a hybrid, self-improving pattern recognition system. The purpose of this project is to explore methods of combining multiple classifiers into a Hybrid Intelligent Perception (HIP) System. The central research issue to be addressed for a multiclassifier hybrid system is whether such a system can perform better than the two classifiers taken by themselves. ANNs and ESs have different strengths and weaknesses, which are being exploited in this project in such a way that they are complementary to each other: Strengths in one system make up for weaknesses in the other, and *vice versa*. There is presently considerable interest in the AI community in ways to exploit the strengths of these methodologies to produce an intelligent system which is more robust and flexible than one using either technology alone. Perception, which involves both data-driven (bottom-up) and concept-driven (top-down) processing, is a process which seems especially well-suited to displaying the capabilities of such a hybrid system. This work has been funded for the past six months by an Oak Ridge National Laboratory seed grant, and most of the system components are operating in both the PC and the hypercube computer environments. Here we report on the efforts to develop the low-level ANNs and a graphic representation of their knowledge, and discuss ways of using an ES to integrate and supervise the entire system.

Research sponsored by Director's R&D Seed Money.

3.45

A HYBRID ARTIFICIAL INTELLIGENCE ARCHITECTURE AS AN INTELLIGENT INTERFACE IN HIERARCHICAL SUPERVISORY CONTROL

P. F. Spelt

[Abstract of paper presented at the Second Workshop on Neural Networks, Auburn University, Auburn, AL, February 11–13, 1991; Proc. pp. 713–721 (1991)]

This paper discusses the use of a hybrid artificial intelligence (AI) architecture as an interface between a human operator and a hierarchical automated process control system. This hybrid architecture combines artificial neural networks (ANNs) and an expert system (ESs) into a hybrid, self-improving AI system. Such a system uses several AI capabilities to help an operator cope with problems associated with modern automated process control. While the focus of this paper is the control rooms of advanced nuclear reactors, the general principles are applicable to any setting in which a human operator confronts an automated control system using locally intelligent distributed control devices.

Research sponsored by U.S. Department of Energy.

3.46

A HYBRID ARTIFICIAL INTELLIGENCE ARCHITECTURE FOR DIAGNOSIS AND DECISION MAKING IN MANUFACTURING

P. F. Spelt H. E. Knee
C. W. Glover

[Abstract of *Journal of Intelligent Manufacturing* (in press)]

This paper presents an architecture which combines Artificial Neural Networks (ANNs) and an Expert System (ES) into a hybrid, self-improving artificial intelligence (AI) system. The purpose of this project is to explore methods of combining multiple AI technologies into a hybrid intelligent diagnostic and advisory system. ANNs and ESs have different strengths and weaknesses, which can be exploited in such a way that they are complementary to each other: Strengths in one system make up for weaknesses in the other, and vice versa. There is presently considerable interest in the AI community in ways to exploit the strengths of these methodologies to produce an intelligent system which is more robust and flexible than one using either technology alone. Any process which involves both data-driven (bottom-up) and concept-driven (top-down) processing is especially well-suited to displaying the capabilities of such a hybrid system. The system can take an incoming pattern of signals, as from various points in an automated manufacturing process, and make intelligent process control decisions on the basis of the pattern as preprocessed by the ANNs, with rule-based heuristic help or corroboration from the ES. Patterns of data from the environment which can be classified by either the ES or a human consultant can result in a high-level ANN being created and trained to recognize that pattern on future occurrences. In subsequent cases in which the ANNs and the ES fail to agree on a decision concerning the environmental situation, the system can resolve those differences and retrain the networks and/or modify the models of the environment stored in the ES. Work on a hybrid system for perception in machine vision has been funded initially by an Oak Ridge National Laboratory seed grant, and most of the system components are operating presently in a parallel distributed computer environment.

Research sponsored by U.S. DOE Office of Basic Energy Sciences.

3.47

HOW WOULD YOU KNOW AN INTELLIGENT SYSTEM IF YOU SAW ONE?

C. W. Glover

[Abstract of paper presented at the Fifth Annual Aerospace Applications of Artificial Intelligence Conference, Dayton, OH, October 23-27, 1989; Proc. Vol. 1, pp. 20–28, J. R. Johnson, Ed. (1989)]

This paper advocates that the study of intelligent systems is a science in its infancy, and there is an urgent need to reduce the ambiguity in definitions of the terms used throughout intelligent systems science. For example, researchers do not agree on what an "intelligent system" is, or how to measure the intelligence within a system. This paper, as an exercise, presents a strawman definition and measure of a system's intelligence, and

discusses some of the problems that can arise when measuring intelligence. Not everyone is expected to agree with the strawman definition of intelligence. The primary purpose for presenting it is to stimulate thought, and to challenge the readers to continue the exercise and develop their own measure of intelligence. Maybe, at some point we as researchers can converge on a working quantitative measure of intelligence.

Research sponsored by U.S. Air Force Wright Aeronautical Laboratory and U.S. DOE Office of Basic Energy Sciences.

HUMAN INTERFACES TO COMPLEX SYSTEMS

3.48

THE ADVANCED CONTROLS PROGRAM AT THE OAK RIDGE NATIONAL LABORATORY

H. E. Knee J. D. White*

[Abstract of paper presented at the International Conference on Supercomputing in Nuclear Applications, Mito City, Japan, March 12–16, 1990; Proc. pp. 490–495 (1990)]

The Oak Ridge National Laboratory (ORNL), under sponsorship of the U.S. Department of Energy (DOE), is conducting research that will lead to advanced, automated control of new liquid-metal-reactor (LMR) nuclear power plants. This program of research entitled, "Advanced Controls Program," involves five principal areas of research activities: 1) Demonstrations of Advanced Control System Designs, 2) Development of an Advanced Controls Design Environment, 3) Development of Advanced Control Strategies, 4) Research and Development (R&D) in Human-System Integration for Advanced Control System Designs, and 5) Testing and Validation of Advanced Control System Designs. Discussion of the research in these five areas will form the basis of this paper. Also included in this paper will be a description of the research directions of the program.

Research sponsored by U.S. DOE Office of Technology Support Programs.

*Instrumentation and Controls Division.

3.49

HUMAN FACTORS ISSUES ASSOCIATED WITH ADVANCED INSTRUMENTATION AND CONTROLS TECHNOLOGIES IN NUCLEAR PLANTS

R. J. Carter R. E. Uhrig*

(Abstract of ORNL/TM-11319, NUREG/CR-5439, June 1990)

A survey of advanced instrumentation and controls (I&C) technologies and associated human factors issues in the U.S. and Canadian nuclear industries was carried out by a team from Oak Ridge National Laboratory to provide background for the development of regulatory policy, criteria, and guides for review of advanced I&C systems as well as human engineering guidelines for evaluating these systems. The survey found those components of the U.S. nuclear industry surveyed to be quite interested in advanced I&C, but very cautious in implementing such systems in nuclear facilities and power plants. The trend in the facilities surveyed is to experiment cautiously when there is an intuitive advantage or short-term payoff. A number of safety-related human factors issues were derived from the results of this survey. They include: Is an advanced I&C guideline equivalent to NUREG-0700 needed? What changes will there be in the role of the control room operator? The potential problem of information overload needs to be addressed. How should existing training technology be made applicable for advanced I&C? How will operator acceptance and trust be accomplished?

Research sponsored by U.S. DOE and Division of Systems Research, Office of Nuclear Regulatory Research, U.S. Nuclear Regulatory Commission.

*Instrumentation and Controls Division.

3.50

SUPERCOMPUTING FOR NUCLEAR DESIGN WITH AN EMPHASIS ON INSTRUMENTATION AND CONTROLS

H. E. Knee

[Abstract of paper presented at the International Conference on Supercomputing in Nuclear Applications, Mito City, Japan, March 12–16, 1990; Proc. pp. 650–652 (1990)]

During the past decade, developments that have emerged in the area of supercomputing technologies have provided a new potential with respect to design. First, supercomputing technologies have provided means for the development of new design tools and environments that may be utilized for more optimal designs. Second, supercomputing technologies themselves are being utilized within particular designs as a means for realizing more optimal systems. The potential impact of supercomputing power is just beginning to be perceived, and is just starting to be assimilated into industrial environments.

With regard to the nuclear industry and supercomputing: the commercial industry within the U.S. seems to have been relatively slow (if not stagnant) to embrace such technologies. This is not surprising given the relatively stringent regulatory environment within the U.S., and the lack of motivation (by the regulatory agencies and the utilities) to introduce advanced instrumentation, controls, or superomputing capabilities into the industry. Although the U.S. commercial nuclear industry has demonstrated a relative paucity with respect to the use of advanced technologies [advanced instrumentation and controls (I&C), including supercomputing], there has been some relatively creative utilization of such technologies with respect to new advanced reactor design concepts, and within the design process itself.

Research sponsored by U.S. DOE Office of Technology Support Programs.

3.51

HUMAN FACTORS SURVEY OF ADVANCED INSTRUMENTATION AND CONTROLS TECHNOLOGIES IN NUCLEAR PLANTS

R. J. Carter

[Abstract of *Nuclear Engineering and Design* (in press)]

A survey of advanced instrumentation and controls (I&C) technologies and associated human factors issues was conducted. The objective of the survey was to provide background for the development of regulatory policy, criteria, and guides for review of advanced I&C systems as well as human engineering guidelines for evaluating these systems. The survey was administered at five U.S. nuclear utilities, two advanced reactor and three light water reactor (LWR) vendors, and a Canadian utility and vendor. The nuclear industry appears to have addressed a number of the human factors concerns and potential problems discussed during the survey. It has started to seriously consider the human factors implications of the introduction of advanced I&C into the control room. There are, however, a number of safety-related human factors issues that still need to be investigated. They include: Is an advanced I&C guideline for the interface of the human with displays and controls needed? What changes will there be in the role of the control room operator? The potential problem of information overload needs to be addressed. How can existing training technology be made applicable for advanced I&C? How will operator acceptance and trust be accomplished? The purpose of this paper is to summarize the human factors results from the survey and to identify and discuss the derived human factors issues.

Research sponsored by the U.S. Nuclear Regulatory Commission, Office of Nuclear Regulatory Research and the U.S. Department of Energy.

3.52

FY 1990 HUMAN FACTORS ENGINEERING SUPPORT FOR THE NEW HEAVY WATER PRODUCTION REACTOR

R. J. Carter P. F. Spelt

(Abstract of ORNL/NPR-90/50, December 1990)

The Department of Energy (DOE) is supporting the design of a new heavy water production reactor (HWPR). Oak Ridge National Laboratory (ORNL) furnished on-site human factors engineering expertise to the HWPR project during fiscal year 1990. Human factors work performed concentrated on seven areas: identification and review of nuclear-related human factors engineering guidelines; development of human factors engineering features for the specific requirements information packages (SRIP); identification and review of human factors engineering standards and guidelines for advanced technology; review of Ebasco Services' human factors engineering conceptual design documents; generation of human factors engineering-related material for the Savannah River Site's (SRS); development of a human factors engineering program plan (HFEPP) for the HWPF; and performance of a feasibility study for the subsequent development of a HWPF simulation code. As a result of the human factors engineering support provided, a number of recommendations were derived. They include General Physics Corporations (GPC) HFEPP for the HWPR should be modified, updated, and adopted; the lessons learned survey conducted by GPC should be modified, expanded, and administered to reactor operators and maintenance personnel, Savannah River Site's (SRS) human factors engineering role, mission, and responsibilities in regard to the HWPR should be defined succinctly; DOE should make a substantial commitment to the incorporation of human factors engineering principles and criteria into the HWPR design; an evaluation/verification human-machine testbed should be developed and constructed in order to validate human factors engineering concepts being developed by Ebasco Services/Combustion Engineering; the nuclear-related human factors engineering guidelines and the human factors engineering standards and guidelines for advanced technology should be used as guidance during the HWPR development; ORNL's development effort in regards to human factors engineering SRIP features should be continued; the SRIP features should be approved by DOE; Ebasco Services/Combustion Engineering's human factors engineering program should be monitored and reviewed closely; the HFEPP, developed by ORNL for the HWPF, should be implemented by SRS; the human factors engineering programs of the HWPF contractors should be monitored and reviewed closely; and a human factors engineering simulation model of the HWPF should be developed.

Research sponsored by U.S. DOE Office of New Production Reactors.

3.53

TEAM-COMPUTER INTERFACES IN COMPLEX TASK ENVIRONMENTS

M. Terranova

(Abstract of ORNL/TM-11592, September 1990)

This research focused on the interfaces (media of information exchange) teams used to interact about the task at hand. This report is among the first to study humam-system interfaces in which the human component is a team, and the system functions as a part of the team. Two operators dynamically shared a simulated fluid flow process, coordinating control and failure detection responsibilities through computer-mediated communication. Different computer interfaces representing the same system information were used to affect the individual operators' mental models of the process. Communication was identified as the most critical variable, consequently future research is being designed to test effective modes of communication. The results have relevance for the development of team-computer interfaces in complex systems in which responsibility must be shared dynamically among all members of the operation.

Research sponsored by U.S. Department of Energy.

3.54

COMPUTER INTERFACES FOR TEAM TASKS: COMMUNICATION AND DISPLAY DESIGN

M. Terranova **D. Hartley***
B. G. Coury† **K. Hooper†**

(Abstract of paper presented at the 34th Annual Meeting of the Human Factors Society, Orlando, FL, October 8-12, 1990)

The purpose of this paper is to report the results of two experiments designed to study computer interfaces for a task shared between two human operators. Specifically, the experiments address the effects of system representations and communication on team performance. The first experiment has been completed and is primarily concerned with team performance. The second experiment, which is currently underway, focuses more precisely on the differences between individual and team performance. In both experiments two operators supervise a simulated fluid flow process, coordinating system control and failure detection responsibilities through their communication. Each of the operators in the experiment had independent access to a computer interface that represented system information either in a graphic or an alphanumeric format. Operators were assigned to a team based on display format. In the first experiment, teams were comprised of operators using a graphic, alphanumeric, or a combination of both graphic and alphanumeric information. In that experiment, fifty reservists from a Navy and Marine Reserve Center served as operators in this study. The teams communicated via explicit, computer-mediated communication. The results identified communication as the most critical variable for team performance. In the second experiment voice-mediated communication is being studied, and operators are trained to supervise the system using either a graphic display or an alphanumeric display. Performance comparisons will be made between operators performing as individuals and in teams. Protocol analysis, specifically using a think aloud methodology, will be used in order to study the cognitive strategies used by operators to supervise the system, and identify the types of strategies that lead to the best performance. In the second phase of the research, operators will be paired into teams to supervise the system. Team communication will be analyzed and related to system performance. It is expected that both the amount of communication and content of the communication will be related to cognitive strategies and effective team performance. Discussion will focus on the application of these results to the design of advanced controls rooms, operator interfaces, and operator communication.

Research sponsored by U.S. Department of Energy.

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3.55

PART-TASK TRAINERS FOR COMPLEX COGNITIVE SKILLS: EVALUATION OF THE USER INTERFACE

D. Hartley* **M. Terranova**
R. J. Carter **C. E. Snyder†**

(Abstract of paper presented at the Conference on Human Factors in Computing Systems, Seattle, WA, April 1-5, 1990)

The research reported here is an evaluation of the user interface of a computer-based part-task (PTT) for Navy weapons operators. Navy weapons operators are required to perform tasks that range in difficulty from simple, ordered procedural tasks to highly complex tasks that are dependent on cognitively-based decision skills. For training system success, the training must focus on the mental operations that must be performed in order to utilize the information required by the task. As the Navy becomes more reliant upon sophisticated, complex defense systems to meet mission requirements, there is an increased need to improve the user interface design that supports the portrayal of complex cognitive tasks. The objective of this evaluation is to provide enhancements to the user interface so that it supports the effectiveness of the training.

The intent of the analyses that will be outlined in this presentation and the ongoing work, is to provide data that contributes to the optimization of the user interface that effectively supports training for complex cognitive skills. Implications for future enhanced trainers will be discussed.

Research sponsored by Pacific Missile Test Center.

*University of Tennessee, Knoxville, TN.

†Data System Research Development Division.

3.56

THE PART TASK TRAINER FOR AIRBORNE WEAPONS SYSTEMS: HUMAN FACTORS EVALUATION OF THE USER INTERFACE

M. Terranova D. E. Hartley*

(Abstract of ORNL/TM-11635, September 1990)

This research examined and evaluated the human factors aspects of a part-task trainer's user interface. Questionnaires, interviews, and observational techniques were used. A number of established human factors attributes were investigated such as user control and trainer fidelity. Recommendations were given for a variety of issues such as screen design (e.g., design log-on process and procedures for user identification to be as simple as possible); text display (e.g., avoid sentences exceeding 20 words); and training for cognitive skills (e.g., train time-sharing skills for dealing with high workload environments). The results and recommendations for future enhancements were reported. An installation process was documented and comments regarding its effectiveness were included.

Research sponsored by U.S. Department of Energy and the Department of the Navy, Pacific Missile Test Center.

*University of Tennessee, Knoxville, TN.

3.57

OBJECT-ORIENTED QUALITATIVE SIMULATION OF HUMAN MENTAL MODELS OF COMPLEX SYSTEMS

J. C. Schryver

[Abstract of *IEEE Transactions on Systems, Man, and Cybernetics* (in press)]

A qualitative model of an expert's mental model of a complex system (advanced nuclear power plant) was developed from the qualitative physics of confluences. This model was implemented as a qualitative simulation using an object-oriented extension to Common Lisp (Flavors). An existing method for dynamic constraint satisfaction was found to be inadequate for complex systems. Invisible connections for flow compatibility, control connections, iterative propagation, and embedded propagation were among the new features provided for derivation of causal ordering. Deterministic output was guaranteed through stochastic state transition. A parametric Monte Carlo simulation study was performed using a fictitious loop fragment, and changes were observed in flow rate change through a pump. State transition models provided excellent fits to the simulation data. The state models showed that all conditions converged to steady state. Strictly forward (with the flow) propagation facilitated consistency within intermediate pre-equilibrium states and convergence as compared to forward propagation with limited backward propagation. Uncertainty bias inhibited propagation of premature incorrect values. The psychological plausibility of qualitative simulation models was evaluated. A further extension of mythical causality is suggested, for which constraint propagation executes on multiple levels of aggregation.

Research sponsored by U.S. DOE Office of Technology Support Programs.

3.58

JOB PLANNING AND EXECUTION MONITORING FOR A HUMAN-ROBOT SYMBIOTIC SYSTEM

L. E. Parker

(Abstract of ORNL/TM-11308, November 1989)

The human-robot symbiosis concept has the fundamental objective of bridging the gap between fully human-controlled and fully autonomous systems to achieve true human-robot cooperative control and intelligence. Such a system would allow improved speed, accuracy, and efficiency of task execution, while retaining the human in the loop for innovative reasoning and decision-making. Earlier research has resulted in the development of a robotic system architecture facilitating the symbiotic integration of teleoperative and automated modes of task execution. This architecture reflects a unique blend of many disciplines of artificial intelligence into a working system, including job or mission planning, dynamic task allocation, human-robot communication, automated monitoring, and machine learning. This report focuses on two elements of this architecture: the Job Planner and the Automated Monitor.

Research sponsored by U.S. DOE Office of Basic Energy Sciences.

3.59

HUMAN FACTORS CONSIDERATIONS FOR EXPERT SYSTEMS

R. J. Carter

[Abstract of *Expert Systems* (in press)]

Two studies which were oriented towards identifying the human factors issues and concerns in regard to expert systems are presented. During the studies, discussions and interviews were conducted with nuclear plant regulators, vendors, and utilities. Issues identified include: adequacy of the knowledge base, acquisition of expert knowledge, simplicity, clarity, and understandability of the human-expert system interface, user's perspectives and mental models, function allocation and division of labor, manner of implementation, impact on workload. effect on human performance, and user's reaction. These and other issues are described and discussed. The human factors-expert systems issues need to be studied further and evaluated thoroughly.

Research sponsored by U.S. Department of Energy.

INTELLIGENT SYSTEMS FOR BIOMEDICAL APPLICATIONS

3.60

PATTERN RECOGNITION IN DNA SEQUENCES: THE INTRON-EXON JUNCTION PROBLEM

R. J. Mural* R. C. Mann
E. C. Uberbacher†

[Abstract of paper presented at the First International Conference on Electrophoresis, Supercomputing, and the Human Genome, Tallahassee, FL, April 7, 1990; Proc. pp. 164–172, C. R. Cantor and H. A. Liu, Eds., World Scientific Publishing Co. (1991)]

One of the fundamental problems facing the field of genomic sequence analysis is the difficulty in locating relatively small coding regions of DNA within the much larger non-coding regions. Neural networks, linguistic analysis and various types of expert systems have been used with various degrees of success to address this problem. We have developed several methods for recognizing the presence of splice junctions and coding DNA which are based on artificial intelligence, linguistic and statistical approaches. The triplet vocabulary in and around splice junctions has been analyzed for primates, and the occurrences of preferred triplets in potential junctions seems to be a very selective method for distinguishing true junctions from otherwise similar sequences. Given a 50% mix of true and false junctions, this method scores 93%–95% correct. Several approaches have been used to identify exons. These include a frame bias matrix algorithm and an algorithm which estimates the fractal dimension of dinucleotide usage. Attempts are underway to combine the outputs of the various methods using a rule-based approach to improve the overall performance of these predictors.

Research sponsored by U.S. Department of Energy.

*Biology Division.

†University of Tennessee, Knoxville, TN and the Biology Division.

3.61

A NEURAL NETWORK — MULTIPLE SENSOR BASED METHOD FOR RECOGNITION OF GENE CODING SEGMENTS IN HUMAN DNA SEQUENCE DATA

E. C. Uberbacher* R. C. Mann
R. C. Hand, Jr.* R. J. Mural*

(Abstract of ORNL/TM-11741, February 1991)

A central focus of the Human Genome Project is to locate and characterize genes within genomic DNA sequence data. Of particular importance are genes related to cancer and other major human genetic diseases. Identification of gene segments within the DNA sequence currently relies upon tedious and time-consuming experimental methods. A new computational method developed at Oak Ridge National Laboratory (ORNL) represents an efficient alternative to these experimental procedures. This method combines a set of statistical

sensors and a neural network into a single structure which is capable of locating gene segments with considerable speed and accuracy. The approach provides a powerful tool for investigators searching for disease genes.

Research sponsored by U.S. DOE Director's R&D.

*Biology Division.

3.62

ON PARALLEL SEARCH OF DNA SEQUENCE DATABASES

X. Guan*　R. Mural†
R. C. Mann　E. Uberbacher†

[Abstract of paper presented at the 5th SIAM Conference on Parallel Processing for Scientific Computing, Houston, TX, March 25-27, 1991; Proc. p. A2 (1991)]

This paper describes the development of large scale parallel search methods for DNA databases using dynamic programming algorithm on an Intel iPSC/860 parallel computer. The performance of these methods has been measured and several strategies for improving performance are discussed.

Research sponsored by U.S. DOE Office of Health and Environmental Research.

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†Biology Division.

3.63

TWO-DIMENSIONAL GEL ELECTROPHORESIS OF CYTOPLASMIC PROTEINS IN CONTROL AND TRANSFORMED 10T$\frac{1}{2}$ AND CVP CELLS AFTER BENZO[A]PYRENE TREATMENT

J. K. Selkirk*　B. K. Mansfield*
D. J. Riese†　A. Nikbakht†
R. C. Mann

[Abstract of paper presented at the Twenty-Seventh Hanford Symposium on Health and the Environment, Richland WA, October 18-21, 1988; Proc. pp. 299-304 (1989)]

It is generally accepted that environmental chemical carcinogens require metabolic activation to reactive intermediates to express their carcinogenic effect. In recent years, the metabolism of different chemical carcinogens has been carefully characterized with the result that the metabolite profile is essentially identical in all species and cells for a given carcinogen. These metabolite profiles are independent of the relative susceptibility to malignant transformation. To understand the relative transformation potential, it is necessary to develop new strategies to comprehend the critical biochemical differences that determine carcinogen susceptibility between cell types and in humans and experimental animals.

We have used two-dimensional gel electrophoresis to characterize gene products in various cell types, including those undergoing differentiation and in transformable cells treated with benzo[a]pyrene (BaP). Utilizing Friend erythroleukemia cells undergoing differentiation, we have observed a number of induced and repressed gene products with image analysis methodology on digitized fluorographs of two-dimensional electrophoresis gels of cytoplasmic proteins.

Eventually, the polypeptide data base will be large enough so that it can be probed for possible elucidation of the cascade of subtle biochemical events that result in cellular commitment to malignancy following exposure to chemical carcinogens.

Research sponsored by U.S. DOE Office of Basic Energy Sciences.

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†Biology Division.

COMPUTER SECURITY

3.64

TESTING COMPUTER SECURITY ANOMALY DETECTION

G. E. Liepins H. S. Vaccaro*

[Abstract of *Computers and Security* (in press)]

This paper addresses three main security monitoring questions: "What are we trying to detect?" "How might we do it?" "How do we know if we're successful?" A framework for total computer security is outlined. The distinct, yet complementary purposes of anomaly detection and misuse detection are clarified in terms of a probability model. Relative density estimation is explained to be the basis of anomaly detection and the use of historical transactions to estimate density is elaborated. Because of drawbacks to density estimation based directly on a sample of historical data (difficulties with extensions to chains of related transactions, and inefficiency with highly multivariate data), alternative approaches have been developed. One of these, called W&S, is briefly summarized. Empirical and simulation methods for testing anomaly detection performance are introduced. Preliminary results of empirical testing of W&S suggest that W&S provides near optimal anomaly detection for low dimensional categorical transactions. Testing with higher dimensional data is planned for the near term.

Research sponsored by U.S. Department of Energy.

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HAZARDOUS WASTE MANAGEMENT

3.65

ENVIRONMENTAL PROTECTION FOR HAZARDOUS MATERIALS INCIDENTS

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J. E. Dobson* C. E. Easterly*
P. S. Ogle* A. K. VanCleave†

(Abstract of ORNL/TM-11421, February 1990)

This document was prepared to provide the U.S. Air Force fire protection community with an integrated program for handling hazardous materials (HAZMAT)s and hazardous material incidents.

The goal of the project was to define and identify a computer system for the base fire departments that would facilitate hazard assessment and response during HAZMAT emergencies, provide HAZMAT incident management guidelines, and provide a training tool to simulate emergency response during normal times. To reach this goal, site visits to Air Force bases were made to observe existing HAZMAT related organizations, their methods and procedures used in HAZMAT management, and to collect personnel input for the development of the computerized Hazardous Materials Incident Management System (HMIMS). In a following phase, the study concentrated on defining strategic areas of concern to emergency response personnel. Particular emphasis was given to such areas as responsibilities and roles for response agencies; personnel requirements to handle HAZMAT incidents; procedures to follow during HAZMAT incidents and decontamination; personnel evacuation; postincident evaluation and feedback; emergency response personnel participation in installation restoration program; personal protective clothing; mutual aid requirements; and training. In light of federal regulations and good HAZMAT management practices, future recommendations were made for purchase, use, storage, disposal, and management of HAZMATs during their life cycle on bases and during incidents. This detailed technical report and the HMIMS are expected to meet the integrated HAZMAT program needs primarily of Air Force fire departments and secondarily in other response agencies.

Research sponsored by U.S. DOE, Hazardous Waste Remedial Actions Program.

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ENERGY ANALYSIS

3.66

THE HYBRID APPROACH TO DEMAND MODELING

D. B. Reister

[Abstract of *Energy - The International Journal* 15(3/4), 249 (1990)]

This paper presents an engineering-economic approach for developing energy demand models. The approach combines the economic theory of production with engineering process data. We review the economic theory of production, the Constant Elasticity of Substitution (CES) function, and the Logit function. Using the Oak Ridge Industrial Model (ORIM) as a case study, we show how the Logit function can be used to specify a fuel share model and how the CES function can be used to specify an energy conservation model. Shephard's lemma is a key result of the economic theory of production. The lemma can be used to derive input-output coefficients from a cost function. We use CES cost functions because they have good global properties. To obtain more flexibility, we use nested CES cost functions. To identify the parameters in a nested CES structure, we assume that the multilevel cost function corresponds to a multistage production process. When input-output coefficients are derived from a cost function, the tradeoffs between the factors satisfy the law of diminishing returns. Energy conservation occurs when capital, labor, or materials are substituted for energy service. In most cases, the substitution obeys the law of diminishing returns. Thus, a CES cost function can be used to specify an energy conservation model. Normally, perfect substitutes do not obey the law of diminishing returns. Since we include all of the costs for each option (the options use fuel and provide energy service) in ORIM, the options are perfect substitutes and do not satisfy the law of diminishing returns. Since the options are perfect substitutes, we use the Logit function to specify the ORIM fuel share model.

Research sponsored by U.S. DOE Office of Fossil Energy.

3.67

ENERGY TECHNOLOGY R&D: WHAT COULD MAKE A DIFFERENCE? PART 1 - END-USE TECHNOLOGY PART 2 - SUPPLY TECHNOLOGY PART 3 - CROSSCUTTING SCIENCE AND TECHNOLOGY

W. Fulkerson* D. B. Reister
J. T. Miller†

(Abstract of ORNL-6541/V2/P1, ORNL-6541/V2/P2, and ORNL-6541/V2/P3, December 1989)

Early in 1988, the management of Oak Ridge National Laboratory (ORNL) decided to organize an internal study to review the status of energy technologies and to identify the research and development opportunities that could make a difference for both the United States and the rest of the world. More than 100 ORNL staff members were organized into teams to review the status of technology in 18 areas covering energy use, energy supply, and crosscutting science. Each team attempted to identify significant technological advances that could be made within a reasonable time and cost.

The results of the study are being published in two volumes. The first volume is the synthesis report, while the second volume is the collection of the 18 team reports. The three parts of Vol. 2 review (1) end-use technology, (2) supply technology, and (3) crosscutting science and technology.

Research sponsored by U.S. Department of Energy.

*Energy Division.

†Publications Division.

3.68

OIL VULNERABILITY AND INTERMEDIATE PRICE FLUCTUATIONS: A PRELIMINARY ASSESSMENT AND PROPOSAL

T. R. Curlee* **D. B. Reister**

(Abstract of ORNL/TM-11259, September 1989)

Most of the work on oil vulnerability has focused on the implications and appropriate public and private responses to short-term oil price spikes. This report focuses on the possibility that the world oil market is inherently more prone to large intermediate price fluctuations that are often triggered by short-term disturbances.

The purposes of this report are to (1) pose the question of whether large and repeated intermediate price swings are a likely outcome, given our knowledge of the world oil market, (2) address how the effectiveness of policy instruments designed to mitigate the impacts of oil vulnerability may change in a world in which large intermediate oil price fluctuations are expected, and (3) propose future research that would address in greater detail the potential for, and appropriate responses to, large intermediate price swings on the world and domestic oil markets.

The report concludes that there are plausible conceptualizations under which oil prices may fluctuate over the intermediate term. It is suggested that a major focus of future work should be on how the structure of the oil market may itself change over time, causing oil prices to go up and down. The report also concludes that the implications of such price swings may be significant for both the types and quantities of mitigation measures held by the public and private sectors. Finally, it is argued that the current world oil market provides a valuable opportunity for studying how oil prices may fluctuate over the intermediate term and how U.S. energy policies can best be structured to cope with oil vulnerability.

Research sponsored by U.S. Department of Energy.

*Energy Division.

Section 4

NUCLEAR ANALYSIS AND SHIELDING

4.0. INTRODUCTION

D. T. Ingersoll

The Nuclear Analysis and Shielding Section is comprised of four groups whose major research activities include: (1) computational analysis and experiments for fission reactor radiation transport and shielding, (2) methods development and analysis for fission reactor core physics, (3) development of computer methods and models for high-energy radiation and particle transport and detection, and (4) mathematical modeling and computer analysis of ground- and spaced-based defensive systems. The Oak Ridge Detector Center, which is also organizationally contained in the section, was established to facilitate ORNL's involvement in the development, design, and engineering of physics detectors for the Superconducting Super Collider (SSC).

The long-established expertise in the reactor shielding group continued to draw support from a diversity of reactor programs including: (1) large-scale shielding analysis for the high-temperature gas-cooled reactor programs (commercial and production concepts) and the liquid-metal-cooled reactor program, (2) prediction of neutron and gamma-ray transport in the beam tubes and cold source of the proposed Advanced Neutron Source (ANS), and (3) prediction of gamma-ray dose rates in a proposed demonstration fuel reprocessing plant. Several neutronics analyses were also performed to support the operation and Safety Analysis Report of the ORNL High Flux Isotope Reactor and the Halden Reactor Project in Norway. A particularly gratifying accomplishment was the resumption of the joint U.S./Japan program of shielding experiments supporting the liquid-metal-cooled reactor program after an extended shutdown of the Tower Shielding Facility.

Activities in the reactor physics group focused on two primary programs: (1) performance and design analyses for the ANS, including control concepts, fuel grading options, and nuclear heating, and (2) methods development, benchmark analyses, and design methodology verification for the gas-cooled reactor concept for the New Production Reactor program. Also, a program was moved into the group from another section to continue the development and application of automated adjoint methods for sensitivity and uncertainty analysis. The acquisition of an IBM RISC/6000 workstation to facilitate reactor physics analyses has led to a renewed effort to adapt and extent our physics codes to an interactive computing environment and has spurred the purchase of additional workstations.

Projects in the high-energy physics area included further developments and improvements to physics models and nuclear data base for the HETC high-energy radiation and particle transport code. One staff member (T. A. Gabriel) was selected to serve as director of the newly formed ORNL center for SSC detector development. The center, which operates in conjunction with other laboratories and universities in the southeast region of the United States, coordinates basic research support of general high-energy detection systems and specific development support for the Solenoidal Detector Collaboration and the L* Collaboration.

The advanced systems group continued to explore opportunities to develop new methods and to apply traditional methods to new applications. Our long-term development and analysis support for the Defense Nuclear Agency was greatly expanded, with the focus of the current program being to improve, verify, and apply adjoint Monte Carlo methods used to predict the radiation hardness of armored vehicles. As part of this effort, new graphical interfaces are being developed to aid the construction and display of three-dimensional geometry models for transport analyses. The TORT three-dimensional discrete ordinates code continues to be developed and applied under an increasing diversity of sponsorships. Exploratory studies continued for the mathematical modeling of nonlinear systems, including the use of coupled nonlinear partial differential equations to describe the behavior of combative forces. Also, a small effort was directed toward the adaptation of transport and diffusion methods to different parallel computer architectures.

NOTE: The Department of Energy has categorized a substantial part of our work for the reactor programs as "Applied Technology," so explicit references to this work cannot be included in this report.

RADIATION TRANSPORT AND PHYSICS FOR FISSION REACTORS

4.1

PHYSICS OF THE CONCEPTUAL DESIGN OF INTENSE STEADY NEUTRON SOURCES

F. C. Difilippo

[Abstract of *Nucl. Sci. Eng.* 107, 82 (1991)]

Because of the demand for intense neutron beams for applications in basic and applied sciences, several design concepts have appeared in the literature recently. It is, therefore, appropriate to present a theory that connects the large variety of possible designs in order to individualize the main parameters from the neutronic point of view; the theory is validated with results from numerical analysis that simulate the transport of neutrons in such drastically different systems as spallation and fission sources. The theory is used to present scoping studies for the production of thermal neutron fluxes around and beyond $10^{20}/m^2{\cdot}s$.

Research sponsored by U.S. DOE Office of Basic Energy Sciences.

4.2

THE CORRELATION BETWEEN FISSION NEUTRONS AND THE CALCULATION OF STOCHASTICS DESCRIPTORS APPLICATION TO THE ^{252}Cf RATIO METHOD

F. C. Difilippo

[Abstract of *Nucl. Sci. Eng.* (in press)]

Stochastics descriptors are calculated using the method of the equivalent source of correlated noise. The results are then applied to analyze the ^{252}Cf ratio method to measure subcriticalities from the point of view of the total specification of the source of noise in phase space $(\vec{r}, \vec{v})$. After using several hypotheses it is shown that this ratio method is sensitive to the specification of the equivalent source of noise, so available experimental data is used to choose the best hypothesis. It was found that the source of noise has to include explicitly the correlations between two fission neutrons coming from the same fission which is an experimental fact overlooked until now by the stochastic theory of neutron transport.

Research sponsored by U.S. Department of Energy.

4.3

ANSL-V: ENDF/B-V BASED MULTIGROUP CROSS-SECTION LIBRARIES FOR ADVANCED NEUTRON SOURCE (ANS) REACTOR STUDIES

W. E. Ford* **J. W. Arwood***
N. M. Greene* **D. L. Moses†**
L. M. Petrie* **R. T. Primm, III**
C. O. Slater **R. M. Westfall***
R. Q. Wright*

(Abstract of ORNL-6618, September 1990)

Pseudo-problem-independent, multigroup cross-section libraries were generated to support Advanced Neutron Source (ANS) Reactor design studies. The ANS is a proposed reactor which would be fueled with highly enriched uranium and cooled with heavy water. The libraries, designated ANSL-V (Advanced Neutron Source Cross Section Libraries based on ENDF/B-V), are data bases in AMPX master format for subsequent generation of problem-dependent cross-sections for use with codes such as KENO, ANISN, XSDRNPM, VENTURE, DOT, DORT, TORT, and MORSE. Included in ANSL-V are 99-group and 39-group neutron, 39-neutron-group 44-gamma-ray-group secondary gamma-ray production (SGRP), 44-group gamma-ray interaction (GRI), and coupled, 39-neutron group 44-gamma-ray group (CNG) cross-section libraries. The neutron and SGRP libraries were generated primarily from ENDF/B-V data; the GRI library was generated from DLC-99/HUGO data, which is recognized as the ENDF/B-V photon interaction data. Modules from the AMPX and NJOY systems were used to process the multigroup data. Validity of selected data from the fine- and broad-group neutron libraries was satisfactorily tested in performance parameter calculations.

Research sponsored by U.S. Department of Energy.

*Computing and Telecommunications Division.

†Engineering Technology Division.

4.4

DESIGN CALCULATIONS FOR THE ANS COLD NEUTRON SOURCE

R. A. Lillie R. G. Alsmiller, Jr.

[Abstract of *Nucl. Instrum. Methods Phys. Res.* **A295**, 147 (1990)]

Calculated results, obtained using two-dimensional discrete ordinates methods, are presented for a variety of cases of interest in the design of a neutron cold source for the Advanced Neutron Source. The methodology that was developed to carry out the calculations is described.

A liquid deuterium cold source of radius 190 mm with and without reentrant cavities is considered. Results are presented for various cavity lengths and radii, for various radii of the void tube that connects the cold source to the guide tube, and for various guide tube radii. In an appendix, a combined liquid nitrogen-15, liquid deuterium cold source is considered.

Research sponsored by U.S. DOE Office of High Energy and Nuclear Physics.

4.5

PARAMETER AND FLUENCE-RATE COVARIANCES IN LEPRICON

R. E. Maerker

(Abstract of paper presented at the Seventh ASTM-EURATOM Symposium on Reactor Dosimetry, Strasbourg, France, August 27–31, 1990)

The LEPRICON code system is now available from the Radiation Shielding Information Center at ORNL as PSR-277. The system consists of modules that involve both the calculation of neutron fluence rates through PWR pressure vessels and the adjustment of these fluence rates with reduced uncertainties based on surveillance dosimetry. This paper describes in detail the manner in which important parameter uncertainties are partitioned and quantified as part of the input to the adjustment procedure, and to what degree they are applicable to all reactor designs.

Research sponsored by the Nuclear Regulatory Commission and by the U.S. Department of Energy.

4.6

REACTOR DESIGN OF THE ADVANCED NEUTRON SOURCE

J. M. Ryskamp* D. L. Selby†
R. T. Primm, III

[Abstract of *Nucl. Tech.* **93(3)**, 330 (1991)]

The ongoing reactor design of the Advanced Neutron Source (ANS) is explored. The Advanced Neutron Source is being designed for materials sciences, isotope production, and fundamental physics research. A reactor design based on previously developed technology can meet the performance requirements set by the user community for a new ANS to serve all fields of neutron science. These requirements include the capability of producing a peak thermal neutron flux over five times higher than in any currently operating steady-state facility. Achievement of these ultra-high flux levels involves many interesting aspects of reactor design.

The reactor characteristics of the current reference design are presented. The attainment of this design was reached by following a design strategy that best met the safety and user requirements. The design has evolved over the last four years from two concepts proposed in 1985. The trade-offs and selection of many reactor parameters are described to illustrate how and why the current design was achieved. Further reactor design is planned, leading to an Advanced Neutron Source operating by 1999 for use by scientists of many disciplines.

Research sponsored by U.S. Department of Energy.

*Idaho National Engineering Laboratory, Idaho Falls, ID.

†Central Management Division.

4.7

TWO-DIMENSIONAL DORT DISCRETE ORDINATES X-Y GEOMETRY NEUTRON FLUX CALCULATIONS FOR THE HALDEN HEAVY BOILING WATER REACTOR CORE CONFIGURATIONS

C. O. Slater

(Abstract of ORNL/TM-11513, July 1990)

Results are reported for two-dimensional discrete ordinates, X-Y geometry calculations performed for seven Halden Heavy Boiling Water Reactor core configurations. The calculations were performed in support of an effort to reassess the neutron fluence received by the reactor vessel. Nickel foil measurement data indicated considerable underprediction of fluences by the previously used multigroup removal-diffusion method. Therefore, calculations by a more accurate method were deemed appropriate.

For each core configuration, data are presented for (1) integral fluxes in the core and near the vessel wall, (2) neutron spectra at selected locations, (3) isoflux contours superimposed on the geometry models, (4) plots of the geometry models, and (5) input for the calculations.

The initial calculations were performed with several mesh sizes. Comparisons of the results from these calculations indicated that the uncertainty in the calculated fluxes should be less than 10%. However, three-dimensional effects (such as axial asymmetry in the fuel loading) could contribute to much greater uncertainty in the calculated neutron fluxes.

Research sponsored by U.S. Department of Energy.

4.8

THERMOLUMINESCENT DOSIMETER MEASUREMENTS OF RADIATION HEATING IN SODIUM AND STAINLESS STEEL SHIELDS

P. N. Stevens* F. J. Muckenthaler W. Yoon*

(Abstract of ORNL-5329, February 1990)

This report describes two different measurements using Thermoluminescent Dosimeters (TLDs) and an iron-equivalent ion chamber as dosimeters to define the radiation energy deposition in a series of Fe and stainless steel mockups. These measurements, performed in late 1975 and early 1976, followed an earlier (1974) not-so-successful series of measurements in typical Clinch River Breeder Reactor (CRBR) mockups. Between these two time periods, a considerable effort was spent to develop a procedure for measurement and readout of the TLD chips that would lead to consistency with minimal error.

Measurements were made using four monoenergetic isotopic gamma-ray sources and different thicknesses of iron to establish a procedure that would give good repeatability as well as provide a basis for calculation of the 1/f spectral correction factors. The technique was then applied to a second series of measurements using typical CRBR mockups of sodium and stainless steel with the Tower Shielding Reactor II (TSR-II) as a source.

The measurements indicated that this procedure was capable of determining the energy deposited within the shield to an absolute accuracy of $\pm 3\%$ with a fractional standard deviation of about 1%.

Research sponsored by the U.S. Department of Energy.

*Nuclear Engineering Department, University of Tennessee, Knoxville, TN.

4.9

USING A DATA BASE TO EXAMINE A NUCLEAR PLANT'S COMPONENT RELIABILITY

D. H. Wood

(Abstract of paper presented at the Southeastern Student ANS Conference, University of Florida, Gainesville, FL, March 7–10, 1991)

The reliability of nuclear plant components is of fundamental importance to plant designers and maintenance engineers. The Centralized Reliability Data Organization (CREDO) at the Oak Ridge National Laboratory is a data base which collects and analyzes component engineering, component event, and facility operating data for liquid metal cooled reactors and test facilities. These data are used by Probabilistic Risk Assessment groups, plant designers, and preventive maintenance staff in reliability, availability, and maintainability (RAM) studies of advanced reactor systems. Information furnished to these users varies from component failure rate information to mean time to repair, once an event occurs. A failure rate is defined as the total number of events for a particular component search specification (e.g., liquid metal globe valves in FFTF's main heat transport loop) divided by the total hours of operation summed for all components in this category. A CREDO reportable event considers component functional degradation which requries some maintenance action to restore it to its proper state. This paper will give a brief description of how data are collected by CREDO, how these data are processed, and how they may be used for RAM analyses. The latter item will be illustrated by discussing a recent study of the life periods of liquid metal centrifugal pumps.

Research sponsored by U.S. Department of Energy.

HIGH ENERGY RADIATION AND PARTICLE TRANSPORT

4.10

CALCULATED INCLUSIVE NEUTRON PRODUCTION FROM 400 GeV PROTON-NUCLEUS COLLISIONS

R. G. Alsmiller, Jr. **F. S. Alsmiller**
O. W. Hermann*

[Abstract of *Nucl. Instrum. Methods Phys. Res.* **A286**, 73 (1990)]

Calculated inclusive neutron production from 400 GeV proton-nucleus collisions is presented and compared with experimental data. Target nuclei H, Be, Cu, and Pb are considered and the comparisons cover the laboratory energy range of 20–400 GeV, and angular range 0.7–10 mrad. Moderately good agreement between the calculated and experimental data is found, but the agreement in the case of Be, Cu, and Pb is significantly better than in the case of H.

Research sponsored by U.S. DOE Office of High Energy and Nuclear Physics.

*Computing and Telecommunications Division.

4.11

CALCULATED NEUTRON SPECTRUM IN THE TEVATRON TUNNEL AND COMPARISON WITH EXPERIMENTAL DATA

R. G. Alsmiller, Jr. **F. S. Alsmiller**
T. A. Gabriel **O. W. Hermann***
J. M. Barnes*

[Abstract of *Nucl. Instrum. Methods Phys. Res.* **A295**, 99 (1990)]

Calculated results of the longitudinal distribution as a function of energy of neutrons and the neutron spectrum with energy $\geq$ 40 keV in the TEVATRON tunnel are presented and compared with experimental data. The source in the calculations and the experiment was the interaction of the 900 GeV proton beam with N_2 gas. Some disagreement between the calculated and measured neutron flux distribution as a function of distance is found, but the calculated and measured neutron spectrum are in good agreement.

Research sponsored by U.S. DOE Office of High Energy and Nuclear Physics.

*Computing and Telecommunications Division.

4.12

THE HIGH-ENERGY TRANSPORT CODE HETC88 AND COMPARISONS WITH EXPERIMENTAL DATA

R. G. Alsmiller, Jr. **F. S. Alsmiller**
O. W. Hermann*

[Abstract of *Nucl. Instrum. Methods Phys. Res.* **A295**, 337 (1990)]

An upgraded verison, HETC88, of the previously available High-Energy Transport Code HETC is briefly described. In the upgraded code, the particle production model from hadron-nucleus nonelastic collisions at energies greater than 5 GeV has been revised. At nucleon and pion energies below 5 GeV, HETC88 is not different from the code previously available. In particular, provision is still made to allow neutrons with energies $\leq$20 MeV to be transported by one of the many available codes designed for low-energy neutron transport.

Calculated results for 29.4 GeV protons incident on a large iron-air target are presented and compared with experimental data and with results obtained with the Monte Carlo code FLUKA87. Calculated results are also presented and compared with experimental data for 300 GeV protons incident on targets of iron-film and lead-film. For 20 TeV protons incident on a large cylindrical iron target, calculated "star" density results from HETC88, FLUKA87, CASIM, and MARS10 are also compared.

Research sponsored by U.S. DOE Office of High Energy and Nuclear Physics.

*Computing and Telecommunications Division.

4.13

LOW-ENERGY PARTICLE PRODUCTION AND TRANSPORT FOR 200 GeV/c PROTONS IN IRON AND COMPARISONS WITH EXPERIMENTAL DATA

R. G. Alsmiller, Jr. **F. S. Alsmiller**

[Abstract of *Nucl. Instrum. Methods Phys. Res.* (in press)]

Calculated results for 200 GeV/c protons incident on an iron, calorimeter-like, target are presented and compared with experimental data. The calculations were carried out with the hadron transport code HETC88.

The quantities that are compared are the production per unit volume of ^{18}F and ^{24}Na in aluminum and the production per unit volume of ^{115m}In in indium as a function of depth and radius in the target. œThe production of ^{24}Na and ^{115m}In is due primarily to the low energy ($\lesssim$ 20 MeV) neutron flux, and thus the comparisons here test the capability of HETC88 for producing and transporting these low-energy neutrons or more precisely for predicting the flux per unit energy of these low-energy neutrons as a function of depth and radius in the target.

The calculated results are in good agreement with the ^{18}F production data (energies $\gtrsim$ 40 MeV) and the ^{24}Na production data (energies $\gtrsim$ 5 MeV) and in moderate agreement with the ^{115m}In production data (energies $\gtrsim$ 0.4 MeV).

Research sponsored by U.S. DOE Office of Basic Energy Sciences.

4.14

WORKSHOP ON SCIENTIFIC AND INDUSTRIAL APPLICATIONS OF FREE ELECTRON LASERS

F. C. Difilippo **R. B. Perez**

(Abstract of ORNL/TM-11380, May 1990)

A workshop on scientific and industrial applications of free electron lasers was organized to address potential uses of a free electron laser in the infrared wavelength region. A total of 13 speakers from national laboratories, universities, and the industry gave seminars to an average audience of 30 persons during June 12 and 13, 1989.

The areas covered were: Free Electron Laser Technology, Chemistry and Surface Science, Atomic and Molecular Physics, Condensed Matter, and Biomedical Applications, Optical Damage, and Optoelectronics.

Research sponsored by U.S. Department of Energy.

4.15

CALOR89: CALORIMETRY ANALYSIS AND BENCHMARKING

T. A. Gabriel **R. G. Alsmiller, Jr.**
B. L. Bishop* **C. Y. Fu**
T. Handler† **J. K. Panakkal‡**
J. Proudfoot‡ **L. Cremaldi§**
B. Moore§ **J. J. Reidy§**

(Abstract of paper presented at the International Conference on Calorimetry in High Energy Physics, Batavia, IL, October 29–November 1, 1990)

The CALOR89 code system has been utilized for extensive calorimeter benchmarking and design calculations. Even though this code system has previously demonstrated its power in the design of calorimeters, major revisions in the form of better collision models and cross-section data bases have expanded its capabilities. The benchmarking has been done with respect to the ZEUS and DO calorimeters. For the most part, good agreement with experimental data has been obtained. The design calculations presented here were done for a variety of absorbers (depleted uranium, lead, and iron) of various thickness, for a given scintillator thickness and for a fixed absorber thickness using various thickness for the scintillator. These studies indicate that a compensating calorimeter can be built using uranium or lead as the absorber, whereas a purely iron calorimeter would be non-compensating. One possibly major problem exists with the depleted uranium calorimeter due to the large number of neutrons produced and due to the large capture cross-section of uranium. These captured neutrons will produce a signal in the scintillator due to secondary gamma rays for many hundreds of nanoseconds and this may contribute substantially to background noise and pile up.

Research sponsored by U.S. Department of Energy.

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4.16

CALOR89 CALORIMETER SIMULATIONS, BENCHMARKING, AND DESIGN CALCULATIONS

T. Handler* **J. Panakkal†**
J. Proudfoot† **L. Cremaldi‡**
B. Moore‡ **J. J. Reidy‡**
R. G. Alsmiller, Jr. **C. Y. Fu**
T. A. Gabriel

(Abstract of paper presented at the Symposium on Detector Research and Development for the Superconducting Super Collider, Ft. Worth, TX, October 15–18, 1990)

Results on CALOR89 benchmarking and design calculations utilizing the CALOR89 programs are presented. The benchmarking is done with respect to the ZEUS and DO calorimeters. The design calculations were done for a variety of absorbers (depleted uranium, lead, and iron) of various thicknesses for a given scintillator thickness and for a fixed absorber thickness using various thicknesses for the scintillator. These studies indicate that a compensating calorimeter can be built using lead as the absorber, whereas a purely iron calorimeter would be non-compensating. A depleted uranium calorimeter would possibly be unsuitable if used in a large configuration and a high luminosity machine because of the delayed energy release from capture gammas.

Research sponsored by U.S. Department of Energy.

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4.17

DETERMINATION OF THE NEUTRON ENERGY AND ANGULAR RESPONSE FUNCTION OF THE ORIENTED SCINTILLATION SPECTROMETER EXPERIMENT (OSSE)

C. M. Jensen* **T. A. Gabriel**
J. D. Kurfess† **W. N. Johnson†**
R. L. Kinzer†

(Abstract of paper presented at the 1989 Nuclear Science Symposium, IEEE/NSS, San Francisco, CA, October 27–29, 1989)

The neutron energy and angular response function of OSSE, one of four instruments to be launched on NASA's Gamma-Ray Observatory (GRO), has been modeled from 10 MeV to 200 MeV and at discrete angles from 0 to 180 degrees. The response has been determined from Monte Carlo calculations, using a system of codes including HETC, EGS, and MORSE, and compared with experimental data collected at the Indiana University Cyclotron Facility.

Research sponsored by U.S. Department of Energy.

*Applied Research Corporation, Landover, MD.

†Naval Research Laboratory, Washington, DC.

4.18

SIMULATION STUDIES FOR DESIGN OPTIMIZATION OF A SCINTILLATOR PLATE CALORIMETER

J. Proudfoot* **P. K. Job***
H.-J. Trost* **T. Handler†**
T. A. Gabriel

(Abstract of paper presented at the Symposium on Detector Research and Development for the Superconducting Super Collider, Ft. Worth, TX, October 15–18, 1990)

Results on simulations studies relating to the optimization of a sampling scintillator plate calorimeter for an SSC detector system are presented. These studies show that whereas a compensating sampling geometry can be obtained using a variety of configurations using either lead or depleted uranium as the principal absorber, no configuration based on a pure iron absorber is compensating. Unlike in a lead system, delayed energy release from long lived shower products produced in a uranium system pose a serious pile up problem. Therefore we advocate the use of lead as the principal absorber in this calorimeter. Work on optimization of the mechanical structure is in progress and results are presented on issues such as structural support, tolerances and on the degradation in response due to other detector material within the volume of the calorimeter.

Research sponsored by U.S. Department of Energy.

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4.19

REACTION RATE DISTRIBUTIONS AND RELATED DATA IN THE FUSION NEUTRON SOURCE PHASE II EXPERIMENTS: COMPARISON OF MEASURED AND CALCULATED DATA

R. T. Santoro **R. G. Alsmiller, Jr.**
J. M. Barnes*

[Abstract of *Fusion Technology* 19(3), Part I, 449 (1991); also ORNL/TM-11481, July 1990]

Neutronics parameters including the source neutron spectrum, activation rates, and the tritium breeding in the Li_2O test zone of the Fusion Neutron Source Phase II experiment performed at the Japan Atomic Energy Research Institute are calculated using the Monte Carlo code MORSE with ENDF/B-V transport and reaction cross sections. Favorable comparisons between the measured and calculated results are achieved for the ^{27}Al(n,α), ^{58}Ni(n,p), ^{93}Nb(n,2n), and ^{197}Au(n,2n) reactions. Calculated ^{58}Ni(n,2n) and ^{197}Au(n,γ) reactions do not agree with measured values within 10 to 40%. For the nickel reaction, the differences may be due to poor data in the ORACT files, while discrepancies for the gold data may be due to unknown quantities of hydrogen-rich epoxy used to coat the Li_2CO_3 blocks used in the test assembly walls. The calculated tritium breeding in the Li_2O agrees with experimental values within ±10% for ^{6}Li and ±15 to 20% for ^{7}Li.

Research sponsored by U.S. Department of Energy and Harry Diamond Laboratory.

*Computing and Telecommunications Division.

MATHEMATICAL MODELING AND CODE DEVELOPMENT

4.20

A COMPARISON BETWEEN THE PROPAGATORS METHOD AND THE DECOMPOSITION METHOD FOR NONLINEAR EQUATIONS

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(Abstract of ORNL/TM-11316, January 1990)

Recently, a new formalism for solving nonlinear problems has been formulated. The formalism is based on the construction of advanced and retarded propagators that generalize the customary Green's functions in linear theory. Onc of the main advantages of this formalism is the possibility of transforming nonlinear differential equations into nonlinear integral equations that are usually easier to handle theoretically and computationally. The aim of this paper is to compare, on an example, the performances of the propagator method with other methods used for nonlinear equations, in particular, the decomposition method. The propagator method is stable, accurate, and efficient for all initial values and time intervals considered, while the decomposition method is unstable at large time intervals, even for very conveniently chosen initial conditions.

Research sponsored by U.S. Department of Energy.

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4.21

ON THE ADEQUACY OF MESSAGE-PASSING PARALLEL SUPERCOMPUTERS FOR SOLVING NEUTRON TRANSPORT PROBLEMS

Y. Y. Azmy

[Abstract of paper presented at the Supercomputing '90, New York, NY, November 12–16, 1990; Proc. p. 693, IEEE Computer Society Press (1990)]

A coarse-grained, static-scheduling parallelization of the standard iterative scheme used for solving the discrete-ordinates approximation of the neutron transport equation is described. The parallel algorithm is based on a decomposition of the angular domain along the discrete ordinates, thus naturally producing a set of completely uncoupled systems of equations in each iteration. Implementation of the parallel code on Intel's iPSC/2 hypercube, and solutions to test problems are presented as evidence of the high speedup and efficiency of the parallel code. The performance of the parallel code on the iPSC/2 is analyzed, and a model for the CPU time as a function of the problem size (order of angular quadrature) and the number of participating processors is developed and validated against measured CPU times. The performance model is used to speculate on the potential of massively parallel computers for significantly speeding up real-life transport calculations at acceptable efficiencies. We conclude that parallel computers with a few hundred processors are capable of producing large speedups at very high efficiencies in very large three-dimensional problems.

Research sponsored by U.S. DOE Office of High Energy and Nuclear Physics.

4.22

ON THE DYNAMICS OF A DISCRETE REACTION-DIFFUSION SYSTEM

Y. Y. Azmy V. Protopopescu

[Abstract of *Numerical Methods for Partial Differential Equations* (in press)]

We investigate various aspects of the dynamics of a discrete reaction-diffusion system. First, we examine the effect of the boundary conditions on the spatially uniform fixed point at locations far from the boundaries by using an asymptotic expansion. We show that except for a few computational cells adjacent to the boundary, the fixed point practically coincides with the one calculated by using reflective boundary conditions (equivalent to an infinite domain). Next, we introduce a classification of the fixed points based on the wavelength in the infinite medium approximation of the system. We use the symbolic manipulator MACSYMA to analytically calculate the amplitude of several such classes of fixed points and we generate bifurcation diagrams for their members.

Also, we consider two special classes of periodic solutions; we calculate their amplitude analytically in the infinite medium approximation, and generate bifurcation diagrams that shed new light on some previous confusing results. Finally, we present an analysis of fictitious periodic solutions that have been previously reported and incorrectly interpreted.

Research sponsored by U.S. Department of Energy.

4.23

INTEGRAL METHODS FOR SOLVING FOKKER-PLANCK-TYPE EQUATIONS

V. Protopopescu

(Abstract of paper presented at the Second International Conference on Integral Methods in Science and Engineering, Arlington, TX, May 15–18, 1990)

Fokker-Planck-type equations occur quite often in different domains of physics and applied mathematics as various realizations of a generic degenerate parabolic equation. Even in the simplest situations, the analysis of the general Fokker-Planck equation is difficult and has been mostly confined to the linear case, where partial results have been obtained in showing existence, uniqueness, regularity, and completeness of eigenfunctions. In the present paper, we present a canonical integral approach that solves, in principle, the most general linear or nonlinear Fokker-Planck-type equations. The method is formal in the sense that it does not provide *per se* the means to prove existence and uniqueness of the solution in an abstract setting. The formalism is based on the Green's functions and their natural extensions to nonlinear systems and allows one to compute the solution (assumed to exist uniquely), by using a canonical iterative scheme. We present several applications of the integral approach in connection with previously developed methods and results.

Research sponsored by the U.S. Department of Energy.

4.24

PREDICTION, CONTROL, AND DECISION-MAKING ASPECTS FOR CHAOTIC SYSTEMS

V. Protopopescu

(Abstract of paper presented at the 8th International Congress on Cybernetics and Systems, New York, June 11–15, 1990)

Several examples of chaotic systems are discussed for which occurrence of chaos, information recovery, control, and decision-making processes appear in a new, sometimes counterintuitive light. From case to case, explanations, conjectures, and/or possible applications are indicated.

Research sponsored by U.S. Department of Energy.

4.25

LINEAR VS NONLINEAR AND INFINITE VS FINITE: AN INTERPRETATION OF CHAOS

V. Protopopescu

(Abstract of ORNL/TM-11667, October 1990)

An example of a linear infinite-dimensional system is presented that exhibits deterministic chaos and thus challenges the presumably unquestionable connection between chaos and nonlinearity. Via this example, the roles of, and relationships between, linearity, nonlinearity, infinity and finiteness in the occurrence of chaos are investigated. The analysis of these complementary but related aspects leads to: (i) a new interpretation of chaos as the manifestation of incompressible and thus unprocessible information and (ii) a conjecture about the nonexistence of operationally accessible linear systems.

Research sponsored by U.S. Department of Energy.

4.26

TORT: A THREE-DIMENSIONAL DISCRETE ORDINATES NEUTRON/PHOTON TRANSPORT CODE

W. A. Rhoades **R. L. Childs***

[Abstract of *Nucl. Sci. Eng.* **107(4)**, 397 (1991)]

TORT calculates the flux or fluence of particles throughout a two- or three-dimensional geometric system from particles incident on the system from extraneous sources or generated internally as a result of interaction with the system. The principal application is for the deep-penetration transport of neutrons and photons. Certain reactor eigenvalue problems can also be solved. Numerous printed edits of the results are available, and many results can be transferred to output files for subsequent analysis.

Research sponsored by Defense Nuclear Agency.

*Computing and Telecommunications Division.

ANALYTIC MODELING OF CONFLICT

4.27

PARAMETER IDENTIFICATION FOR GENERALIZED LANCHESTER'S EQUATIONS

J.-C. Culioli* **V. Protopopescu**

(Abstract of ORNL/TM-11367, March 1990)

The validation of analytic combat models is hindered by the almost complete lack of *a priori* knowledge about the aggregated attrition coefficients serving as inputs in such models. To overcome this difficulty we discuss the applicability of two methods that use empirical data (combat outcomes) to identify the unknown attrition coefficients. Both methods are based on the minimization of an optimization criterion (equation error criterion or output error criterion).

Research sponsored by Defense Nuclear Agency.

*Laboratoire d'Automatique, Fontainebleau, France.

4.28

ANALYTIC MODELING OF LOW INTENSITY CONFLICT USING PARTIAL DIFFERENTIAL EQUATIONS

V. Protopopescu **R. T. Santoro**

(Abstract of paper presented at the 14th Annual Symposium on Special Operations/Low Intensity Conflict, Arlington, VA, December 4–5, 1989)

Analytic models currently in use for studying low intensity conflict and special operations are Lanchester models based on the use of ordinary differential equations that describe only the temporal evolution of engaged forces. In this paper, we present a new model based on the use of nonlinear partial differential equations (PDE) wherein both the spatial and temporal dependence of the opposing force troop concentrations are taken into account. This model has the capability to provide a more realistic description of the interactions between conventional and unconventional forces, including the special features of guerrilla and counter-guerrilla operations. It can treat the opposition of both homogeneous forces (i.e., each force employs a single weapon system) or heterogeneous forces (each force employs multiple weapon systems). The principal strength of

the model lies in its capabilities to (i) obtain rapid solutions of engagement scenarios that include the effects of both direct and area fire and (ii) perform sensitivity studies to define optimum force and fire-power ratios.

A detailed description of the PDE model emphasizing its mathematical aspects, its range of capabilities, and application for replicating low intensity type engagements are described. Included are the results of numerical parametric studies carried out using a one-dimensional version of the model and the presentation of classical tactical maneuvers, (e.g., frontal attack, envelopment, infiltration, etc.) that are reproduced by a two-dimensional version of the model.

Finally, some related aspects are discussed pertaining to (i) validation problems related to the model, (ii) several new capabilities and characteristics of its discrete version, and (iii) developments to include the essential elements of C^3I and logistics.

Research sponsored by U.S. DOE and Air Force Weapons Laboratory.

4.29

PDE MODELS FOR COMBAT: POTENTIAL APPLICATIONS TO LIC

V. Protopopescu R. T. Santoro
Y. Y. Azmy

(Abstract of paper presented at the 14th Annual Symposium on Special Operations/Low Intensity Conflict, Arlington, VA, December 4-5, 1989)

Acute or subdued conflict situations (ranging from fierce combat to peaceful competition) are modeled by using nonlinear partial differential equations that account for both temporal and spatial evolution of the system. One- and two-dimensional applications to conventional warfare are reported. The discretized version of the model resulting in a nonlinear map is used to investigate the chaotic aspects of a conflict situation. The comparison between our model and a wargame exercise yields excellent agreement and provides a strong validation basis for further developments.

Research sponsored by U.S. DOE and Defense Advanced Research Projects Agency.

4.30

COMBAT MODELING WITH PARTIAL DIFFERENTIAL EQUATIONS — THE BIDIMENSIONAL CASE

V. Protopopescu R. T. Santoro
R. Cox* P. Rusu†

(Abstract of ORNL/TM-11343, January 1990)

The system of partial differential equations recently introduced to model combat in one spatial dimension has been extended to include two spatial dimensions and has been numerically integrated to demonstrate its capability to describe maneuver. Engagement scenarios wherein the attacking force(s) employs the frontal attack, turning movement, envelopment, or infiltration against a fixed defensive force are presented for various combinations of troop and firepower ratios. The time and spatial distributions of the forces are displayed in graphical form along with approximate attrition rates as a function of battle duration. The results establish that the PDE formalism replicates these maneuver forms within the constraints and present development of the model.

Research sponsored by U.S. Department of Energy.

*Computing and Telecommunications Division.

†University of Colorado, Boulder, CO.

4.31

RECENT ADVANCES IN ANALYTIC COMBAT SIMULATION: FROM MODELING TO VALIDATION AND BEYOND

V. Protopopescu R. T. Santoro
Y. Y. Azmy

[Abstract of *PHALANX* p. 49 (1990); also paper presented at the 58th Military Operations Research Society Symposium, Annapolis, MD, June 12-14, 1990]

A new analytic approach is presented that models acute or subdued conflict situations (ranging from fierce combat to peaceful competition) by using nonlinear partial differential equations. One- and two-dimensional applications to conventional warfare are reported which replicate

successfully both attrition and maneuver. The comparison between the analytic model and a wargame exercise yields excellent agreement and provides a strong validation basis for further developments and applications.

Research sponsored by Defense Advanced Research Projects Agency.

4.32

RECENT ADVANCES IN VALIDATING ANALYTIC COMBAT MODELS

V. Protopopescu R. T. Santoro
Y. Y. Azmy B. L. Kirk

(Abstract of paper presented at the MORS Mini-Symposium "Simulation Validation," Albuquerque, NM, October 15-18, 1990)

A considerable effort has been devoted to quantify, understand, and predict processes associated with conventional and modern war by using analytic models, simulations, and wargames, or combinations thereof. Although there are more than 450 identified active military models, many of which are in extensive use, their validation/accredidation, let alone verification, is still far from being satisfactorily carried out.

In this paper we discuss some of the outstanding problems in validating analytic combat models. We present cross-validation results between analytic models based on partial differential equations (PDEs) and standard wargames, for compatible scenarios and tactical situations. The results show very good agreement and provide a strong validation framework for further developments and applications. Based on these preliminary results, the PDE analytic model appears to be the best available candidate to execute quick sensitivity analyses for testing, training, and decision-making.

Research sponsored by U.S. Department of Energy.

4.33

ANALYTIC MODELING VS. WARGAMING: AN ATTEMPT AT CROSS-VALIDATION

R. T. Santoro Y. Y. Azmy
V. Protopopescu

[Abstract of *Signal*, p. 49 (July 1990)]

An attempt to compare and correlate results obtained using two different combat simulation methods for a specific engagement scenario is discussed. Calculated results obtained using the ORNL PDE code, WAR, are compared with data obtained using the JANUS wargame code for the assault by a RED armored regiment on a prepared defensive position occupied by BLUE armor and anti-tank weapons. The calculated time dependent losses obtained using both models agree within 10% or better over the duration of the battle.

Research sponsored by U.S. DOE and Defense Advanced Research Projects.

SENSITIVITY AND UNCERTAINTY ANALYSIS

4.34

MATRIX REDUCTION ALGORITHMS FOR GRESS AND ADGEN

J. E. Horwedel*

(Abstract of ORNL/TM-11261, November 1989)

The GRESS Version 0.0 code system was developed to automate the implementation of derivative-taking capabilities in existing FORTRAN 77 computer models. The GRESS CHAIN option is used to calculate and report first derivatives of model results with respect to user selected input data by application of the calculus chain rule. The GRESS ADjoint matrix GENerator (ADGEN) option is used to calculate first derivatives of selected model results with respect to all input data. The first part of this paper presents the mathematical foundations and algorithms as presently implemented in GRESS Version 0.0. Examples are used to describe the implementation of both the CHAIN and ADGEN options. Due to excessive execution time and memory requirements

with the CHAIN option users are often limited to propagating derivatives for just a few parameters. The ADGEN option allows an almost unlimited number of parameters (i.e., input ddata); however, the data storage requirement for an ADGEN application was more then 322 megabytes for a code that executes in one minute on a VAX 8600 computer.

The purpose for this paper is to present three new algorithms that could easily be implemented in GRESS Version 0.0 to dramatically reduce the data storage requirements and execution time for application of the ADGEN option. The new algorithms are described with examples. Test versions of these algorithms were implemented and tested. The application of these algorithms to the GRESS enhancement of the PRESTO-II computer model resulted in a significant reduction in execution time and a reduction in data storage requirements from 322 megabytes to 97 megabytes without any loss in the generality of the approach.

Research sponsored by U.S. DOE National Low-Level Waste Management Program.

*Computing and Telecommunications Division.

4.35

AUTOMATED SENSITIVITY ANALYSIS WITH THE GRADIENT ENHANCED SOFTWARE SYSTEM (GRESS)

J. E. Horwedel*

(Abstract of paper presented at the ACM Fall Conference, Gatlinburg, TN, November 9–10, 1989)

GRESS is an efficient automated software system for calculating sensitivities of model results to input data in existing FORTRAN 77 computer models. In a FORTRAN program, variables are a function of previously defined variables and data through mathematical operations. GRESS automates the analytic calculation of the partial derivatives of the term on the left-hand side of an equation with respect to those on the right. The GRESS CHAIN option is used to calculate and report first derivatives of model results with respect to data by application of the calculus chain rule. The GRESS ADjoint matrix GENerator (ADGEN) option is used to calculate first derivatives of a selected model result with respect to all input data. With the ADGEN application, data storage is a major limiting factor. The data storage for a code that executes in one minute on a VAX 8600 computer exceeded 322 megabytes.

The purpose for this presentation is to describe GRESS and to report on the development of two new algorithms that dramatically reduce the data storage requirements for an ADGEN application. The new algorithms are described with examples. Results from the application of these algorithms to the GRESS enhancement of a major computer model will be presented.

Research sponsored by U.S. DOE and Air Force Weapons Laboratory.

*Computing and Telecommunications Division.

4.36

SENSITIVITY ANALYSIS OF AIRDOS-EPA USING ADGEN WITH MATRIX REDUCTION ALGORITHMS

J. E. Horwedel* **R. J. Raridon***
R. Q. Wright*

(Abstract of ORNL/TM-11373, November 1989)

ADGEN was developed to automate the calculation of sensitivities of a few model results to all input data in existing FORTRAN 77 computer models. ADGEN is now included as one of two options available to users of the Gradient Enhanced Software System (GRESS). GRESS was initially developed to automate the calculation of sensitivities of all model results to a few input parameters by application of the calculus chain rule during the forward run of the computer model. The ADGEN option automates the application of adjoint sensitivity theory to calculate first derivatives of model results to input data by first creating, and then solving, an adjoint equation for the computer model. The purpose of this report is twofold: (1) to present the development of two algorithms that significantly improve the application of ADGEN; and (2) to demonstrate the application of ADGEN to the AIRDOS-EPA computer model.

Research sponsored by U.S. DOE National Low-Level Waste Management Program.

*Computing and Telecommunications Division.

4.37

SENSITIVITY ANALYSIS OF EQ3

J. E. Horwedel* R. Q. Wright*
R. E. Maerker

(Abstract of ORNL/TM-11407, January 1990)

A sensitivity analysis of EQ3, a computer code which has been proposed to be used as one link in the overall performance assessment of a national high-level waste repository, has been performed. EQ3 is a geochemical modeling code used to calculate the speciation of a water and its saturation state with respect to mineral phases. The model chosen for the sensitivity analysis is one which is used as a test problem in the documentation of the EQ3 code. Sensitivities are calculated using both the CHAIN and ADGEN options of the GRESS code compiled under G-float FORTRAN and the VAX/VMS and verified by perturbation runs. The analyses were performed with a preliminary Version 1.0 of GRESS which contains several new algorithms that significantly improve the application of ADGEN.

Use of ADGEN automates the implementation of the well-known adjoint technique for the efficient calculation of sensitivities of a given response to all the input data. Application of ADGEN to EQ3 results in the calculation of sensitivities of a particular response to 31,000 input parameters in a run time of only 27 times that of the original model. Moreover, calculation of the sensitivities for each additional response increases this factor by only 2.5 percent. This compares very favorably with a running-time factor of 31,000 if direct perturbation runs were used instead.

Research sponsored by U.S. Department of Energy.

*Computing and Telecommunications Division.

4.38

AUTOMATED SENSITIVITY ANALYSIS WITH THE GRADIENT ENHANCED SOFTWARE SYSTEM (GRESS)

J. E. Horwedel*

(Abstract of ORNL/M-1121, May 1990)

GRESS automates the implementation of the well-known adjoint method for performing a comprehensive sensitivity analysis of existing FORTRAN 77 computer models. The GRESS ADjoint matrix GENerator (ADGEN) option is used to calculate first derivatives and sensitivities of selected model results with respect to all input data. This report provides a small sample problem used to exercise most of the major program options for a GRESS/ADGEN application. A description of the input and output from each processing step as well as the method for controlling the application is presented. The report is designed to aid users of the GRESS ADGEN option.

Research sponsored by U.S. DOE National Low Level Waste Management.

*Computing and Telecommunications Division.

NUCLEAR WEAPON EFFECTS

4.39

NUCLEAR WEAPONS EFFECTS FOR CIVIL DEFENSE CONSIDERATIONS

C. M. Haaland

[Abstract of a series of journal articles that appeared in Vol. 23 of *J. of Civil Defense* (February, April, June, August, October, and December 1990)]

A brief review of the historical development of nuclear weapons is followed by a treatise on their destructive effects, and how protective measures may be taken for the civilian population.

Research sponsored by U.S. Department of Energy.

4.40

ANALYSIS OF THE RADIOLOGICAL TEST CONFIGURATION (RTK) EXPERIMENTS USING THE MONTE CARLO CODE SYSTEM — MASH

J. O. Johnson

(Abstract of ORNL/TM-11410, March 1990)

The capability to accurately assess and predict the effectiveness of shielding materials on vehicles, structures, trenches, and other shield configurations represents an important interest to various government agencies. A joint research effort involving several institutions has worked towards providing this capability for several years, resulting in the first code system called the Vehicle Code System (VCS) and the successor code system VCS, referred to as the Monte Carlo Adjoint Shielding Code system - MASH. The purpose of this report is to present the results of radiation transport calculations for a steel rectangular box with sloping sides identified as the Radiological Test Configuration (RTK) using the MASH code system.

As part of the ongoing research program, the MASH code system utilizing the combinatorial geometry package (MASH-CG) and an initial version of the MASH code system utilizing the GIFT5 geometry package (MASH-G) have been prepared. The verification of MASH-CG and MASH-G is being accomplished through comparisons with differential and integral data obtained from the three dimensional discrete ordinates code TORT and from data obtained in experimental measurements performed at the Army Pulse Radiation Facility (APRF) reactor. In this report, the comparison of the MASH results to the results from experimental measurements performed at the APRF reactor is presented and discussed.

The concerns expressed in this report will be investigated to determine their significance with respect to the validity and applicability of the MASH code system. Resolution of these concerns, coupled with future testing will contribute towards a fully verified version of the MASH code system.

Research sponsored by Foreign Science and Technology Center.

4.41

ACTIVATION OF COBALT BY NEUTRONS FROM THE HIROSHIMA BOMB

G. D. Kerr* F. F. Dyer†
J. F. Emery† J. V. Pace
R. L. Brodzinski‡ J. Marcum§

(Abstract of ORNL-6590, February 1990)

A study has been completed of cobalt activation in samples from two new locations in Hiroshima. The samples consisted of a piece of steel from a bridge located at a distance of about 1300 m from the hypocenter and pieces of both steel and concrete from a building located at approximately 700 m. The concrete was analyzed to obtain information needed to calculate the cobalt activation in the two steel samples.

Close agreement was found between calculated and measured values for cobalt activation of the steel sample from the building at 700 m. It was found, however, that the measured values for the bridge sample at 1300 m were approximately twice the calculated values. Thus, the new results confirm the existence of a systematic error in the transport calculations for neutrons from the Hiroshima bomb.

Research sponsored by U.S. Department of Energy.

*Health and Safety Division.

†Analytical Chemistry Division.

‡Pacific Northwest Laboratories, Richland, WA.

§R&D Associates, Marina del Rey, CA.

4.42

EFFECTS OF X-RADIATION ON THE LAMPSHADE ORBITAL DEBRIS SATELLITE SHIELD–II

M. S. Smith R. T. Santoro

(Abstract of ORNL/TM-11514, April 1990)

One-dimensional thermo-hydrodynamic calculations have been performed to estimate the response of the lead (Pb) bumper plate and aluminum (Al) foam liquidator screen of the LAMPSHADE orbital debris satellite shield. Mass fractions in the solid, liquid, and vapor phases as a function of time after irradiation for two incident x-ray spectra, were calculated using the PUFF-TFT code. Material losses due to phase changes did not exceed 3%, but fracture and spallation may seriously reduce the performance of the lead component against incident debris.

Research sponsored by Air Force Weapons Laboratory.

Section 5

ENGINEERING PHYSICS AND MATHEMATICS INFORMATION CENTERS

5.0. INTRODUCTION

R. W. Roussin

Information analysis and data management, important activities of the division since its inception, comprise a significant fraction of the division's program. Under the management umbrella of Engineering Physics Information Centers (EPIC), we operated two activities during the reporting period, September 1, 1989 – March 31, 1991. The Radiation Shielding Information Center (RSIC), founded in FY 1963, serves the international scientific community as a technical institute for shielding design and analysis. The second activity, begun in FY 1990, involves participation in the shielding analysis part of the Safety Analysis Reports for Packaging for the Y-12 radioactive material container and shipment program.

Radiation Shielding Information Center (RSIC)

During this reporting period, RSIC continues to be widely used as attested by current user statistics. Usage reported at the end of FY 1990 showed that the total number of requests processed during the year (3832) exceeded those in FY 1989 (3419) by 12%. The statistics indicate that the individual user is requesting more products and/or services; activities required to fill the requests increased by 13% (14,289 vs 12,660). The increased usage is largely attributed to environment, safety, health, and defense-related programs.

Established to promote the exchange of radiation transport technology, RSIC acts as a resource base for both government and civilian agencies in the United States and in foreign countries and performs such diverse functions as testing, assembling, and distributing computer codes; preparing, testing and distributing multigroup cross-section libraries, both fine-group and broad-group; collecting and distributing other types of data bases; holding seminars to educate the community of particular techniques, especially computer-based techniques for solving radiation transport or nuclear data problems; helping to establish shielding benchmark problems and shielding standards; providing bibliographic information; and generally providing problem assistance to requesters. Staff members also engage in radiation transport developments and perform radiation transport studies, often in collaboration with staff members in EPMD as well as other institutions.

The RSIC scope includes the physics of interaction of radiation with matter; radiation production, protection, and transport; radiation detectors and measurements; engineering design techniques; shielding materials properties; computer codes useful in research and design; and nuclear data compilations. The goals of RSIC are to function as a technical institute to provide information (computer codes, technical advice, bibliographic and other data,) upon request; collect, evaluate, enrich, distill, and repackage information to extend the state of the art, bringing into the public domain technology more usable and more valuable than the sum of the input; and to initiate and effect research and development in appropriate areas of need.

During this reporting period work has continued in the development of fine- and broad- group cross-section data libraries. The 174 neutron, 38 photon group VITAMIN-E general-purpose cross-section library based on ENDF/B-V now contains 94 materials. It has been used with success for fusion neutronics, fast reactor core and shielding applications, and various other radiation transport calculations within the division and externally. During the reporting period, an upgrade for VITAMIN-E, based on ENDF/B-VI data, was initiated. It will contain 174 neutron and 42 photon groups.

RSIC has continued to participate in the work of the Cross Section Evaluation Working Group (CSEWG), with the Methods and Formats Subcommittee chaired by the RSIC director. Other staff members are actively involved with the ANS in developing radiation protection and shielding standards and standards for scientific computer programming and its documentation.

In the area of computing technology, RSIC now makes available 896 computer code packages and 160 data packages. The RSIC Newsletter is currently mailed monthly to 1785 people. A total of 74 persons came during the reporting period for an orientation visit and /or to use the center's facilities.

In terms of reciprocity in international information exchange, a significant percentage of all incoming computing technology (codes and data) comes from foreign contributors, with Japan and France continuing in the lead. Much of the new technology is of domestic interest.

The RSIC computer-based information system (SARIS), containing more than 24,000 literature references, is used in support of internal research activities and user services. Seven consecutive indexed bibliographies have been published and data files have been constructed in preparation for publication of the eighth in the series. SARIS, formerly accessible nationally on the now-defunct DOE RECON system, is currently accessible for a search on demand service.

RSIC interacts daily with, and continues to have the support of, its user community. Participants contributed their publications and 164 transmissions of technology as follows: 86 new computer codes and data libraries; 9 replacements of existing code/data packages with newly-frozen versions; 21 new hardware versions or other extensions to existing code/data packages; 37 updates to improve existing code/data packages; and 11 corrections to fix errors in existing code/data packages.

Announcement of availability was made for 130 transportable, tested packages of new or revised computer code systems and data libraries, including contributions received in the previous fiscal year. It should be noted that the same evaluation, computer testing, and packaging is followed for updates to existing code packages as for new technology.

Safety Analysis Reports for Packaging

EPIC staff members are in charge of performing the radiation shielding analysis and preparing the shielding chapter for all the Safety Analysis Reports for Packaging (SARPs) for the Y-12 Plant radioactive material container and shipment program. Besides the initial draft, three separate chapter versions are prepared: issued for comment (IFC), issued for approval (IFA), and issued approved (IA). Each version must be approved by three review committees for compliance with the Code of Federal Register (CFR) Title 10 Part 71, dealing with the packaging and transportation of radioactive material. These committees are (1) an independent MMES group at K-25, (2) an Albuquerque-based group reporting to DOE Albuquerque Operations, and (3) a group from LLNL reporting to DOE

Headquarters. Upon approval of the SARP from all committees, a transportation certificate for the package is issued by DOE.

Thirteen SARP shielding chapters have been prepared, and the backlog that existed before EPIC began this work has been eliminated. In addition to the analysis and chapter preparation, EPIC personnel defend, both in writing and oral presentations, all chapter versions as they proceed through the review process. One SARP has been given final approval and a certificate, one is in the IA version, eight are in the IFA version and three are in the IFC version. In addition there are at present seven chapters in the initial draft stage.

RADIATION TRANSPORT DEVELOPMENTS

5.1

AN OPTIMIZED ALGORITHM FOR THE NODAL DIFFUSION METHOD ON SHARED MEMORY MULTIPROCESSORS

B. L. Kirk Y. Y. Azmy

[Abstract of paper presented at the International Conference on Supercomputing in Nuclear Applications, Mito City, Japan, March 12–16, 1990; Proc. pp. 325–329 (1990)]

We discuss an iterative method for solving the one-group neutron nodal diffusion equation in two dimensional geometry. We apply this method on a parallel computer and consider mesh sizes of the form $M \times N$. For $M \neq N$, the effects of dynamic scheduling on speedup and efficiency are presented. A model for the CPU time broken down into its serial and parallel components is also discussed.

Research sponsored by U.S. DOE Office of Nuclear Energy.

5.2

AN ITERATIVE ALGORITHM FOR SOLVING THE MULTIDIMENSIONAL NEUTRON DIFFUSION NODAL METHOD EQUATIONS ON PARALLEL COMPUTERS

B. L. Kirk Y. Y. Azmy

[Abstract of *Nucl. Sci. Eng.* (in press)]

The one-group steady-state neutron diffusion equation in two-dimensional Cartesian geometry is solved using the nodal method technique. By decoupling sets of equations representing the neutron current continuity along the length of rows or columns of computational cells a new iterative algorithm is derived that is more suitable for solving large practical problems. To accelerate the method, successive overrelaxation is applied. This algorithm is highly parallelizable and is implemented on the Intel iPSC/2 hypercube and Sequent Balance 8000 parallel computers. Speedup was achieved. However, the efficiency of the hypercube is very low when many processors are used. This leads to the conclusion that the hypercube is not as well suited for this algorithm as shared memory machines.

Research sponsored by U.S. DOE Office of Magnetic Fusion.

5.3

A SPATIAL DOMAIN DECOMPOSITION OF THE NODAL NEUTRON DIFFUSION EQUATIONS FOR PARALLEL COMPUTERS

B. L. Kirk Y. Y. Azmy

[Abstract of paper presented at the 5th SIAM Conference on Parallel Processing for Scientific Computing, Houston, TX, March 25–27, 1991; Proc. p. A25 (1991)]

The nodal method for the neutron diffusion problem is composed of loosely coupled, algebraic equations. These can be solved iteratively, where the bulk of the computation is comprised of solving one tridiagonal system per row or column of computational cells. Thus the spatial domain decomposition occurs naturally in the parallel, as well as sequential, algorithm that we implemented on modern day parallel computers of the distributed and shared memory types. Reasonable efficiencies and speedups factors are achieved on the hypercube, while excellent efficiencies are obtained on shared memory computers. Models for the CPU time are developed and verified in order to accurately predict parallel performance in non-test situations.

Research sponsored by U.S. Department of Energy.

5.4

A CALCULATIONAL METHOD OF PHOTON DOSE EQUIVALENT BASED ON THE REVISED TECHNICAL STANDARDS OF RADIOLOGICAL PROTECTION LAW

S. Tanaka* **T. Suzuki***

(Abstract of ORNL/TR-90/29, March 1991)

The effective conversion factor for photons from 0.03 to 10 MeV were calculated to convert the absorbed dose in air to the 1 cm, 3 mm, and 70 μm depth dose equivalents behind iron, lead, concrete, and water shields up to 30 mfp thickness. The effective conversion factor changes slightly with thickness of the shields and becomes nearly constant at 5 to 10 mfp. The difference of the effective conversion factor was less than 2% between plane normal and point isotropic geometries. It is suggested that the present method, making the data base of the exposure buildup factors useful, would be very effective as compared to a new evaluation of the dose equivalent buildup factors.

Research sponsored by U.S. Department of Energy.

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RADIATION TRANSPORT STUDIES

5.5

MONTE CARLO ANALYSIS OF A NEUTRON STREAMING EXPERIMENT

S. N. Cramer **T. Y. Lee***

[Abstract of *Nucl. Sci. Eng.* 107, 180 (1991)]

The analysis of neutron spectra emitted from a 14-MeV source and streaming through a void steel duct embedded in concrete is carried out using a multigroup Monte Carlo code on a small computer. The calculated results are compared with experimental results and with other calculational analyses involving continuous energy Monte Carlo methods. The computational methods agree when the P_N expansion of the multigroup method is sufficiently extended. Some discrepancies with the experimental results, found in earlier analyses, still remain; and these are investigated with regard to the use of a new modification of the evaluated iron data, the spreading of the calculated results for comparison with experimental spectra, and various other modeling details.

Research sponsored by U.S. DOE Office of Fusion Energy.

*Korean Atomic Energy Research Institute, Seoul, Korea.

5.6

INVESTIGATION OF RADIATION EFFECTS IN HIROSHIMA AND NAGASAKI USING A GENERAL MONTE CARLO-DISCRETE ORDINATES COUPLING SCHEME

S. N. Cramer **C. O. Slater**

(Abstract of ORNL/TM-11532, May 1990)

A general Monte Carlo-discrete ordinates radiation transport coupling procedure has been created to study effects of the radiation environment in Hiroshima and Nagasaki due to the bombing of these two cities. The forward two-dimensional free-field air-over-ground flux is coupled with an adjoint Monte Carlo calculation. The size, orientation, or translation of the Monte Carlo geometry is unrestricted. The radiation effects calculated are the dose in the interior of a large concrete building in Nagasaki and the activation production of Co-60 and P-32 in Hiroshima.

Research sponsored by U.S. Defense Nuclear Agency.

5.7

TIME DEPENDENT MONTE CARLO CALCULATIONS OF THE ORELA TARGET NEUTRON SPECTRUM

S. N. Cramer F. G. Perey

(Abstract of paper presented at the MC Methods for Neutron and Photon Transport Calculations, Budapest, Hungary, September 25-28, 1990)

The time dependent spectrum of neutrons in the water-moderated Oak Ridge Electron Linear Accelerator (ORELA) target has been calculated using a modified version of the MORSE multigroup Monte Carlo code with an analytic hydrogen scattering model. Distributions of effective neutron distance traversed in the target are estimated with a time and energy dependent algorithm from the leakage normal to the target face. These data are used in the resonance shape analyses of time-of-flight cross section measurements to account for the experimental resolution function. The 20 MeV-10 eV energy range is adequately represented in the MORSE code by the 174 group VITAMIN-E cross section library with a P_5 expansion. An approximate representation of the ORELA positron source facility, recently installed near the target, has been included in the calculations to determine any perturbations the positron source might create in the computed neutron distributions from the target. A series of coupled Monte Carlo calculations was performed from the target to the positron source and back to the target using a next-event estimation surface source for each step. The principal effect of the positron source was found to be an increase in the distance for the lower energy neutron spectra, producing no real change in the distributions where the ORELA source is utilized for experiments. Different configurations for the target were investigated in order to simulate the placement of a shadow bar in the neutron beam. These beam configurations included neutrons escaping from: (1) the central tantalum plates only, (2) the entire target with the tantalum plates blocked out, and (3) only a small area from the water. Comparisons of the current data with previous calculations having a less detailed model of the tantalum plates have been satisfactory.

Research sponsored by U.S. DOE Office of Fusion Energy.

5.8

GAMMA-RAY ATTENUATION IN THE VICINITY OF THE K EDGE IN MOLYBDENUM, TIN, LANTHANUM, GADOLINIUM, TUNGSTEN, LEAD, AND URANIUM

Y. Harima* D. K. Trubey
Y. Sakamoto† S. Tanaka

[Abstract of *Nucl. Sci. Eng.* 107, 385 (1991)]

The values of gamma-ray buildup factors and attenuation coefficients rise steeply as the source energy decreases near the K edge in heavy materials and discontinuously fall at the K edge. However, the exposure rate attenuation factor, $A(E,r) = D(E)B(E,\mu r)\exp^{-\mu r}$, given as a function of the penetration depth in centimeters, is relatively constant in the vicinity of the K edge. The development of a model that employs 4 K-shell X rays for the source shows that such behavior results from the large contribution of fluorescence radiation to the buildup factor for source photons of energies just about the K edge. In addition, an uncertainty in the extrapolation formula of the K parameter of the geometric progression buildup factor fitting function was removed for the energy range near the K edge.

Research sponsored by U.S. DOE and the Office of Administration and Resource Management, U.S. Nuclear Regulatory Commission.

*Tokyo Institute of Technology, Tokyo, Japan.

†Japan Atomic Energy Research Institute, Tokai-mura, Ibaraki-ken, Japan.

5.9

INVESTIGATION OF 1 CM DOSE EQUIVALENT FOR PHOTONS BEHIND SHIELDING MATERIALS

H. Hirayama* **S. Tanaka†**

(Abstract of ORNL/TR-90/28, March 1991)

The ambient dose equivalent at 1-cm depth, assumed equivalent to the 1-cm dose equivalent in practical dose estimations behind shielding slabs of water, concrete, iron or lead for normally incident photons having various energies was calculated by using conversion factors for a slab phantom. It was compared with the 1-cm depth dose calculated with the Monte Carlo code EGS4. It was concluded from this comparison that the ambient dose equivalent calculated by using the conversion factors for the ICRU sphere could be used for the evaluation of the 1-cm dose equivalent for the sphere phantom within 20% errors.

Average and practical conversion factors are defined as the conversion factors from exposure to ambient dose equivalent in a finite slab or an infinite one, respectively. They were claculated with EGS4 and the discrete ordinates code PALLAS. The exposure calculated with simple estimation procedures such as point kernel methods can be easily converted to ambient dose equivalent by using these conversion factors. The maximum value between 1 and 30 mfp can be adopted as the conversion factor which depends only on material and incident photon energy. This gives the ambient dose equivalent on the safe side.

Research sponsored by U.S. Department of Energy.

*National Laboratory for High Energy Physics, Oho, Tsukuba-shi, Ibaraki-ken, Japan.

†Japan Atomic Energy Research Institute, Tokai-mura, Ibaraki-ken, Japan.

INFORMATION ANALYSIS CENTER ACTIVITIES

5.10

ACTIVITIES OF THE RADIATION SHIELDING INFORMATION CENTER AND A REPORT ON CODES/DATA FOR HIGH ENERGY RADIATION TRANSPORT

R. W. Roussin

[Abstract of paper presented at the Sixth Seminar on Software Development in Nuclear Energy Research, Tokai, Japan, October 31, 1990; Proc. pp. 63-81 (1991)]

The presentation and paper will focus on the long-standing and beneficial relationship between the Radiation Shielding Information Center (RSIC) and numerous organizations in Japan. It will also stress the activities of RSIC related to computer code and data library packages useful for high energy radiation transport.

From the very early days in its history RSIC has been involved with high energy radiation transport. The National Aeronautics and Space Administration was an early sponsor of RSIC until the completion of the Apollo Moon Exploration Program. In addition, the intranuclear cascade work of Bertini at Oak Ridge National Laboratory provided valuable resources which were made available through RSIC. Over the years, RSIC has had interactions with many of the developers of high energy radiation transport computing technology and data libraries and has been able to collect and disseminate this technology. The current status of this technology will be reviewed and prospects for new advancements will be examined.

Research sponsored by U.S. Department of Energy.

APPENDICES

PERSONNEL CHANGES

NEW STAFF MEMBERS

A. Scientific Staff

J. E. Baker, Ph.D., Computer Science, Vanderbilt University
A. L. Bangs, B.A., Computer Engineering, Harvard College
C. [illegible]. Beasley, Ph.D., Physics, University of Wisconsin
E. F. D'Azevedo, Ph.D., Computer Science, University of Waterloo
J. M. Donato (Householder Fellow), Ph.D., Applied Mathematics, University of California-LA
O. H. Doerum (post-doc), Ph.D., Robotics Vision, Norwegian Institute of Technology
J. E. Finger, B.S., Mathematics, University of Tennessee
K. Fujimura, Ph.D., Computer Science, University of Maryland
J. A. Green, B.S., Computer Science, Tennessee Technological University
X. Guan (post-doc), Ph.D., Computer Science, Washington State University
H. T. Hunter, M.S., Nuclear Engineering, University of Washington
E. R. Jessup (Householder Fellow), Ph.D., Computer Science, Yale University
T. H. Rowan, Ph.D., Computer Science, University of Texas, Austin
R. F. Sincovec, Ph.D., Applied Mathematics, Iowa State University
P. F. Spelt, Ph.D., Experimental Psychology, University of Pittsburgh
M. A. Unseren, Ph.D., Electrical Engineering, Purdue University
D. W. Walker, Ph.D., Physics, Queen Mary College, University of London
J. Yoon (post-doc), Ph.D., Robotics, Korea Atomic Energy Research Institute

B. Administrative and Technical Support Staff

A. J. Alton, secretary
J. A. Atchley, Engineering Assistant
Y.-C. Chan, co-op student
M. A. Hacker, secretary
L. G. Jordan, secretary
M. A. Moore, secretary
S. P. Shriner, secretary
B. J. Snow, secretary

STAFF TRANSFERS OUT AND TERMINATIONS

A. Scientific Staff

O. W. Christian (retired)
K. Fujimura (Ohio State)
R. Gwin (retired)
M. T. Heath (University of Illinois)
E. R. Jessup (University of Colorado)
R. L. Macklin (retired)
F. C. Maienschein (retired)

V. W.-K. Ng (IT Corp)
P. J. Otaduy (transfer to Engineering Technology Division)
F. G. Perey (retired)
R. B. Perez (transfer to Instrumentation & Controls Division)
B. D. Rooney (Newport News Shipbuilding)
M. A. Terranova (Concord Associates)
D. K. Trubey (retired)
V. R. R. Uppuluri (retired)
D. G. Wilson (IBM)

B. Administrative and Technical Support Staff

C. B. Anthony (retired)
M. V. Denson (other employment)
M. C. Evans (other employment)
M. J. Fraley (co-op assignment completed)
R. F. Harbison (transfer to Y-12 Plant)
E. S. Howe (retired)
D. K. Hensley (transfer to Solid State Division)
R. A. Lexvold (co-op assignment completed)
R. S. Pattay (co-op assignment completed)
S. R. Simmons (summer student)
A. L. VanHull (co-op assignment completed)
L. C. Whitman (retired)

DISTINGUISHED SCIENTIST

J. J. Dongarra, University of Tennessee

GUESTS AND SHORT-TERM APPOINTMENTS

University/Industry Research Collaborators

A. Scientific Staff

M. A. Abidi, Computer Engineering, University of Tennessee
Z. Bai, Computer Science, University of Tennessee
J. L. Barlow, Computer Science, Penn State University, University Park, Pennsylvania
A. Benzoni, Mathematics, IBM-ECSEC, Rome
J. R. S. Blair, Computer Science, University of Tennessee
H. D. Booth, Computer Science, University of Tennessee
J. Borenstein, Nuclear Engineering, University of Michigan
C. L. Bowman, Mathematics, Ball Systems Engineering Division
R. W. Brockett, EPM Advisory Committee, Electrical Engineering/Computer Science, Harvard University

R. H. Brown, Physics, Luther College, Decorah, Iowa
W. M. Bugg, Physics, University of Tennessee
B. Carlson, Computer Science, Vanderbilt University
R. F. Carlton, Physics, Middle Tennessee State University, Murfreesboro, Tennessee
B. W. Char, Computer Science, University of Tennessee
C.-X. Chen, Computer Engineering, University of Tennessee
E. Chu, Computer Sciences, University of Waterloo
T. C. Collins, Physics, University of Tennessee
J. C. Courtney, Nuclear Engineering, Louisiana State University
B. G. Coury, Cognitive Science, University of Massachusetts
C. D. Crane, Mechanical Engineering, University of Florida
G. R. Dalton, Nuclear Engineering, University of Florida
G. J. Davis, Mathematics, Georgia State University
D. J. Dean, Physics, Vanderbilt University
B. Denby, Physics, Fermi Laboratory
Y. Deng, Computer Science, New York University, Stony Brook
N. R. Desai, Systems Engineering, University of Virginia
J. J. Dorning, EPM Advisory Committee, Nuclear Engineering/Engineering Physics, University of Virginia
L. W. Dowdy, Computer Science, Vanderbilt University
R. E. Ewing, Computer Science, University of Wyoming
E. A. Fleishman, Cognitive Science, George Mason University
T. B. Fowler, Nuclear Engineering (retiree)
J. A. George, Computer Science, University of Waterloo
J. Glimm, Computer Science, New York University, Stony Brook
G. H. Golub, Mathematics, Stanford University
A. T. Goshaw, Physics, Duke University
C. E. Guthrie, Computer Science, University of Tennessee
R. Gwin, Physics (retiree)
P. M. Haas, Cognitive Science, Concord Associates, Knoxville
A. Haghighat, Computer Science, Pennsylvania State University
T. Handler, Physics, University of Tennessee
H. J. Hargis, Physics, University of Tennessee
E. L. Hart, Physics, University of Tennessee
D. E. Hartley, Cognitive Science, University of Tennessee
L. Hermanto, Physics, National Atomic Energy Agency
P. Huray, Computer Science, University of South Carolina
T. E. Hutchinson, Physics, University of Virginia
A. R. Ingraffea, Computer Science, Cornell University
S. S. Iyengar, Computer Science, Louisiana State University
N. O. Jorgensen, Electrical Engineering, Aalborg University, Denmark
F. Kertesz, Chemistry (retiree)
A. I. Khuri, Statistics, University of Florida
E. Komori, Reactor Engineering, Power Reactor and Nuclear Fuel Development Corp., Japan
Y. Koren, Robotics, University of Michigan

K. Kurisaka, Nuclear Engineering, Power Reactor and Nuclear Fuel Development Corp., Japan
M. A. Langston, Computer Science, University of Tennessee
J. E. Leiss, EPM Advisory Committee, Physics, Department of Energy (retired)
B. Lindquist, Computer Science, New York University, Stony Brook
R. L. Macklin, Physics (retiree)
R. L. Macklin, Nuclear Engineering, University of Tennessee
R. J. Manchek, Computer Science, University of Tennessee
L. T. Mashburn, History, University of Tennessee
B. F. Maskewitz, Mathematics (retiree)
G. R. Montry, Physics. Southwest Software, Albuquerque, New Mexico
N. Moray, EPM Advisory Committee, Mechanical/Industrial Engineering/Psychology, University of Illinois
M. C. Moxon, Physics, UKAEA, AERE-Harwell, England
D. C. Mutchler, Computer Science, University of Tennessee
B. Newman, Physics, Los Alamos National Laboratory
J. M. Ortega, Mathematics, University of Virginia
L. Palko, Cognitive Science, JBF Associates, Knoxville
F. G. Perey, Physics (retired Martin Marietta Fellow)
J. H. Poore, Computer Science, University of Tennessee
D. A. Poplawski, Computer Science, Michigan Technological University
S. V. Rao, Computer Science, Old Dominion University
E. L. Redmond, Nuclear Engineering, Massachusetts Institute of Technology
K. N. Reid, Robotics, Oklahoma State University
J. J. Reidy, Physics, University of Mississippi
J. P. Reihs, Physics, University of Vienna
H. J. Schmiedmayer, Physics, Technical University of Wien, Austria
R. A. Schrack, Physics, National Institute of Standards and Technology
S. Serbin, Applied Mathematics, University of Tennessee
L. R. Shenton, Computer Science, University of Georgia
A. Shono, Nuclear Engineering, Power Reactor and Nuclear Fuel Development Corp., Japan
K. N. Sigmon, Mathematics, University of Florida
R. W. Sliger, Mechanical Engineering, Automated Sciences Group
J. C. Sluder, Electrical Engineering, University of Tennessee
G. W. Snashall, Mathematics, Ball Systems Engineering Division
A. D. Solomon, Computer Science, Israel (retiree)
C. Sparrow, Mississippi State University
R. Sreedhar, Robotics, University of Texas
R. Stohler, Kaman Sciences Corporation, Albuquerque, New Mexico
K. Storjohann, Computer Vision, University of Mainz, Germany
M. G. Thomason, Electrical Engineering, University of Tennessee
S. Thompson, Mathematics, Radford University, Radford, Virginia
S. L. Tosunoglu, Robotics, University of Texas
B. Tourancheau, Computer Science, INP-Grenoble, France
M. M. Trivedi, Robotics, University of Tennessee
D. K. Trubey, Computer Science (retiree)

B. W. Turnbull, Statistics, Cornell University
E. C. Uberbacher, Computer Science, University of Tennessee
R. A. van de Geijn, Computer Science, University of Tennessee
University Corporation for Atmospheric Research
H. A. Vasseur, Robotics, Ecole Nationale des Ponts, Paris
M. D. Vose, Computer Science, University of Tennessee
E. L. Wachspress, Mathematics, University of Tennessee
T. Wagner, Computer Science, Vanderbilt University
O. A. Wasson, Physics, National Institute of Standards
H. Watanabe, Computer Science, University of North Carolina
Y. Watanabe, Robotics, University of Tsukuba, Tsukuba, Japan
T. E. Weymouth, Computer Science, University of Michigan
M. F. Wheeler, EPM Advisory Committee, Computer Science, Rice University
J. R. White, Nuclear Engineering, University of Lowell
M. A. Williams, Mathematics, IBM
R. R. Winters, Physics, Denison University
J. Wu, Physics, University of Tennessee
Z. Zhao, Nuclear Physics, Institute of Atomic Energy, Beijing
J. P. Ziebarth, Aerospace Engineering, University of Alabama

B. Graduate Students

E. C. Anderson, Computer Science, University of Tennessee
L. S. Auvil, Math/Computer Science, Alderson-Broaddus College, Philipi, West Virginia
S. Balvja, Computer Science, University of Virginia
C. R. Bidlack, Electrical Engineering, University of Tennessee
C. P. Breashears, Computer Science, University of Tennessee
C.-X. Chen, Computer Vision, University of Tennessee
D. J. Dean, Physics, Vanderbilt University
H. P. Gadagkar, Computer Vision, University of Tennessee
R. J. Gray, Computer Science, University of Tennessee
C. E. Guthrie, Mathematics, University of Tennessee
D. E. Hartley, I/O Psychology, University of Tennessee
E. S. Kirsch, Computer Science, University of Tennessee
S. Kopecky, Physics, Institut fur Kernphysik, Vienna
L. C. Leal, Physics, University of Tennessee
J. W. H. Liu, Computer Science, York University, North York, Ontario
S. B. Marapan, Robotics/Computer Vision, University of Tennessee
J. S. Nicholas, Mathematics, University of Tennessee
L. S. Ostrouchov, Computer Science, University of Tennessee
G. Rajeev, Computer Science, University of Tennessee
S. Ramakrishnan, Electrical Engineering, University of Tennessee
E. L. Redmond, Nuclear Engineering, Massachusetts Institute of Technology
Y. Roth-Tabak, Computer Science, University of Michigan
M. M. Sidani, Computer Science, University of Tennessee
J. C. Sluder, Robotics, University of Tennessee
R. Siddarthan, Computer Science, University of Tennessee

E. Smith, Forestry, Tennessee Valley Authority
J. Speck, Cognitive Science, University of Virginia
R. N. Stewart, Mathematics/Statistics, University of Tennessee
C. Tan, Computer Engineering, University of Tennessee
C. A. York, Mathematics Education, University of Tennessee
K. S. Yu, Cognitive Engineering, University of Virginia

C. Oak Ridge Associated Universities - Faculty Research Participation Program

J. S. Bay, Electrical Engineering, Ohio State University
K. W. Bowyer, University of South Florida, Tampa, Florida
J. C. Courtney, Nuclear Engineering, Louisiana State University
G. J. Davis, Mathematics, Georgia State University, Atlanta
M. S. Jones, Industrial Engineering, Virginia Polytechnic Institute
H. N. Narang, Applied Mathematics, Tuskegee University
V. J. Rego, Computer Science, Michigan State University
V. S. Sunderam, Computer Science, Emory University
S. Thompson, Computer Science, Radford University, Virginia
W. Torres, Computer Science, Metropolitan University, San Juan, Puerto Rico
G. G. Vining, Statistics, University of Florida
M. L. Williams, Nuclear Engineering, Louisiana State University
R. R. Winters, Physics, Denison University, Granville, Ohio

D. Oak Ridge Associated Universities - Post-Doctoral Program

E. F. D'Azevedo, Computer Science, University of Waterloo
O. H. Doerum, Robotics Vision, Norwegian Institute of Technology
X. Guan, Computer Science, University of Tennessee
J. Yoon, Robotics, Korea Atomic Energy Research Institute

E. Oak Ridge Associated Universities - Graduate Student Research Partipation Program

C. A. Leete, Applied Mathematics, University of Virginia
R. R. Murphy, Computer Science, Georgia Institute of Technology
E. Stuck, Robotics, University of Minnesota

F. Oak Ridge Associated Universities - Student Research Participation Program

S. Belvja, Computer Science, University of Virginia
J. M. Banoczi, Mathematics, Youngstown State University
H. Chen, Computer Science, Hope College, Holland, Michigan
C. J. Cox, Computer Science, University of Alabama
M. D. Dewing, Physics, Michigan Technological University
C. F. Dumas, Mathematics, Tennessee Technological University
T. L. Duncan, Physics, University of Illinois
M. A. Iverson, Computer Engineering, Michigan State
K. D. Katzman, Cognitive Science, Wellesley College

J. E. Luntz, Mechanical Engineering, State University of New York - Buffalo
J. L Painter, Mathematics/Computer Science, East Tennessee State University
J. W. Pospisil, Mathematics/Computer Science, Nebraska Wesleyan
C. San Soucie, Mathematics, Louisiana State University
E. L. Sedlacek, Mathematics/Computer Science, Ohio Northern University
R. N. Stewart, Mathematics/Statistics, University of Tennessee
G. R. Torrez, Mathematics, New Mexico Highlands University

G. Oak Ridge Associated Universities - Science and Engineering Research Semester

G. W. Hunt, Mathematics, University of Montevallo, Montevallo, Alabama
T. J. Jones, Mathematics, Lindenwood College
K. A. Macko, Mathematics, Allegheny College, Meadville, Pennsylvania
L. L. Manne, Mathematics, Otterbein College, Westerville, Ohio
R. Melancon, Computer Science, University of Southern Louisiana
W. R. Rourk, Electrical Engineering, Clemson University
E. L. Saltzen, Computer Science, California State University
G. R. Torrez, Computer Science, New Mexico Highlands, Espanola, New Mexico

H. Oak Ridge Associated Universities - Professional Internship Program

R. A. Cacheiro, Electrical Engineering, Tennessee Technological University
C. F. Dumas, Mathematics, Tennessee Technological University

I. Oak Ridge Associated Universities - Summer Internship Program

J. L. Kirk, Electrical Engineering, Memphis State University
S. R. Simmons, Engineering Science, University of Tennessee
M. S. Winstead, Mathematics, University of Virginia

J. Teacher Research Program

J. T. Atkins, Education, Lincoln Memorial University, Rutledge High School
J. R. Beckett, Mathematics, Farragut High School, Farragut, Tennessee

K. University of Tennessee Post Doctoral Program

A. L. Beguelin, Computer Science, University of Colorado
W.-K. Kim, Mechanical Engineering, University of Texas

L. National Science Foundation Undergraduate Research Program

K. W. Broman, Mathematics, University of Wisconsin
J. V. Butera, Mathematics, Clemson University

M. U.S. Military Service Academy Research Associates

D. J. Durn, Systems Engineering, U.S. Naval Academy

N. Special Program for Gifted High School Students

J. A. Grimm, Mathematics/Computer Science, Oak Ridge High School
H. F. Tsai, Mathematics, Oak Ridge High School

O. University of Tennessee/ORNL Science Alliance Program

S. B. Hill, Physics, Washington University, Clayton, Missouri
R. L. Marsa, Physics, University of Tennessee

P. University of Tennessee/Mathematical Sciences Section Research Assistantship Program

J. S. Nicholas, Mathematics, University of Tennessee

Q. Great Lakes College Association - Science Semester

H. Chen, Computer Science, Hope College, Holland, Michigan
J. R. Coleman, Robotics, Albion College, Albion, Michigan
M. E. Hribar, Mathematics, Albion College, Albion, Michigan
M. R. Hribar, Mathematics, Albion College, Albion, Michigan
J. J. Kruse, Physics/Mathematics, Monmouth College, Monmouth, Illinois
C. L. Rakich, Mathematics, Albion College, Albion, Michigan

R. Undergraduate Students

M. D. Dewing, Physics, Michigan Technological University, Grantsburg, Michigan
C. Fellner, Physics, Technical University of Wien, Austria
C. M. Teichtmeister, Physics, Technical University of Vienna

SCIENTIFIC AND PROFESSIONAL ACTIVITIES

September 1, 1989 — March 31, 1991

V. Alexiades

Invited paper

— "A Weak Formulation for Phase-Change Problems with Bulk Movement Due to Unequal Densities of the Phases," International Conference on Free Boundary Problems: Theory and Applications, University de Montreal, Montreal, Canada, June 1990.

Professor

— Mathematics Department, University of Tennessee, Knoxville, TN.

Award

— UTK-ORNL Science Alliance Research Incentive Award, 1986–1990.

Reviewer

— *Mathematics Reviews*

Referee

— *Applicable Analysis*

— *SIAM Journal of Mathematical Analysis*

— *Nonlinear Analysis*

— *International Journal of Heat and Mass Transfer*

— *ASME Journal of Heat Transfer*

— NSF and DOE Proposals

F. S. Alsmiller

Referee

— *Nuclear Instruments and Methods*

R. G. Alsmiller, Jr.

Chairman

— DOE-ER Advisory Panel on Accelerator Radiation Safety (APARS) for the Review of the Continuous Electron Beam Accelerator Facility (CEBAF) End Stations.

— DOE-ER Committee for the Restart Review of the AGS at BNL.

— DOE-ER Committee for the Technical Safety Review of the Los Alamos Meson Physics Facility.

Member

- Subcommittee on Dosimetry of the National Research Council Advisory Committee on the Radiation Effects Research Foundation.
- DOE-ER APARS for the Review of the LINAC Upgrade at FNAL.
- DOE-ER APARS for the Review of the AGS Booster Project at BNL.
- DOE-EH Committee to Investigate the Unusual Occurrence Report 90-11 at the BNL AGS.
- Committee appointed by Los Alamos National Laboratory Management to Review the Shielding of the Los Alamos Meson Physical Facility.
- National Committee of Radiological Protection Scientific Committee 52 on Conceptual Basis of the Calculation on Dose Distributions.

Referee

- *Nuclear Science and Engineering*
- *Nuclear Instruments and Methods in Physical Research*
- *Physics in Medicine and Biology*
- *Health Physics*
- *Radiation Research*
- *Fusion Nuclear Technology*

Y. Y. Azmy

Treasurer

- Mathematics and Computation Division of the American Nuclear Society.

Referee

- *Nuclear Science and Engineering*

Visiting scientist

- University of Bologna, Italy, invited by the Italian National Council for Research.

J. J. Beauchamp

Instructor

- Oak Ridge Graduate School of Biomedical Sciences, University of Tennessee, Knoxville, TN.

Recipient

- Certificate of Appreciation for Participation in the National Acid Precipitation Assessment Program.

Referee

- *The American Statistician*
- *Environmental Management*
- *Canadian Journal of Fisheries and Aquatic Sciences*
- *Communications in Statistics*

K. O. Bowman

Member

- Advisory Committee on Equal Opportunities in Science and Engineering, National Science Foundation.
- Advisory Board, *Journal of Statistical Computation and Simulation.*
- International Editorial Board, Communications in Statistics.
- Proposal Review Panel, National Science Foundation.
- National Science Foundation Task Force on Persons with Disabilities.

Chair

- Subcommittee on Persons with Disabilities, Equal Opportunities in Science and Engineering, National Science Foundation.
- Coordinating Committee on Equal Opportunities in Statistics, American Statistical Association.

Invited papers

- "The Approximate Distribution of Four Moment Statistics from Type III Distribution," (with L. R. Shenton) *Commun. Statist. Theory and Methods* **19(4)** 1511 (1990).
- "Statistical Quality Control Technology in Japan," (with T. Hopp, R. N. Kacker, and R. J. Lundegard) *Chance* (in press).

Contributing editor

- *Current Index to Statistics*

Grant

- National Science Foundation

Reviewer

- *Science, American Association for the Advancement of Science*
- Research Proposal, National Science Foundation

Referee

- *Communications in Statistics*
- *American Statistician*
- *Journal of Statistical Computation and Simulation*

R. J. Carter

Member

- Human Factors Society Publications Committee.
- Human Factors Society Best Bulletin Article Award Committee.

Chair

- Human Factors Society Best Bulletin Article Award Committee.

Editor

- *Human Factors Society Bulletin*

Session organizer

- Computer-Based Human Decision-Making Aids, ANS Topical Meeting on Advances in Human Factors Research on Man/Computer Interactions: Nuclear and Beyond.
- Hands-On Demonstrations of Computer Models, ANS Topical Meeting on Advances in Human Factors Research on Man/Computer Interactions: Nuclear and Beyond.

Invited lecture

- "Expert System Interface and Other Human Factors Issues," ANS Workshop on Expert System Development, Validation, and Experience, Nashville, TN, June 9, 1990.

Invited papers

- "Advanced Instrumentation and Controls Technology, Survey Results," (with R. E. Uhrig), Nuclear Safety Research Review Committee's Subcommittee Meeting on Human Factors and Reliability, Massachusetts Institute of Technology, Cambridge, MA, November 20, 1989.
- "Human Factors Survey of Advanced Instrumentation and Controls," Nuclear Regulatory Commission Water Reactor Safety Information Meeting, Rockville, MD, October 24, 1989.

G. de Saussure

Member

- International Program Committee International Topical Meeting on the Physics of Reactor Operation, Design, and Computation: Physor '90 (1990).

Honorary professor

— Nuclear Engineering Department, University of Tennessee.

Referee

— *Nuclear Science and Engineering*

— *The Physical Review*

— *Nuclear Safety*

J. K. Dickens

Member

— American Nuclear Society Standards Working Group 5.1, Decay Heat Standard.

— American Nuclear Society Standards Working Group 5.2, Fission Product Yields.

— American Nuclear Society Standards Working Group 5.8, Delayed Neutrons Standard.

— Nuclear Energy Agency Task Force on Decay Heat Predictions.

— Oak Ridge National Laboratory Speakers Bureau.

— Oak Ridge Associated Universities Tennessee Visiting Scientist Roster.

Correspondent

— Designated by IAEA Working Group on Fission Product Nuclear Data as correspondent on worldwide experimental measurements of fission product decay heat (1977–continuing).

Invited paper

— "Proposed Improvements to ANSI/ANS-5.1, Decay Heat Power In Light Water Reactors," *Trans. Am. Nucl. Soc.* **62**, 536 (1990).

Invited lectures

— "Reactor Safety and the Status of Commercial Nuclear Power in the U.S.," Southwestern University Physics Department, Austin, TX, November 20, 1989.

— "Cold Fusion: Fact and Fiction," University of North Texas, Physics Department, January 22, 1990.

— "Reactor Safety and the Status of Commercial Nuclear Power in the U.S.," South Texas Energy Research and Development Center, Texas A&I University, Kingsville, TX, January 23, 1990.

Referee

— *Nuclear Science and Engineering*

— *IEEE Nuclear Science Transactions*

— *Nuclear Instruments and Methods*

F. C. Difilippo

Member

— Program Committee Reactor Physics Division American Nuclear Society.

Invited lecture

— "Design of the Advanced Neutron Source Reactor," University of Tennessee, Knoxville, TN, March 15, 1991.

Invited paper

— "Theoretical Analysis of Reactivity Measurements with the ^{252}Cf-Source Ratio Method," International Topical Meeting on Safety Margins in Criticality Safety, San Francisco, CA, November 26–30, 1989.

Organizer

— Special Session of Winter 1990 American Nuclear Society Meeting on the Advanced Neutron Source.

Fellow

— American Nuclear Society

Listed

— International Directory of Nuclear Criticality Safety Personnel.

Academic

— Adjunct Professor, Department of Nuclear Engineering, University of Tennessee, Knoxville, TN.

— Thesis Advisor at the University of Tennessee, Knoxville, TN, and the University of Buenos Aires, Argentina.

Referee

— *Nuclear Science and Engineering*

— *Journal of Nuclear Materials*

W. W. Engle, Jr.

Special assignment

— On assignment at the OECD-NEA Data Bank, Saclay, France, August 1988 through June 1990.

E. L. Frome

Member

— American Statistical Association Committee on Statistics and the Environment.

— Statistics Test Panel for Data Management Systems in Genetic Toxicology Sponsored by U.S. EPA.

— ORAU/University of North Carolina Research Planning Group for DOE Health and Mortality Studies.

— Information Systems Working Group for the DOE Comprehensive Epidemiologic Data Resource.

Associate professor

— Department of Biostatistics, University of North Carolina, Chapel Hill, NC.

Associate editor

— *The American Statistician*, 1983–present.

Referee

— *The American Journal of Epidemiology*

— *Statistics in Medicine*

— *The American Statistician*

— *Radiation Research*

— *Biometrics*

C. Y. Fu

Chairman

— Task 1.1, NEACRP/NEANDC Task Force on International Nuclear Data Evaluation Coordination.

Member

— Cross Section Evaluation Working Group (CSEWG).

— NEANDC Activation Cross Section Working Group.

— Task 1.2 NEANDC/NEACRP Task Force on International Nuclear Data Evaluation Coordination.

Invited papers

— "Pairing Interaction Effects in Exciton Level Densities," NEANDC Specialists' Meeting on Level Densities, Bologna, Italy, November 15-17, 1989.

— "Improvements in ENDF/B-VI Iron and Possible Impacts on Pressure Vessel Surveillance Dosimetry," Seventh ASTM-EURATOM Symposium on Reactor Dosimetry, Strasbourg, France, August 27-31, 1990.

Referee

— *Nuclear Science and Engineering*

K. Fujimura

Member

— *IEEE Computer Society*

— *Association for Computing Machinery*

— *American Association for Artificial Intelligence*

T. A. Gabriel

Director

— Oak Ridge Detector Center

Member

— Steering Committee of the Southern Association for High Energy Physics (SAHEP).

Co-initiative manager

— High Energy Physics Research

Publicity chairman

— Organizing Committee for the Southeastern Conference on the Superconducting Super Collider (SSC) (November 1991).

Co-chairman

— Conference on Detector Simulation for the SSC (August 1992).

— Inner Tracking Simulation Session at the Workshop on Major SSC Detectors, Tucson, AZ, February 19–23, 1990.

Chairman

— Computing and Simulations Session at the Symposium on SSC Detector R&D, Fort Worth, TX, October 15–18, 1990.

— Central Tracking Simulation Session at the Workshop on Major SSC Detectors, Tucson, AZ, February 19–23, 1990.

Co-session organizer

— Workshop on Major SSC Detectors, Tucson, AZ, February 19–23, 1990.

Organizer

— Workshop on Calorimetry for the L*Collaboration, Oak Ridge National Laboratory, January 26–28, 1990.

— Workshop on Mechanical Engineering for the Central Tracking Chamber of the Solenoidal Detector, Oak Ridge National Laboratory, April 9, 1990.

— Expression of Interest Workshop for L*, Oak Ridge National Laboratory, April 26–28, 1990.

— Workshop on Simulation Studies on Compensating Scintillator Plate Calorimeters, Oak Ridge National Laboratory, June 19–20, 1990.

— Workshop on the Scintillating Fiber Central Tracker, Oak Ridge National Laboratory, July 17, 1990.

— SSC Session at the WATTec '91 Meeting, Knoxville, TN, February 19–22, 1991.

— Solenoidal Detector Collaboration Tracking Workshop, Oak Ridge National Laboratory, February 11–13, 1991.

Invited lectures

— "High Energy Physics, The SSC, and ORNL," dinner presentation for the local IEEE, December 19, 1989.

— "The SSC, ORDC, and Detector Design Research," Monthly Symposium, Memphis State University, November 9, 1990.

— "Will Radiation Damage be the End of SSC Detectors?" Hybrid Central Tracking Workshop, Duke University, January 16–18, 1991.

— "Radiation Damage in Plastic Scintillator," Tracking Workshop, Oak Ridge National Laboratory, February 11–13, 1991.

Invited papers

— "The Coupling of CALOR89 and GEANT," (with J. J. Reidy) Workshop on Simulation Software Packages for the SSC, Dallas, TX, January 8–19, 1990.

— "CALOR89: Lead/Plastic Calorimetry and Benchmarking," (with T. Handler) Workshop on Major SSC Detectors, Tucson, AZ, February 19–23, 1990.

— "Damage Simulations," (with T. Handler) Workshop on Radiation Hardness of Plastic Scintillator, Florida State University, March 19–21, 1990.

— "Radiation Damage in Various Components of an SSC Detector," SDC Meeting at SSCL, Dallas, TX, January 10–12, 1991.

Fellow

— American Physics Society.

G. A. Geist

Member

— NAC Committee

— Workstation Advisory Board

— SIAM Society

Invited talks

— "Getting High Performance from Distributive Memory Computers," Daresbury Laboratory, United Kingdom, November 9, 1990.

— "Experiences with the Intel iPSC/860 at Oak Ridge National Laboratory," IBM Research Center, Yorktown, NY, January 24, 1991.

— "PICL: A Portable Instrumented Communication Library," Houston, TX, March 28, 1991.

Awards

— 1990 Cray Gigaflop.

— 1990 Gorden Bell Award.

— First Place 1990 IBM Supercomputer Competition.

L. J. Gray

Invited talks

— "Electroplating at Corners," BETECH 90, University of Delaware, Newark, DE, July 10–12, 1990.

— "Boundary Element Fracture Analysis," FFA, the Aeronautical Research Institute of Sweden, Stockholm, Sweden, October 3, 1990.

— "Boundary Element Analysis of the Dirichlet Problem," IBM Bergen Scientific Centre, Bergen, Norway, October 8, 1990.

— "Evaluation of the Boundary Stress Tensor," (with E. D. Lutz and A. R. Ingraffea) IABEM-90 Symposium, Rome, Italy, October 15–18, 1990.

— "Boundary Element Fracture Analysis," IBM Rome Scientific Centre, Rome, Italy, October 19, 1990.

— "Applications of Hypersingular Integral Equations," University of Bath, Bath, England, October 24, 1990.

— "Applications of Hypersingular Integral Equations," University of Wisconsin, Madison, WI, November 6, 1990.

Invited papers

— "Hypersingular Integrals and the Two Dimensional Helmholtz Equation," Proc. of Japan/USA Symposium, June 5–7, 1990, Palo Alto, CA, Computational Mechanics.

— "Electroplating Corners," Computational Engineering with Boundary Elements, Vol. 1, Proc. of BETECH 90, Newark, DE, Editors, S. Grilli, C. A. Brebbia, and A. Cheng, Computational Mechanics, Boston, MA.

Editorial board

— Engineering Analysis with Boundary Elements

— Electrosoft

— Boundary Elements: Abstracts and Newsletters

Referee

— *International Journal for Numerical Methods in Engineering*

Member

— Scientific Organizing Committee for the 12th International Boundary Element Conference, Sapporo, Japan, September 1990 and the Japan/USA Boundary Element Symposium, Palo Alto, May 1990.

C. M. Haaland

Advisor

— National Council for Radiation Protection and Measurements Scientific Committee #63, Radiation Exposure Control in a Nuclear Emergency, Lewis V. Spencer, Chairman.

Member

— American Physical Society

— Institute of Electrical and Electronics Engineers

— Sigma Xi

Referee

— *Journal of Civil Defense*

— *Journal of Health Physics*

J. A. Harvey

Member

— ORNL Accelerators and Radiation Sources Review Committee.

— Panel on Basic Nuclear Data Compilations National Research Council.

— Committee on Membership, American Physical Society.

Labor coordinator

— Engineering Physics and Mathematics Division.

Safety officer

— Engineering Physics and Mathematics Division.

Radiation control officer

— Engineering Physics and Mathematics Division.

Referee

— *Physical Review C*

— *Physical Review Letters*

— *Nuclear Science and Engineering*

D. T. Ingersoll

Member

— Nuclear Energy Agency Committee on Reactor Physics (NEACRP).

— ORNL Nuclear Energy Panel.

— DOE/SEI Life Support Working Group.

Chairman

— Radiation Protection and Shielding Division, American Nuclear Society.

— Shielding Data Testing Subcommittee, Cross-Section Evaluation Working Group (CSEWG).

— U.S.–JASPER Shielding Program Working Group.

Reviewer

— DOE Nuclear Engineering Research Program.

— Nuclear Technology Journal.

Invited paper

— "Current U.S. Activities and Directions in Shielding Technology for Liquid-Metal-Cooled Reactors," ANS Winter Meeting, Washington, DC, November 11–15, 1990.

B. L. Kirk

Membership chairman

— American Nuclear Society, Radiation Protection and Shielding Division.

Member

— American Nuclear Society (ANS-10 Standards Committee).

— Society for Industrial and Applied Math Special Interest Group on Supercomputing.

Secretary

— American Nuclear Society, Oak Ridge/Knoxville Chapter.

H. E. Knee

Member

- Executive Committee: Human Factors Division of the American Nuclear Society.
- American Nuclear Society.
- Smoky Mountain Chapter of the Human Factors Society.
- EPRI Chapter 10 Man/Machine Interface Requirements Committee.
- EPRI Reactor Upgrade Planning Review Committee.

Technical chairman

- ANS Topical Meeting on Advances in Human Factors Research on Man-Computer Interactions: Nuclear and Beyond (June 1990).
- ANS Topical Meeting on Nuclear Plant Instrumentation Control and Man-Machine Interface Technologies (April 1993).

D. C. Larson

Member

- Department of Energy Nuclear Data Committee.
- NEANDC International Task Force on Evaluation Cooperation.
- Evaluation Methods Subcommittee, Cross Section Evaluation Working Group (CSEWG).
- Resonance Region Subcommittee, CSEWG.

Chairman

- Working Group A, Office of Nuclear Physics Committee on Nuclear Data for Fusion Reactor Applications.
- Working Group 2, IAEA Specialist's Meetings on Fusion Evaluated Nuclear Data Library.
- Co-chairman of General Purpose Evaluations Subcommittee, CSEWG.

Proposal reviewer

- Office of Nuclear Physics, Department of Energy, Low Energy Nuclear Physics.

Referee

- *Nuclear Science and Engineering*

R. A. Lillie

Chairman

- ORNL Reactor Experiments Review Committee.

Referee

— *Nuclear Technology*

— *Nuclear Technology/Fusion*

— *Journal of Fusion Energy*

— *Nuclear Science and Engineering*

— *Nuclear Instruments and Methods*

R. E. Maerker

Member

— ASTM E10.05 Subcommittee Member Ad-Hoc Committee to Prepare Guide on LWR-RPV' Surveillance Analysis for NRC.

— American Nuclear Society.

Invited papers

— "Parameter and Flux Covariances in LEPRICON," to be published in Proceedings of the Seventh ASTM-EURATOM Symposium on Reactor Dosimetry, Strasbourg, France, August 27-31, 1990.

— "Analysis of the VENUS-3 Experiments," (with P. D'hondt, L. Lenders, and A. Fabry) to be published in Proceedings of the Seventh ASTM-EURATOM Symposium on Reactor Dosimetry, Strasbourg, France, August 27-31, 1990.

— "Development and Application of a New Deterministic Method for Calculating Computer Model Result Uncertainties," (with B. A. Worley) *Trans. Am. Nucl. Soc.* **60**, 591 (1989).

Referee

— *Nuclear Science and Engineering*

— *Journal of Nuclear Materials*, Amsterdam, Holland

R. C. Mann

Member

— Advisory Committee for the Universidad del Turabo, Puerto Rico, Engineering Curriculum Development.

Invited lecture

— "Intelligent Robots for Hazardous Environments," Colloquium at Johns Hopkins University, Applied Physics Laboratory, April 13, 1990.

Chairman

— DOE SEI Robotics Working Group

Reviewer

- *IEEE Trans. Systems, Man, Cybernatics*
- *IEEE Computer*
- *IEEE J. Robotics & Automation*
- DOE SBIR Program

M. D. Morris

Member

- Editorial Review Board - *Journal of Quality Technology*

E. Ng

Invited lectures

- "Parallel Direct Solution of Sparse Linear Systems," Department of Computer Science, University of Alberta, Edmonton, Alberta, Canada, March 12, 1990.
- "Parallel Direct Solution of Sparse Linear Systems," Department of Computer Science, University of British Columbia, Vancouver, British Columbia, Canada, March 14, 1990.
- "Algorithms for the Direct Solution of Sparse Nonsymmetric Linear Systems," Institute for Computer Research, University of Waterloo, Waterloo, Ontario, Canada, April 25, 1990.
- "Direct Solution of Sparse Linear Systems on Multiprocessor Architectures," Southern Ontario Numerical Analysis Day, University of Waterloo, Waterloo, Ontario, Canada, April 26, 1990.
- "Algorithms for the Direct Solution of Sparse Nonsymmetric Linear Systems," Workshop on Sparsity in Large Scale Scientific Computation, IBM Europe Institute, Oberlech, Austria, August 6–10, 1990.

Invited papers

- "Solution of Sparse Positive Definite Systems on a Hypercube (with A. George, M. T. Heath, and J. Liu), *J. of Computational and Applied Mathematics* **27**, 129–156 (1989).
- "Parallel Sparse Gaussian Elimination with Partial Pivoting," (with A. George) *Annals of Operations Research* **22**, 219–240 (1990).
- "Parallel Algorithms for Matrix Computations (with K. Gallivan, M. T. Health, J. Ortega, B. Peyton, R. Plemmons, C. Romine, A. Sameh, and R. Voigt), SIAM Publications (1990).
- "Experiments with an Ordinary Differential Equation Solver in the Parallel Solution of Method of Lines Problems on a Shared Memory Parallel Computer (with D. K. Kahaner, W. E. Schiesser, and S. Thompson), to be published in the Proceedings of the Chicago 1990 AICHE Annual Meeting (1991).

G. Ostrouchov

Associate editor

— *Journal of Statistical Computation and Simulation*

R. W. Peelle

Member

— Cross Section Evaluation Working Group (CSEWG) Executive Committee.

— U.S. Member to International Nuclear Data Committee.

— International Advisory Committee for 1991 Jülich Conference on Nuclear Data.

— Working Group for the DOE-NSF Nuclear Science Advisory Committee 1989 Long Range Plan.

Chairman

— CSEWG Covariance Data Subcommittee.

Reviewer

— Small Business Incentive Research Grant Programs of the Department of Energy Office of Energy Research and of the National Science Foundation.

Referee

— *The Physical Review*

— *Nuclear Science and Engineering*

B. W. Peyton

Invited lecture

— "Parallel Sparse Cholesky Algorithms," Cray Research Inc., December 1990.

Reviewer

— *SIAM Journal Scientific and Statistical Computing*

— *SIAM Journal Matrix Anal. Appl.*

F. G. Pin

Program chairman

— Robotics and Intelligent Interfaces, the International Conference on Engineering and Industrial Application of AI and Expert Systems, Tullahoma, TN, June 6–9, 1990.

Technical program committee

— IEEE International Workshop on Intelligent Robots and Systems, IROS '89, Tsukuba, Japan, September 4–9, 1989.

- IEEE International Workshop on Intelligent Robots and Systems, IROS '90, Tuschuria, Japan, October 29–November 2, 1990.
- IEEE International Workshop on Intelligent Motion Control, Istanbul, Turkey, August 20–22, 1990.
- International Symposium on Robotics and Manufacturing, ISRAM '90, Vancouver, BC, July 10–12, 1990.

Editorial board

- *International Journal of Robotics and Mechatronic.*
- *Japanese Journal of Advanced Automation Technology.*

Guest editor

- *Computers and Electrical Engineering Journal*

R. T. Primm, III

Member

- Executive Committee Local Section, American Nuclear Society.
- Technical Program Committee, 1990 Annual Meeting of American Nuclear Society.

Treasurer

- Local Section, American Nuclear Society.

Referee

- *Nuclear Science and Technology*

Reviewer

- "Criticality Data and Validation Studies of Arrays of Mixed Oxide Fuel Pins in Aqueous and Organic Solution," by G. R. Smolen, et al.

V. A. Protopopescu

Member

- Editorial Board of the Series *Advances in Mathematics for Applied Sciences.*
- Editorial Board of the Journal *Mathematical Methods and Models in Applied Sciences.*
- Editorial Board of the Journal *Transport Theory and Statistical Physics.*

Award

- 1990 Martin Marietta Special Achievement Award.

Adjunct professor

— Mathematics Department, University of Tennessee, Knoxville, TN.

Invited lectures and talks

— "Propagators for Nonlinear Systems," presented at the University of Louisville, KY, March 2, 1990.

— "Propagators for Nonlinear Systems," presented at the University of Alabama at Birmingham, January 25, 1991.

— "Chaos and Instability in Linear Systems," presented at the Space Institute of the University of Tennessee, Tullahoma, March 13, 1991.

Reviewer

— *Mathematical Reviews*

Referee

— *Journal of Statistical Physics*

— *Transport Theory and Statistical Physics*

— *Nuclear Science and Engineering*

— *Journal of Physics*

W. A. Rhoades

Member

— Scientific Workstation Subcommittee

Referee

— *Nuclear Science and Engineering*

R. W. Roussin

Member

— Panel on Reference Nuclear Data, Representative for American Nuclear Society, Radiation Protection and Shielding Division.

— ANS 6.1.2: Shielding Cross Sections Standards Committee.

— Shielding Data Testing and Applications Subcommittee, Cross Section Evaluation Working Group (CSEWG).

— ORNL Federal Credit Union Board of Directors.

Chairman

— Methods and Formats Committee, Cross Section Evaluation Working Group (CSEWG).

— Photon Interaction Evaluation Subcommittee, CSEWG.

— Subgroup 7, Cross Section Processing, NEANDC/NEACRP Committee on International Evaluation Cooperation.

Referee

- *Nuclear Science and Engineering*
- *Nuclear Technology/Fusion*
- *Trans. of Symposia on Space Nuclear Power Systems*

R. T. Santoro

Member

- ORNL WFO Steering Committee.
- American Nuclear Society Honors and Awards Committee.
- American Nuclear Society, Radiation Protection and Shielding Division Executive Committee.
- ORNL Space Exploration Initiative Task Force.

Invited paper

- "U.S. Shielding and Streaming Experiments: Brief Review," ITER Specialists Meeting on Fusion Reactor Shielding Experiments, Mac Planck Institute, Federal Republic of Germany.

Referee

- *Fusion Technology*
- *Nuclear Science and Engineering*
- *Nuclear Technology/Fusion*

Fellow

- American Nuclear Society.

M. S. Smith

Chairman

- 1992 WATTec Technical Program, American Nuclear Society.

Executive committee

- Oak Ridge/Knoxville Section of American Nuclear Society.

D. K. Trubey

ANS representative

- ANSI Committee N17: Research Reactors, Reactor Physics, and Radiation Shielding.

Chairman

- ANS-6: Radiation Protection and Shielding Subcommittee, Standards Committee, American Nuclear Society.
- ANS-6.4.3: Standards Working Group, Gamma-Ray Attenuation Data.

Computer security officer

— Engineering Physics and Mathematics Division.

SI standards coordinator

— Engineering Physics and Mathematics Division.

Referee

— *Nuclear Science and Engineering*

— *Health Physics*

M. A. Unseren

Invited paper

— "A Rigid Body Model and Decoupled Control Architecture for Two Manipulators Holding a Complex Object," *Computers and Electrical Engineering, An International Journal.*

R. C. Ward

Member

— ORNL Working Group on Computing.

— Program Committee: The Fifth Distributed Memory Computing Conference, Charleston, SC, April 8–12, 1990.

— College of Engineering Advisory Council, North Carolina State University, 1991–93.

— Advisory Committee, Applied Linear Algebra Year, Institute for Mathematics and Its Applications, University of Minnesota, 1991–92.

Invited papers

— "Numerical Analysis, Mathematics and Parallel Computing," Interdisciplinary Center for Applied Mathematics, VPI&SU, Blacksburg, VA, November 6–7, 1989.

— "Computational Science at Oak Ridge National Laboratory," The 1991 IBM Technical Computing Executive Conference, Orlando, FL, March 11–13, 1991.

Proposal reviewer

— National Science Foundation.

— Department of Energy.

Fellow

— American Association for Advancement of Science.

T. Wright

Member

— American Statistical Association Advisory Committee to the U.S. Bureau of the Census.

— Executive Committee, Section on Survey Research Methods, American Statistical Association.

— Steering Committee, Tennessee Mathematics Coalition.

Editorial board

— *The American Journal of Mathematical and Management Sciences.*

Board of directors and treasurer

— Tennessee Mathematics and Computer Sciences Foundation, Inc.

Project director

— Mentors (and students) for the Mathematical Sciences–Pilot Project (Tennessee Mathematics and Computer Sciences Foundation, Inc.)

Associate professor

— (Mathematics) Knoxville College, Knoxville, TN.

— (Statistics) University of Tennessee, Knoxville, TN.

Reviewer

— *Mathematical Reviews*

Referee

— *Communications in Statistics, Theory and Methods*

— *Communications in Statistics, Simulation and Computation*

— *International Statistical Review*

— *The American Statistician*

— *Naval Research Logistics*

CONFERENCES

1990

"CHAMMP (Computer Hardware, Advanced Mathematics, and Model Physics) Organizing Meeting," May 9–11, 1990, Oak Ridge, Tennessee

Organizer: J. B. Drake

Attendees: 37

Sponsor: ORNL, Mathematical Sciences Section

"Workshop on Mathematics and Environmental Waste Problems," July 23, 1990, Oak Ridge, Tennessee

Organizer: L. J. Gray

Attendees: 48

Sponsors: ORNL, Mathematical Sciences Section

"iPSC/860 Workshop," August 2–3, 1990, Oak Ridge, Tennessee

Organizers: M. R. Leuze

Attendees: 47

Sponsors: ORNL, Mathematical Sciences Section

"Scalable Parallel Libraries: Science and Technology for the '90's," September 6–7, 1990, Oak Ridge, Tennessee

Organizers: M. R. Leuze and G. Weigand

Attendees: 79

Sponsors: DARPA, ORNL, Mathematical Sciences Section

"Oak Ridge CHAMMPions Meeting," October 22–23, 1990, Oak Ridge, Tennessee

Organizer: J. B. Drake

Attendees: 46

Sponsors: ORNL, Mathematical Sciences Section

SEMINARS AT ORNL

M. Beckerman, Y. Y. Azmy, and C. H. Romine were the seminar coordinators during the period covered by this report. The following seminars were held during September 1989 through March 1991.

S. Anghaie, Associate Director, Innovative Nuclear Space Power & Propulsion Institute, College of Engineering, University of Florida, Gainesville, FL, "Space Power and Propulsion with Ultrahigh Temperature Reactors"

I. G. Angus, Northrop Research and Technology Center, "Parallelism, Object Oriented Programming Methods, Portable Software and C++. (A CFD Example)"

R. C. Arkin, Mobile Robot Laboratory, School of Information and Computer Science, Georgia Institute of Technology, Atlanta, GA, "Visual Strategies for Mobile Robot Docking"

L. S. Auvil, Alderson-Broaddus College, Philippi, WV,"Graphical Display on a Scientific Workstation of Parallel Algorithm Behavior"

R. S. Baker, Los Alamos National Laboratory, Los Alamos, NM, "A Fully Coupled Monte Carlo/S_N Technique for Solving Neutron Transport Problems"

J. Barlow, Computer Science Department, Pennsylvania State University, University Park, PA, "Computing Accurate Eigensystems of Scaled Diagonally Dominant Matrices"

A. Beguelin, Department of Computer Science, University of Colorado, Boulder, CO, "Deterministic Parallel Programming Phred"

C. Bischof, Department of Mathematical Sciences, Argonne University, Argonne, IL, "Structured Orthogonal Factorizations of Rank-Deficient Matrices"

B. Bradley, University of Virginia, Charlottesville, VA, "A Survey of Methods in the Optimal Control of the Stefan Problem"

I. Cavers, Department of Computer Science, University of British Columbia, "Using Deficiency Measure for Tiebreaking the Minimum Degree Algorithm"

S. R. Choudhury, Department of Computer Science, Duke University, Durham, NC, "Multirate Numerical Methods for Differential Algebraic Systems and Partial Differential Equations"

A. Cleary, University of Virginia, "The Solution of Narrowly Banded Linear Systems on Parallel Computers by Direct Methods"

B. G. Coury, Department of Industrial Engineering and Operations Research, University of Massachusetts, Amherst, MA, "Cognitive Components of Operator Decision-Making Performance and Implications for the Design of Control Systems"

E. D'Azevedo, Department of Computer Science, University of Waterloo, "On Optimal Triangulation for Piecewise Linear Approximation"

J. Dongarra, Engineering Physics and Mathematics Division, "Influence of High-Performance Computers on Numerical Software for Dense Linear Algebra"

D. L. Donohue, Analytical Chemistry Division, "Positron Ionization Mass Spectrometry of Organic Compounds"

N. Draper, University of Wisconsin, Madison, WI, "Triple Threat Seminar: Selected Topics in Design of Experiments and Regression Analysis"

I. Duff, Rutherford Appleton Laboratory and CERFACS, "Parallel Algorithms for Sparse Matrices"

T. H. Dunigan and C. H. Romine, Engineering Physics and Mathematics Division, "Parallel Processing Short Course"

H. Embrechts, Department of Computer Science, "Component Labeling on a Distributed Memory Multiprocessor"

J. Etheridge, Roanoke College, Salem, VA, "Graphical Animation of Message-Passing Parallel Algorithms"

I. Foster, Argonne National Laboratory, Argonne, IL, "Parallel Programming Language Tutorial"

A. Geist, Engineering Physics and Mathematics Division, "Development of a 1.6 Gflop Superconductivity Application Code on ORNL's iPSC/860 Hypercube"

J. Gilbert, Palo Alto Research Center, Xerox, "Data-Parallel Sparse Matrix Factorization"

J. Glimm, State University of New York, Stony Brook, NY, "Front Tracking Methods and Results"

C. W. Glover, Engineering Physics and Mathematics Division, "Hybrid Neural Network and Rule-Based Pattern Recognition System Capable of Self-Modification"

L. J. Gray, Engineering Physics and Mathematics Division, "Computational Fracture Mechanics"

F. M. Guess, Department of Statistics, University of Tennessee, Knoxville, TN, "Mean Residual Life: Theory and Applications"

G. A. Guiochon, Analytical Chemistry Division and Chemistry Department, University of Tennessee, Knoxville, TN, "Mathematical and Computational Modeling of Preparative Protein Chromatography"

C. M. Haaland, Engineering Physics and Mathematics Division, "Steady-Flow Liquid Metal MHD Electric Generators"

A. Haghighat, Nuclear Engineering Department, Pennsylvania State University, University Park, PA, "Development of Parallel/Vector Algorithms for the S_N Transport Theory Method"

M. T. Heath, Engineering Physics and Mathematics Division, "ParaGraph: A Graphical Performance Visualization Tool for Parallel Computers"

N. Hecker, Harvard University, Cambridge, MA, "Vibrational Anomalies in High-Temperature Superconductors"

E. Jessup, Department of Computer Science, Yale University, New Haven, CT, "Parallel Solution of the Symmetric Tridiagonal Eigenproblem"

L. Kellerher, Ohio Northern University, Ada, OH "A Graphical Interface for a Log-Linear Model"

S. Kim, Department of Chemical Engineering, University of Wisconsin, Madison, WI, "Parallel Computational Strategies for Hydrodynamic Interactions Between Complex Microstructure in Viscous Fluids"

B. Kirk, Engineering Physics and Mathematics Division, "The Neutron Diffusion Nodal Method on Dedicated Parallel Processors"

G. Liepins, Engineering Physics and Mathematics Division, "Credit Assignment for Reinforcement Learning"

G. Liepins, Engineering Physics and Mathematics Division, "Dynamic Properties of Genetic Algorithms"

R. A. Lillie, Engineering Physics and Mathematics Division, "Neutronics Calculations for the ANS Cold Source Optimization"

E. Lusk, Mathematics and Computer Science Division, Argonne National Laboratory, Argonne, IL, "Programming Parallel Computers"

A. Malloney, University of Illinois, Urbana, IL, "Performance Observability: Principle and Practice"

C. L. McCullough, Assistant Professor Electrical Engineering, University of Alabama, Huntsville, AL, "A Neural Net Adaptive Controller for a Class of Nonlinear Systems"

M. D. Morris, Engineering Physics and Mathematics Division, "Factorial Sampling Plans for Preliminary Computational Experiments"

S. Ostrouchov, University of Tennessee, Knoxville, TN, "Modeling Speedup in Parallel Sparse Matrix Factorization"

J. V. Pace, III, Engineering Physics and Mathematics Division, "JASPER—The Friendly, Elusive Ghost"

D. Pierce, Department of Computer Science, Boeing Computer Services, "Multifrontal Householder QR Factorization"

N. Platt, Center for Fluid Mechanics, Turbulence, and Computation, Brown University, Providence, RI, "An Investigation of a Kolmogorov Flow"

D. A. Poplawski, Department of Computer Science, Michigan Technological University, "Two Aspects of Parallel Program/Architecture Characterization"

D. A. Poplawski, Department of Computer Science, Michigan Technological University, "MATRIX-A Parallel Matrix Algorithm Animation Tool"

R. Powell, Allegheny College, Meadville, PA, "A Debugging Interface for a Heterogeneous Network"

V. Protopopescu, Engineering Physics and Mathematics Division, "Chaos in Linear Systems and Related Questions"

L. Reichel, Department of Mathematics, University of Kentucky, Lexington, KY, "A Hybrid GMRES Method for the Iterative Solution of Linear Systems"

C. H. Romine and T. H. Dunigan, Engineering Physics and Mathematics Division, "Short Course on Parallel Computing"

T. H. Rowan, University of Texas, Austin, TX, "Functional Stability Analysis of Numerical Algorithms"

R. T. Santoro, Engineering Physics and Mathematics Division, "Recent Progress in Analytic Combat Models"

W. E. Schiesser, Lehigh University, Bethlehem, PA, and the Superconducting Super Collider Laboratory, Dallas, TX, "Formulas for Higher-Order Spatial Derivatives in the Numerical Method of Lines"

J. Schmiedmayer, Institute for Nuclear Physics, Vienna Technical University, Austria, "Measurement at ORELA of the Electric Polarizability of the Neutron"

J. S. Scroggs, Institute for Computer Applications in Science and Engineering, NASA Langley Research Center, Hampton, VA, "Asymptotic-Induced Numerical Methods for Increased Accuracy and Computational Efficiency"

Dong Hun Shin, Carnegie-Mellon University, Pittsburgh, PA, "High Performance Mobile Robot Path Tracking"

D. Smith, Davis and Elkins College, Elkins, WA, "Acoustic Wave Scattering via Boundary Methods"

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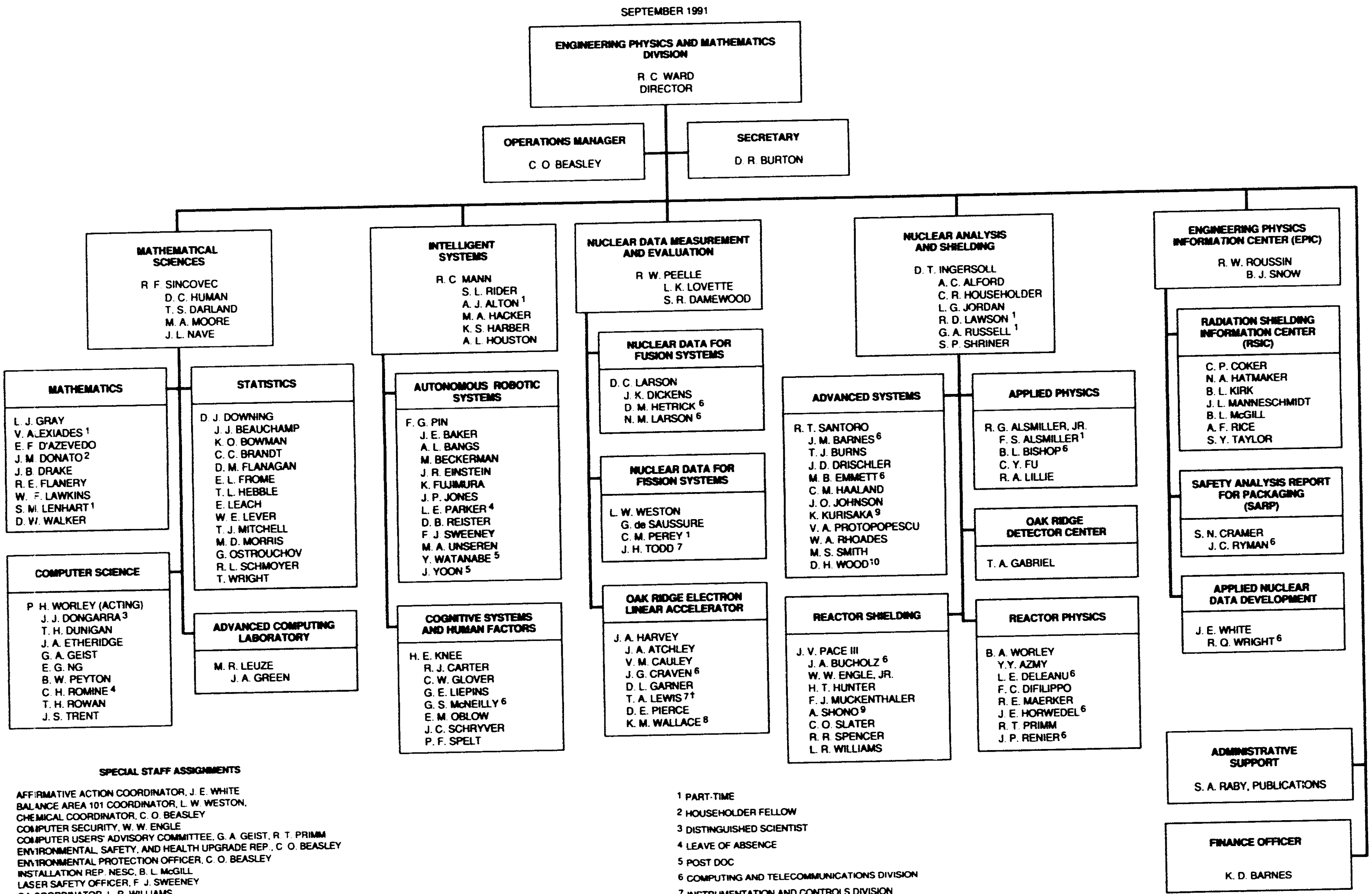

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