ORNL-6868

**OAK RIDGE
NATIONAL
LABORATORY**

**Engineering Physics
and Mathematics Division
Progress Report for Period Ending
December 31, 1994**

R. F. Sincovec, Director

**MANAGED BY
LOCKHEED MARTIN ENERGY SYSTEMS, INC.
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**ENGINEERING PHYSICS AND MATHEMATICS DIVISION
PROGRESS REPORT
FOR PERIOD ENDING DECEMBER 31, 1994**

R. F. Sincovec, Director

Date Published - July 1995

Prepared by the
OAK RIDGE NATIONAL LABORATORY
Oak Ridge, Tennessee 37831
managed by
LOCKHEED MARTIN ENERGY SYSTEMS
for the
U.S. DEPARTMENT OF ENERGY
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PREFACE

This report provides a record of the research activities of the Engineering Physics and Mathematics Division for the period January 1, 1993, through December 31, 1994. This report is the final archival record of the EPM Division. On October 1, 1994, ORELA was transferred to Physics Division and on January 1, 1995, the Engineering Physics and Mathematics Division and the Computer Applications Division reorganized to form the Computer Science and Mathematics Division and the Computational Physics and Engineering Division. Earlier reports in this series are identified on the previous pages, along with the progress reports describing ORNL's research in the mathematical sciences prior to 1984 when those activities moved into the Engineering Physics and Mathematics Division.

The primary mission of the Engineering Physics and Mathematics Division is to develop and apply in concert the principles, methods and data of the engineering, nuclear, mathematical, computational and cognitive sciences to complex research problems of national importance. Partnerships with industry and universities are sought to develop and transfer technology that will improve the nation's competitiveness. The Division's core competency R&D capabilities include: computer science, human engineering, informatics, mathematics, nuclear data measurement and evaluation, nuclear engineering, reactor physics and neutronics, and robotics.

Division staff have been active participants during the reporting period in defining, planning, and implementing the Department of Energy's (DOE) mission and goals relating to our core competencies. In addition, considerable effort has been extended in laying the groundwork for transferring technology developed in our division to the industrial sector.

As in previous reports, our research is described through abstracts of journal articles, technical reports, and presentations organized into sections following the five major operating units in the division: Mathematical Sciences, Intelligent Systems, Nuclear Data and Measurement Analysis, Nuclear Analysis and Shielding, and the Engineering Physics Information Centers. Each section begins with an introduction highlighting honors, awards, and significant research accomplishments in that unit during the reporting period.

The report concludes with appendices on personnel activity including staff additions, staff departures, and guest/short-term appointments, scientific and professional activities of division staff, technical conferences organized and/or sponsored by our division, division seminars, publications of division staff in journals, proceedings, and technical reports, papers presented by division staff at scientific meetings, and seminars by division staff. The report concludes with the division's organization chart, as of October 1, 1994, prior to the reorganizations described above.

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Section 1

MATHEMATICAL SCIENCES

1.0. INTRODUCTION

M. R. Leuze

The Mathematical Sciences Section has three main objectives: to perform research in computer science, mathematics, and statistics germane to the solution of problems of national importance; to collaborate and consult with other scientists and engineers on applications requiring computational science; and to maintain expertise in leading-edge technologies with particular attention to advanced large-scale parallel computing and heterogeneous distributed computing. The Mathematical Sciences Section actively pursues partnerships with industry and with universities to leverage our research programs and to transfer technology. In 1994, to better carry out its objectives, the Section reorganized into six groups: Algorithms, Computer Science, Mathematics, Networking, Statistics, and Visual and Information Sciences.

The research program in computer science has expanded over the past two years and now spans seven broad areas: heterogeneous distributed computing, high speed networking and information infrastructure, computational techniques for parallel applications, evaluation of prototype computer systems, software tools for high performance computing, the development of algorithms for matrix computations, and computational Grand Challenges. Highlights of our heterogeneous distributed computing research includes the continued development of PVM with new features and increased portability, and the development of a graphical interface to PVM called XPVM. Over the past two years PVM has become the world-wide de facto standard for distributed computing. This area of research also includes work on the design of the MPI specification. We have installed experimental ATM and FDDI high speed networks at ORNL. Besides testing network interoperability and performance, we have worked on video conferencing over high speed networks. The Section has a growing effort in the emerging field of information infrastructure technologies, including network protocols and security, distributed visualization and computational steering, software repositories, and client server applications. Recent work in information technologies includes the development of FaME, the Financial Automated Management Environment. We continue to develop new computational techniques and algorithms for parallel applications. A recent highlight in this area is the development of a new algorithm for materials science problems that reduces the time complexity of the application from $O(n^3)$ to $O(n)$. Over the past two years we have evaluated several new computer systems including: the Intel XPS35, KSR, IBM 590, Intel MP node, and the Cray T3D. Software tools research in conjunction with the Center for Computational Sciences has the goal of developing tools that make it easier for scientists to exploit high performance computers. Over the past two years, we continued to maintain our PICL and ParaGraph tools for visualizing the performance of applications on parallel computers. We were involved in the development of the ScaLAPACK parallel linear algebra library for distributed memory computers. We developed the DOLIB/DONIO tools that make porting applications to parallel computers easier and significantly improve the I/O performance on Intel XPS computers. We have developed HeNCE and VPE, two tools to simplify PVM programming. One highlight from this research area was the development of a prototype PVM/AVS library that allows PVM applications to incorporate interactive visualization and computational steering. Recent highlights of the algorithmic research include the development of new algorithms for symbolic factorization of sparse matrices,

the implementation of refined algorithms for numerical factorization of sparse matrices, the development and analysis of scalable algorithms for dense matrix computations, the implementation of iterative methods based on the quasi minimal residual approach, the design and development of a collection of quasi minimal residual related methods (QMRPACK), and the development and analysis of iterative techniques in the context of solving differential-algebraic equations. Five Grand Challenge problems are being worked on in conjunction with the Center for Computational Sciences: groundwater transport, first principles materials calculations, global climate modeling, numeric Tokamak, and laser ablation. These are fundamental problems of particular interest to DOE and to industry.

Research in applied mathematics during the reporting period emphasized the mathematical modeling of environmental problems and their numerical solution on parallel supercomputers. Particularly noteworthy accomplishments are (a) parallel implementation of a groundwater flow model and its application in a study of the WAG-6 waste site at ORNL; (b) improved parallel algorithms for a MIMD implementation of the Global Community Climate Model; and (c) development of optimal control techniques for application in "pump-and-treat" and bioremediation methods. Important ORNL collaborations outside the Mathematical Sciences Section have been with the Solid State Division (parallel molecular dynamics, visualization, thin film stability), Fusion Energy Division (numeric Tokamak), Environmental Sciences Division (groundwater modeling, in-situ vitrification, pore scale analysis), Engineering Physics and Mathematics Division (robotics), and Chemical Technology Division (fluid drop motion).

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 methods for estimating cumulative radiation exposures using historical data that are subject to bias and uncertainty, the development of new methods of DNA sequence analysis based on probabilistic models, the development of discrete Pearson and Johnson system of curves, the development of methodology for Bayesian design for response surface prediction, examination of the role of low pass filtering in the process of attractor reconstruction from chaotic time series data, the development of an algorithm for data-driven global model search with respect to a model optimality criterion within a large user-defined class of models, and the development of a methodology for analyzing large scientific datasets by extracting features indicative of changes in the process worthy of further investigation. 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 methods for determining optimal sampling frequencies for measuring temporal changes in water quality, estimation and testing of hypotheses concerning rare attributes in a finite universe, methods for analyzing screening test data, determination of relationships between truck accidents and measures of road geometry and activity, surveys of truck activity and commodity, statistical simulation and 3-D visualization for analysis and interpretation of soil voc data, and analysis of tree ring data and concomitant time series data to understand reasons for recent growth increases in old-growth longleaf pine trees.

The computational resources of the Mathematical Sciences Section are concentrated in the Advanced Visualization Research Center (AVRC) and the

Center for Computational Sciences (CCS), which together consist of a number of multiprocessor systems and the infrastructure required to support the use of these computers. The primary computational resource of the AVRC is an Intel iPSC/860 with 128 processors, each with 8 MBytes of local memory, and capable of sustained performance in excess of 2 Gflops. This computer is currently being used on some of ORNL's Grand Challenge problems. A high speed link connects the AVRC with the University of Tennessee (UT) Computer Science Department to facilitate the use of computers at both sites. UT computers include a CM-5 with 32 processors and a MasPar MP-2 with 4096 processors. The primary CCS computers are two Intel Paragon computers, one with 512 processors and the other with 66 processors, and a Kendall Square Research KSR-2 with 64 processors. There are a number of other smaller scalable parallel systems available plus an extensive infrastructure of Sun, IBM, and Silicon Graphics workstations on local area networks with various compute, network, file, and print servers.

COMPUTER SCIENCE

General Parallel Computing

1.1

VISUALIZATION AND DEBUGGING IN A HETEROGENEOUS ENVIRONMENT

A. Beguelin* J. J. Dongarra
A. Geist V. Sunderam†

[Abstract of *Computer* (in press)]

PVM is becoming a popular package for doing heterogeneous distributed computing. As its popularity grows so does the need to have good supporting tools for program development in PVM. This paper describes our experiences with visualization and debugging of PVM programs. It includes our early work in this field, the present research, and the future directions of our research in visualization and debugging.

Our present research revolves around the development of a graphical monitoring package called Xab. The basic concept is to instrument every PVM call so that the progress of the parallel program can be displayed in real time or saved in a tracefile for later analysis. Xab can convert its tracefiles to PICL format so that several other graphical tracing packages such as ParaGraph can be used for detailed analysis.

It is recognized that special views are required to understand the complex interactions between tasks in a heterogeneous environment. Problems of network delays and machine loads dynamically changing due to other users are important considerations in trying to debug or improve the performance of a PVM application. We present several ideas for such views and methods for debugging programs in a heterogeneous environment.

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

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1.2

NETLIB SERVICES AND RESOURCES

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S. C. Green* K. Moore*
T. H. Rowan R. C. Wade*

[Abstract of ORNL/TM-12680, April 1994]

The Netlib repository, maintained by the University of Tennessee and Oak Ridge National Laboratory, contains freely available software, documents and databases of interest to the numerical, scientific computing, and other communities. This report includes both the Netlib User's Guide and the Netlib System Manager's Guide, and contains information about Netlib's databases, interfaces, and system implementation. The Netlib repository's databases, include the Performance Database, the Conferences Database, and the NAnet mail forwarding and Whitepages Databases. A variety of user interfaces enable users to access the Netlib repository in the manner most convenient and compatible with their networking capabilities. These interfaces include the Netlib email interface, the Xnetlib X Windows client, the netlibget command-line TCP/IP client, anonymous FTP, anonymous RCP, and gopher.

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

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1.3

DONIO: DISTRIBUTED OBJECT NETWORK I/O LIBRARY

E. F. D'Azevedo C. H. Romine

[Abstract of ORNL/TM-12743, September 1994]

This report describes the use and implementation of DONIO (Distributed Object Network I/O), a library of routines that provide fast file I/O capabilities in the Intel iPSC/860 and Paragon dis-

tributed memory parallel environments. DONIO caches a copy of the file in memory distributed across all processors. Disk I/O routines (such as read, write, and lseek) are replaced by calls to DONIO routines, which translate these operations into message communication to update the cached data. Experiments on the Intel Paragon show that the cost of concurrent disk I/O using DONIO for large files can be 15–30 times smaller than using standard disk I/O.

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

1.4

DOLIB: DISTRIBUTED OBJECT LIBRARY

E. F. D'Azevedo C. H. Romine

(Abstract of ORNL/TM-12744, October 1994)

This report describes the use and implementation of DOLIB (Distributed Object Library), a library of routines that emulates global or virtual shared memory on Intel multiprocessor systems. Access to a distributed global array is through explicit calls to gather and scatter. Advantages of using DOLIB include: dynamic allocation and freeing of huge (gigabyte) distributed arrays, both C and FORTRAN callable interfaces, and the ability to mix shared-memory and message-passing programming models for ease of use and optimal performance. DOLIB is independent of language and compiler extensions and requires no special operating system support. DOLIB also supports automatic caching of read-only data for high performance. The virtual shared memory support provided in DOLIB is well suited for implementing Lagrangian particle tracking techniques. We have also used DOLIB to create DONIO (Distributed Object Network I/O Library), which obtains over a 10-fold improvement in disk I/O performance on the Intel Paragon.

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

1.5

A PROPOSAL FOR A USER-LEVEL, MESSAGE PASSING INTERFACE IN A DISTRIBUTED MEMORY ENVIRONMENT

J. J. Dongarra R. Hempel*
A. G. J. Hey† D. W. Walker

(Abstract of ORNL/TM-12231, February 1993)

This paper describes Message Passing Interface 1 (MPI1), a proposed library interface standard for supporting point-to-point message passing. The intended standard will be provided with Fortran 77 and C interfaces, and will form the basis of a standard high level communication environment featuring collective communication and data distribution transformations. The standard proposed here provides blocking, nonblocking, and synchronized message passing between pairs of processes, with message selectivity by source process and message type. Provision is made for non-contiguous messages. Context control provides a convenient means of avoiding message selectivity conflicts between different phases of an application. The ability to form and manipulate process groups permits task parallelism to be exploited, and is a useful abstraction in controlling certain types of collective communication.

Research sponsored by Applied Mathematical Sciences Research Program, U.S. DOE Office of Energy Research; by the Defense Advanced Research Projects Agency; and by the Center for Research on Parallel Computing.

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1.6

SOFTWARE DISTRIBUTION USING XNETLIB

J. J. Dongarra T. H. Rowan
R. C. Wade

(Abstract of ORNL/TM-12318, June 1993)

Xnetlib is a new tool for software distribution. Whereas its predecessor netlib uses e-mail as the user interface to its large collection of public-domain mathematical software, xnetlib uses an X Window interface and socket-based communica-

tion. Xnetlib makes it easy to search through a large distributed collection of software and to retrieve requested software in seconds.

Research sponsored by Applied Mathematical Sciences Research Program, U.S. DOE Office of Energy Research; by the Defense Advanced Research Projects Agency; and by the Army Research Office.

*University of Tennessee, Knoxville, TN.

1.7

EARLY EXPERIENCES AND PERFORMANCE OF THE INTEL PARAGON

T. H. Dunigan

(Abstract of ORNL/TM-12194, August 1994)

Experiences and performance figures are reported from early tests of the 512-node Intel Paragon XPS35 at Oak Ridge National Laboratory. Computation performance of the 50 MHz i860XP processor as well as communication performance of the 200 megabyte/second mesh are reported and compared with other multiprocessors. Single and multiple hop communication bandwidths and latencies are measured. Concurrent communication speeds and speed under network load are also measured. File I/O performance of the mesh-attached Parallel File System is measured. Early experiences with OSF/Mach and SUNMOS operating systems are reported, as well results from porting various distributed-memory applications. This report also summarizes the second phase of a Cooperative Research and Development Agreement between Oak Ridge National Laboratory and Intel in evaluating a 66-node Intel Paragon XPS5.

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

1.8

MULTI-RING PERFORMANCE OF THE KENDALL SQUARE MULTIPROCESSOR

T. H. Dunigan

(Abstract of ORNL/TM-12331, March 1994)

Performance of the hierarchical shared-memory system of the Kendall Square Research multiprocessor is measured and characterized.

The performance of prefetch is measured. Latency, bandwidth, and contention are analyzed on a 4-ring, 128 processor system. Scalability comparisons are made with other shared-memory and distributed-memory multiprocessors.

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

1.9

PARADIGMS AND STRATEGIES FOR SCIENTIFIC COMPUTING ON DISTRIBUTED MEMORY CONCURRENT COMPUTERS

I. T. Foster* D. W. Walker

[Abstract of paper presented at the High Performance Computing 1994 Conference, LaJolla, CA, April 11-15, 1994; Proc. pp. 252-257 (1994)]

In this work we examine recent advances in parallel languages and abstractions that have the potential for improving the programmability and maintainability of large-scale, parallel, scientific applications running on high performance architectures and networks. This paper focuses on Fortran M, a set of extensions to Fortran 77 that supports the modular design of message passing programs. We describe the Fortran M implementation of a particle-in-cell (PIC) plasma simulation application and discuss issues in the optimization of the code. The use of two other methodologies for parallelizing the PIC application are considered. The first is based on the shared object abstraction as embodied in the Orca language. The second approach is the Split-C language. In Fortran M, Orca, and Split-C the ability of the programmer to control the granularity of communication is important is designing an efficient implementation.

Research sponsored by the Applied Mathematical Sciences Research Program, U.S. DOE Office of Energy Research; by the Office of Scientific Computing; and by the National Science Foundation's Center for Research in Parallel Computation.

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1.10

MPI WORKSHOP**G. A. Geist**

[Abstract of paper presented at Supercomputing '93, Portland, OR, November 18, 1993; Proc. pp. 878-883 (1993)]

This paper presents an overview of MPI, a proposed standard message passing interface for MIMD distributed memory concurrent computers. The design of MPI has been a collective effort involving researchers in the United States and Europe from many organizations and institutions. MPI includes point-to-point and collective communication routines, as well as support for process groups, communication contexts, and application topologies. While making use of new ideas where appropriate, the MPI standard is based largely on current practice.

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

1.11

DISTRIBUTED COMPUTING'S FUTURE**G. A. Geist**

[Abstract of paper presented at Supercomputing '93, Portland, OR, November 18, 1993; Proc. p. 762 (1993)]

As workstations become more powerful and speed and bandwidth of networks increase, parallel computing on a network of heterogeneous systems becomes more attractive. However, heterogeneity makes effective use of resources more difficult. In this talk, we discuss the software assistance required to alleviate these difficulties.

Hiding the complexity of using network communication primitives (e.g. UNIX sockets) within a library is helpful but insufficient. Beguelin and colleagues revealed that future PVM will use the open-system approach to integrate tool modules provided in other environments. In this way, PVM will provide capabilities for debugging, profiling, performance visualization, dynamic process migration, and fault tolerance. In addition, it will support communication of multimedia and computation on MPPs.

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

1.12

PVM A PLATFORM FOR PORTABLE DISTRIBUTED COMPUTING**G. A. Geist**

(Abstract of paper presented at the High Performance Computing Conference '94, National University of Singapore, Singapore, September 29-30, 1994)

PVM (Parallel Virtual Machine) is a byproduct of the heterogeneous network research project going on at Oak Ridge National Laboratory and the University of Tennessee. It is a software package that permits a user defined collection of serial, parallel, and vector computers to appear as one large distributed memory computer. PVM's popularity is quickly making it the worldwide de facto standard for distributed computing. Applications, which can be written in FORTRAN or C, can be parallelized by using simple message-passing constructs common to most distributed-memory computers. By sending and receiving messages, subtasks of an application can cooperate to solve a problem in parallel.

This paper describes the features of the latest release of PVA (version 3.3) and describes the major new research areas we are beginning to explore in heterogeneous network computing. The paper explains how PVM version 3 opens many new opportunities in distributed computing, and how several technical and social challenges must be addressed before we can take distributed computing into the 21st century.

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

1.13

PVM 3 BEYOND NETWORK COMPUTING**G. A. Geist**

[Abstract of paper presented at the Second International Conference of the Austrian Center for Parallel Computation, Gmunden, Austria, October 4-6, 1993; Proc. Lecture Notes in Computer Science 734, pp. 194-203, J. Volkert, Ed., (1993)]

PVM (Parallel Virtual Machine) is a byproduct of the heterogeneous network research project going on at Oak Ridge National Laboratory and the University of Tennessee. It is a software package that permits a user defined collection of serial,

parallel, and vector computers to appear as one large distributed memory computer. PVM's popularity is quickly making it the worldwide de facto standard for distributed computing. Applications, which can be written in FORTRAN or C, can be parallelized by using simple message-passing constructs common to most distributed-memory computers. By sending and receiving messages, sub-tasks of an application can cooperate to solve a problem in parallel. This paper describes the features of the latest release of PVM (version 3.1) and explains the major new research areas we are beginning to explore in heterogeneous network computing. The new features of PVM version 3 open many new opportunities to go beyond simple network computing, but several technical and social issues must be addressed before we can make the next big leap in distributed computing.

Research sponsored by U.S. DOE Office of Energy Research and by the National Science Foundation and Technology Center.

1.14

THE EVOLUTION OF THE PVM CONCURRENT COMPUTING SYSTEM

G. A. Geist V. S. Sunderam*

[Abstract of paper presented at the Compcom '93 Conference, San Francisco, CA, February 25, 1993; Proc. pp. 545-553 (1993)]

Concurrent and distributed computing, using portable software systems or environments on general purpose networked computing platforms, has recently gained widespread attention. Many such systems have been developed, and several are in production use. This paper describes the evolution of the PVM system, a software infrastructure for concurrent computing in networked environments. PVM has evolved over the past three years; it is currently in use at several hundred institutions worldwide for applications ranging from scientific supercomputing to high performance computations in medicine, discrete mathematics, and databases, and for learning parallel programming. We describe the historical evolution of the PVM system, outline the programming model and supported features, present results gained from its use, list representative applications from a variety

of disciplines that PVM has been used for, and comment on future trends and ongoing research projects.

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

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1.15

XPVM: A GRAPHICAL CONSOLE AND MONITOR FOR PVM

J. A. Kohl

(Abstract of paper presented at the 1994 Scalable High Performance Computing Conference, University of Tennessee, Knoxville, TN, May 23-25, 1994)

As technology continues to spawn new supercomputing platforms and more powerful workstation environments, it becomes increasingly important to integrate and apply these diverse collections of computers together to extract the best performance possible. PVM (Parallel Virtual Machine) is gaining wide popularity as a means for realizing the computing power of these heterogeneous systems. PVM is a software package that permits a heterogeneous collection of serial, parallel and vector computers, hooked together by a network, to appear as one large distributed memory computer.

One of the primary difficulties in designing applications for distributed computer systems is identifying precisely what is happening inside a program, as multiple threads of control interact to solve a problem. Often it is useful to provide the user with feedback as to the state of the system, including tasks executing on it. XPVM is a graphical interface to PVM that provides such information to monitor executions and assist in debugging and tuning the performance of PVM programs. XPVM can be used in real time, to observe program activity as it happens, or it can play back saved traces of PVM program executions, for detailed post-mortem analysis.

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

1.16

ANALYZING PICL TRACE DATA WITH MEDEA

A. P. Merlo* P. H. Worley

[Abstract of ORNL/TM-12506, November 1993; also Seventh International Conference on Modeling Techniques and Tools for Computer Performance Evaluation, Vienna, Austria, May 4-6, 1994; Proc. pp. 445-464 Springer-Verlag (1994)]

Execution traces and performance statistics can be collected for parallel applications on a variety of multiprocessor platforms by using the Portable Instrumented Communication Library (PICL). The static and dynamic performance characteristics of performance data can be analyzed easily and effectively with the facilities provided within the MEasurements Description Evaluation and Analysis tool (MEDEA). This report describes the integration of the PICL trace file format into MEDEA. A case study is then outlined that uses PICL and MEDEA to characterize the performance of a parallel benchmark code executed on different hardware platforms and using different parallel algorithms and communication protocols.

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

*University of Pavia, Pavia, Italy.

1.17

GOPHER AND OTHER RESOURCE DISCOVERY TOOLS

G. Ostrouchov

[Abstract of *Statistical Computing and Graphics* 4(1), 16 (1993)]

Several powerful resource discovery tools were recently developed for the Internet. This article attempts to describe Gopher and some other tools of potential interest to statisticians.

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

1.18

THE KSR1: EXPERIMENTATION AND MODELING OF POSTSTORE

E. Rosti* E. Smirni†
T. D. Wagner† A. W. Apon†
L. W. Dowdy†

(Abstract of ORNL/TM-12287, February 1993)

Kendall Square Research introduced the KSR1 system in 1991. The architecture is based on a ring of rings of 64-bit microprocessors. It is a distributed, shared memory system and is scalable. The memory structure is unique and is the key to understanding the system. Different levels of caching eliminates physical memory addressing and leads to the ALLCACHETM scheme. Since requested data may be found in any of several caches, the initial access time is variable. Once pulled into the local (sub)cache, subsequent access times are fixed and minimal. Thus, the KSR1 is a Cache-Only Memory Architecture (COMA) system.

This paper describes experimentation and an analytic model of the KSR1. The focus is on the poststore programmer option. With the poststore option, the programmer can elect to broadcast the updated value of a variable to all processors that might have a copy. This may save time for threads on other processors, but delays the broadcasting thread and places additional traffic on the ring. The specific issue addressed is to determine under what conditions poststore is beneficial. The analytic model and the experimental observations are in good agreement. They indicate that the decision to use poststore depends both on the application and the current system load.

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

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1.19

BROADCASTING ON LINEAR ARRAYS AND MESHES

S. R. Seidel*

(Abstract of ORNL/TM-12356, March 1993)

The well known spanning binomial tree broadcast algorithm is generalized to obtain several broadcast algorithms for linear arrays and meshes. These generalizations take advantage of bidirectional communication, the connectivity of two-dimensional meshes, and the difference between node-to-network and network-to-network bandwidth. It is shown how these algorithms can be further generalized so that any node can be the source of the broadcast message. A partitioning scheme is given that allows these algorithms to be used on linear arrays and meshes of any size. One of these algorithms, the bidirectional spanning tree broadcast, always has lower cost than the recursive halving broadcast for linear arrays. All of these algorithms offer significant performance improvements over the basic spanning tree broadcast. These algorithms do not rely on a knowledge of machine-dependent constants for network bandwidth and latency, so their performance is not as sensitive to changes in machine characteristics as that of hybrid and pipelined algorithms. Performance measurements are given for some of these broadcast algorithms on the Intel Delta mesh.

Research sponsored by Applied Mathematical Sciences Research Program and the Atmospheric and Climate Research Division of the Office of Energy Research U.S. DOE and by NASA Ames Research Center.

*Michigan Technological University, Houghton, MI.

1.20

MEASURING THE EFFECTS OF THREAD PLACEMENT ON THE KENDALL SQUARE KSR1

T. D. Wagner* E. Smirni*
A. W. Apon* M. Madhukar*
L. W. Dowdy*

(Abstract of ORNL/TM-12462, August 1993)

This paper describes a measurement study of the effects of thread placement on memory access times on the Kendall Square multiprocessor, the KSR1. The KSR1 uses a conventional

shared memory programming model in a distributed memory architecture. The architecture is based on a ring of rings of 64-bit superscalar microprocessors. The KSR1 has a Cache-Only Memory Architecture (COMA). Memory consists of the local cache memories attached to each processor. Whenever an address is accessed, the data item is automatically copied to the local cache memory module, so that access times for subsequent references will be minimal.

If a local cache has space allocated for a particular data item, but does not have a current valid copy of that data item, then it is possible for the cache to acquire a valid read-only copy before it is requested by the local processor due to a request by a different processor that happened to pass by on the ring. This automatic prefetching can greatly reduce the average time for a thread to acquire data items. Because of the automatic prefetching, the time required to obtain a valid copy of a data item does not depend simply on the distance from the owner of the data item, but also depends on the placement and number of other processing threads which share the same data item. Also, the strategic placement of processing threads helps programs take advantage of the unique features of the memory architecture which help eliminate memory access bottlenecks for shared data sets. Experiments run on the KSR1 across a wide variety of thread configurations show that shared memory access is accelerated through strategic placement of threads which share data. The results indicate strategies for improving the performance of applications programs, and illustrate that KSR1 memory access times can remain nearly constant even when the number of participating threads increases.

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

*Vanderbilt University, Nashville, TN.

1.21

THE DESIGN OF A MESSAGE PASSING INTERFACE FOR DISTRIBUTED MEMORY CONCURRENT COMPUTERS

D. W. Walker

[Abstract of *Parallel Computing* 20, 657 (1994)]

This paper presents an overview of MPI, a proposed standard message passing interface for MIMD distributed memory concurrent computers. The design of MPI has been a collective effort involving researchers in the United States and Europe from many organizations and institutions. MPI includes point-to-point and collective communication routines, as well as support for process groups, communication contexts, and application topologies. While making use of new ideas where appropriate, the MPI standard is based largely on current practice.

Research sponsored by U.S. Department of Energy.

1.22

AN MPI VERSION OF THE BLACS

D. W. Walker

(Abstract of paper presented at the 1994 Scalable Parallel Libraries Conference, Mississippi State University, Starkville, MS, October 12-14, 1994)

In this paper, issues related to implementing an MPI version of the Basic Linear Communication Subprograms (BLACS) are investigated. A

set of routines, the MPI Linear Algebra Communication Subprograms (MLACS), are presented, and these are used to implement an MPI version of the BLACS. The MLACS provide the same functionality as the BLACS, but extend the functionality of the BLACS to include both blocking and non-blocking communication, and all four of the MPI communication modes.

Research sponsored by the U.S. Department of Energy and by ARPA administered by ARO.

1.23

THE DESIGN OF A STANDARD MESSAGE PASSING INTERFACE FOR DISTRIBUTED MEMORY CONCURRENT COMPUTERS

D. W. Walker

(Abstract of ORNL/TM-12512, October 1993)

This paper presents an overview of MPI, a proposed standard message passing interface for MIMD distributed memory concurrent computers. The design of MPI has been a collective effort involving researchers in the United States and Europe from many organizations and institutions. MPI includes point-to-point and collective communication routines, as well as support for process groups, communication contexts, and application topologies. While making use of new ideas where appropriate, the MPI standard is based largely on current practice.

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

Dense Matrix Computations

1.24

CRPC RESEARCH INTO LINEAR ALGEBRA SOFTWARE FOR HIGH PERFORMANCE COMPUTERS

J. Choi J. J. Dongarra
R. Pozo* D. C. Sorensen†
D. W. Walker

[Abstract of *International Journal of Supercomputer Applications* 8(2), 99 (1994)]

In this paper we look at a number of approaches being investigated in the Center for Research on Parallel Computation (CRPC) to de-

velop linear algebra software for high-performance computers. These approaches are exemplified by the LAPACK, templates, and ARPACK projects. LAPACK is a software library for performing dense and banded linear algebra computations, and was designed to run efficiently on high-performance computers. We focus on the design of the distributed-memory version of LAPACK, and on an object-oriented interface to LAPACK.

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

*University of Tennessee, Knoxville, TN.

†Rice University, Houston, TX.

1.25

**THE DESIGN OF A PARALLEL, DENSE
LINEAR ALGEBRA SOFTWARE
LIBRARY: REDUCTION TO
HESSENBERG, TRIDIAGONAL, AND
BIDIAGONAL FORM**

**J. Choi J. J. Dongarra
D. W. Walker**

[Abstract of paper presented at the Workshop on Environments and Tools for Parallel Scientific Computing, Wal-land, TN, May 26-27, 1994; also paper presented at the 14th IMACS World Congress on Computation and Applied Mathematics, Georgia Institute of Technology, Atlanta, GA, July 11-15, 1994; Proc. pp. 1180-1882 (1994)]

This paper addresses issues in the design and implementation of algorithms that reduce a real general matrix to Hessenberg or bidiagonal form, and a symmetric matrix to tridiagonal form. These three algorithms are part of the ScaLAPACK software library for performing dense linear algebra computations on distributed memory concurrent computers. Upon completion, ScaLAPACK ("Scalable LAPACK") will make available on distributed memory machines the same set of library routines that LAPACK provides for vector and shared memory architectures. ScaLAPACK makes use of block partitioned matrix algorithms to maximize data reuse in the upper levels of memory. A block cyclic data distribution is used to ensure good load balance as rows and columns of a matrix are eliminated from use in the course of an algorithm. ScaLAPACK routines are constructed using three sets of modules: (1) the sequential Basic Linear Algebra Subprograms (BLAS), (2) a set of Basic Linear Algebra Communication Subprograms (BLACS), and (3) the Parallel Block BLAS (PB-BLAS). The PB-BLAS are distributed Level 2 and 3 BLAS routines in which at least one of the matrix sizes is limited to the block size of the data distribution.

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

1.26

**PUMMA: PARALLEL UNIVERSAL
MATRIX MULTIPLICATION
ALGORITHMS ON
DISTRIBUTED MEMORY
CONCURRENT COMPUTERS**

**J. Choi J. J. Dongarra
D. W. Walker**

[Abstract of *Concurrency: Practice and Experience* (in press); also ORNL/TM-12252, August 1993]

This paper describes the Parallel Universal Matrix Multiplication Algorithms (PUMMA) on distributed memory concurrent computers. The PUMMA package includes not only the non-transposed matrix multiplication routine $C=A \cdot B$, but also transposed multiplication routines $C=A^T \cdot B$, $C=A \cdot B^T$, and $C=A^T \cdot B^T$, for a block scattered data distribution. The routines perform efficiently for a wide range of processor configurations and block sizes. The PUMMA together provide the same functionality as the Level 3 BLAS routine xGEMM. Details of the parallel implementation of the routines are given, and results are presented for runs on the Intel Touchstone Delta computer.

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

1.27

**PARALLEL MATRIX TRANSPOSE
ALGORITHMS ON DISTRIBUTED
MEMORY CONCURRENT COMPUTERS**

**J. Choi J. J. Dongarra
D. W. Walker**

(Abstract of ORNL/TM-12309, October 1993; also paper presented at the Scalable Parallel Libraries Conference, Mississippi State, MS, October 6-8, 1993)

This paper describes parallel matrix transpose algorithms on distributed memory concurrent processors. We assume that the matrix is distributed over a $P \times Q$ processor template with a block scattered data distribution. P , Q , and the block size can be arbitrary, so the algorithms have wide applicability.

The communication schemes of the algorithms are determined by the greatest common divisor (GCD) of P and Q . If P and Q are rel-

atively prime, the matrix transpose algorithm involves *complete exchange* communication. If P and Q are not relatively prime, processors are divided into GCD groups and the communication operations are overlapped for different groups of processors. Processors transpose GCD wrapped diagonal blocks simultaneously, and the matrix can be transposed with LCM/GCD steps, where LCM is the least common multiple of P and Q .

The algorithms make use of non-blocking, point-to-point communication between processors. The use of nonblocking communication allows a processor to overlap the messages that it sends to different processors, thereby avoiding unnecessary synchronization.

Combined with the matrix multiplication routine, $C=A \cdot B$, the algorithms are used to compute parallel multiplications of transposed matrices, $C=A^T \cdot B^T$, in the PUMMA package. Details of the parallel implementation of the algorithms are given, and results are presented for runs on the Intel Touchstone Delta computer.

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

1.28

REDUCTION TO CONDENSED FORM FOR THE EIGENVALUE PROBLEM ON DISTRIBUTED MEMORY ARCHITECTURES

J. J. Dongarra R. A. Van de Geijn*

[Abstract of *Parallel Computing* (in press)]

In this paper, we describe a parallel implementation for the reduction of general symmetric matrices to Hessenberg and tridiagonal form, respectively. The methods are based on LAPACK sequential codes and use a panel-wrapped mapping of matrices to nodes. Results from experiments on the Intel Touchstone Delta are given.

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

*University of Texas, Austin, TX.

1.29

SCALABILITY ISSUES AFFECTING THE DESIGN OF A DENSE LINEAR ALGEBRA LIBRARY

J. J. Dongarra R. A. Van de Geijn*
D. W. Walker

[Abstract of *Journal of Parallel and Distributed Computing* 22(3), 523 (1994)]

This paper discusses the scalability of Cholesky, LU, and QR factorization routines on MIMD distributed memory concurrent computers. These routines form part of the ScaLAPACK mathematical software library that extends the widely-used LAPACK library to run efficiently on scalable concurrent computers. To ensure good scalability and performance, the ScaLAPACK routines are based on block-partitioned algorithms that reduce the frequency of data movement between different levels of the memory hierarchy, and particularly between processors. The block cyclic data distribution, that is used in all three factorization algorithms, is described. An outline of the sequential and parallel block-partitioned algorithms is given. Approximate models of algorithms' performance are presented to indicate which factors in the design of the algorithm have an impact upon scalability. These models are compared with timing results on a 128-node Intel iPSC/860 hypercube. It is shown that the routines are highly scalable on this machine for problems that occupy more than about 25% of the memory on each processor, and that the measured timings are consistent with the performance model.

Research sponsored by U.S. Department of Energy.

*University of Texas, Austin, TX.

1.30

THE DESIGN OF LINEAR ALGEBRA LIBRARIES FOR HIGH PERFORMANCE COMPUTERS

J. J. Dongarra D. W. Walker

(Abstract of ORNL/TM-12404, August 1993)

This paper discusses the design of linear algebra libraries for high performance computers. Particular emphasis is placed on the development of scalable algorithms for MIMD distributed mem-

ory concurrent computers. A brief description of the EISPACK, LINPACK, and LAPACK libraries is given, followed by an outline of ScaLAPACK, which is a distributed memory version of LAPACK currently under development. The importance of block-partitioned algorithms in reducing the frequency of data movement between different levels of hierarchical memory is stressed. The use of such algorithms helps reduce the message startup costs on distributed memory concurrent computers. Other key ideas in our approach are the use of distributed versions of the Level 3 Basic Linear Algebra Subprograms (BLAS) as computational building blocks, and the use of Basic Linear Algebra Communication Subprograms (BLACS) as communication building blocks. Together the distributed BLAS and the BLACS can be used to

construct higher-level algorithms, and hide many details of the parallelism from the application developer.

The block-cyclic data distribution is described, and adopted as a good way of distributing block-partitioned matrices. Block-partitioned versions of the Cholesky and LU factorizations are presented, and optimization issues associated with the implementation of the LU factorization algorithm on distributed memory concurrent computers are discussed, together with its performance on the Intel Delta system. Finally, approaches to the design of library interfaces are reviewed.

Research sponsored by Applied Mathematical Sciences Research Program, U.S. DOE Office of Energy Research and by the Advanced Research Projects Agency administered by the Army Research Office.

Sparse Matrix Computations

1.31

ON FINDING MINIMUM-DIAMETER CLIQUE TREES

J. R. S. Blair* B. W. Peyton

[Abstract of *Nordic Journal of Computing* 1, 173 (1994)]

A clique-tree representation of a chordal graph often reduces the size of the data structure needed to store the graph, permitting the use of extremely efficient algorithms that take advantage of the compactness of the representation. Since some chordal graphs have many distinct clique-tree representations, it is interesting to consider which one is most desirable under various circumstances. A clique tree of minimum diameter (or height) is sometimes a natural candidate when choosing clique trees to be processed in a parallel-computing environment. This paper introduces a linear-time algorithm for computing a minimum-diameter clique tree.

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

*United States Military Academy, West Point, NY.

1.32

SPARSE MATRIX LIBRARIES IN C⁺⁺ FOR HIGH PERFORMANCE ARCHITECTURES

J. J. Dongarra A. Lumsdaine*
X. Niu* R. Pozo†
K. A. Remington

(Abstract of paper presented at the Object Oriented Numerics Conference, Sun River, OR, April 24-27, 1994)

We describe an object oriented sparse matrix library in C⁺⁺ designed for portability and performance across a wide class of machine architectures. Besides simplifying the subroutine interface, the object oriented design allows the same driving code to be used for various sparse matrix formats, thus addressing many of the difficulties encountered with the typical approach to sparse matrix libraries. We also discuss the design of a C⁺⁺ library for implementing various iterative methods for solving linear systems of equations. Performance results indicate that the C⁺⁺ codes are competitive with optimized Fortran.

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

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†University of Tennessee, Knoxville, TN.

1.33

SEPARATORS AND STRUCTURE PREDICTION FOR NONSYMMETRIC MATRIX FACTORIZATIONS

J. R. Gilbert* E. G. Ng

(Abstract of paper presented at the Pure and Applied Linear Algebra: The New Generation, The 3rd Conference of the International Linear Algebra Society, University of West Florida and the Pensacola Hilton Hotel, Pensacola, FL, March 17-20, 1993)

How much information about the nonzero pattern of the value of a matrix function can be determined from the nonzero pattern of the argument(s) to the function? The study of this question is sometimes called "structure prediction." Structure prediction is closely related to qualitative matrix theory. Its applications are in efficient algorithms and data structures for sparse matrix computation. Many of its tools come from graph theory: paths, connectivity, matchings, separators.

This talk will discuss some structure prediction problems for the nonsymmetric matrix factorizations $PA=LU$, $A=QR$, and their relatives. In particular, we will combine strands from several different sources to derive new lower bounds that relate the complexity of QR factorization to separators in graphs.

Research sponsored by Applied Mathematical Sciences Research Program, U.S. DOE Office of Energy Research and Xerox Palo Alto Research Center.

*Xerox Palo Alto Research Center, Palo Alto, CA.

1.34

SEPARATORS AND STRUCTURE PREDICTION IN SPARSE ORTHOGONAL FACTORIZATION

J. R. Gilbert* E. G. Ng
B. W. Peyton

[Abstract of *Linear Algebra and Its Applications* (in press)]

In the factorization $A=QR$ of a matrix A , the orthogonal matrix Q can be represented either explicitly (as a matrix) or implicitly (as a sequence of Householder vectors). We compare the nonzero counts of these two representations, for a class of matrices that arise in finite element analysis. We prove both upper and lower bounds on nonzero

counts in terms of the quality of the separators in a particular graph, the column intersection graph of A . This extends earlier work of George and Ng, who proved upper bounds on the nonzero counts of the Householder vectors in the case that A is square and has good separators.

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

*Xerox Palo Alto Research Center, Palo Alto, CA.

1.35

A COMPARISON OF SOME DIRECT METHODS FOR SOLVING SPARSE NONSYMMETRIC LINEAR SYSTEMS

E. Ng

(Abstract of paper presented at the SIAM Conference on Applied Linear Algebra, Minisymposium on Sparse Direct Methods, Snowbird, UT, June 15-18, 1994)

We survey some of the state-of-the-art algorithms for the direct solution of sparse nonsymmetric linear systems. All of these algorithms use Gaussian elimination, but they differ in the choice of data structures and in the design of the algorithms. Using test problems from the Harwell-Boeing sparse matrix collection, we compare these algorithms in terms of storage requirements and execution times.

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

1.36

SPARSITY STRUCTURE IN ORTHOGONAL FACTORIZATION

E. Ng B. W. Peyton

(Abstract of paper presented at the First Panamerican Workshop on Applied and Computational Mathematics, Caracas, Venezuela, January 11-15, 1993)

In this talk we consider the orthogonal factorization of a sparse full-rank matrix A using Householder transformations. In particular, we provide upper bounds on the structures of the following matrices: (a) the upper triangular factor R , (b) a lower trapezoidal matrix H (known as the Householder matrix), which contains the vectors for constructing the Householder transformations, and (c) the orthogonal factor Q .

We show that these bounds are right when A is a strong Hall matrix. Moreover, we show that the structure of H and Q are related. Finally we derive similar tight bounds for general Hall matrices.

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

1.37

IMPROVED SOFTWARE FOR SYMBOLIC FACTORIZATION

E. Ng B. W. Peyton

(Abstract of paper presented at the 14th Annual Meeting of the Canadian Applied Math Society, York University, North York, Ontario, Canada, May 30-June 6, 1993)

The solution of a sparse symmetric positive definite system of linear equations via sparse Cholesky factorization requires four distinct steps. The second of these, the symbolic factorization (SF) step, is the only one of the four which is run by current software packages with *a priori* knowledge of the storage requirement. The reason for this is that until recently the algorithms needed to compute the amount of storage needed was considerably more expensive in practice than the SF step itself. In this paper we present a new approach to the SF step, which is based on an efficient algorithm to compute the number of nonzeros in each row and column of the Cholesky factor introduced recently by the authors and John Gilbert. Advantages of this approach include (1) knowledge of the storage requirement prior to computation of the data structures created by SF, and (2) greater flexibility (due to greater modularity), which is valuable when the software is targeted for current high-speed workstations or vector supercomputers.

The new approach is much more efficient than the implementation found in current sparse matrix software packages. We also present a more efficient implementation of the old approach SF routine used by these packages. The new approach is only slightly less efficient than this new implementation.

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

1.38

ON THE SOLUTION OF STOKES' PRESSURE SYSTEM WITHIN N3S USING SUPERNODAL CHOLESKY FACTORIZATION

E. Ng B. Nitroso*
B. W. Peyton

(Abstract of paper presented at the VIII International Conference on Finite Elements in Fluid, Barcelona, Spain, September 20-24, 1993)

Using a splitting of the operators, the Navier-Stokes equations can be separated into an advection step and a Stokes problem. Finite element discretization of the Stokes problem results in a structured system of linear equations. In this paper we consider the solution of such a linear system using two classic algorithms due to Uzawa and Chorin. Both require solution of a reduced linear system involving a matrix of the form BB^T , where B^T corresponds to a discretization of the pressure gradient. We solve the reduced system using a sparse Cholesky factorization. We compare the performance of such an approach with other approaches available in the code N3S developed at Electricité de France. We demonstrate that the reduced linear system can be solved effectively and reliably using a sparse Cholesky factorization.

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

*Département Laboratoire National d'Hydraulique, Cedex, France.

1.39

CHORDAL-GRAPH ALGORITHMS FOR SPARSE CHOLESKY FACTORIZATION

B. W. Peyton

(Abstract of paper presented at the Seventh SIAM Conference on Discrete Mathematics, Albuquerque, NM, June 22-25, 1994)

We will discuss algorithms that take only the elimination order and the unfilled graph as input, and generate in time "almost proportional" to the input the following:

1. A depth-first spanning tree of the chordal filled graph known as the elimination tree, and
2. The size of the adjacency set of each vertex in the filled graph.

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

1.40

ON THE SOLUTION OF STOKES PRESSURE SYSTEM USING SUPERNODAL CHOLESKY FACTORIZATION

B. W. Peyton E. G. Ng
B. Nitrosso*

(Abstract of paper presented at the Society of Industrial and Applied Mathematics 18th Annual Southeastern Atlantic Section Meeting, Winston-Salem, NC, March 25-26, 1994; also paper presented at the Computer Science Colloquium, Sandia National Laboratory, Albuquerque, NM, June 20, 1994)

Using a splitting of the operators, the Navier-Stokes equations can be separated into an advection step and a Stokes problem. Finite element discretization of the Stokes problem results in a structured system of linear equations. In this talk, we consider the solution of such a linear system using two classic algorithms due to Uzawa and Chorin. Both require solution of a reduced linear system involving a matrix of the form BB' where B' corresponds to a discretization of the pressure gradient. We solve the reduced system with other approaches available in the code N3S developed at Electricite de France. We demonstrate that the reduced linear system can be solved effectively and reliably using a sparse Cholesky factorization.

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

* Cedex, France.

1.41

A CLIQUE TREE ALGORITHM FOR PARTITIONING A CHORDAL GRAPH INTO TRANSITIVE SUBGRAPHS

B. W. Peyton A. Pothen*
X. Yuan†

[Abstract of *Linear Algebra and Its Applications* (in press); also CS-93-27, University of Waterloo Technical Report, July 1993]

A partitioning problem on chordal graphs that arises in the solution of sparse triangular systems of equations on parallel computers is considered. Roughly the problem is to partition a chordal graph G into the fewest transitively orientable subgraphs over all perfect elimination orderings of G , subject to a certain precedence relationship on its vertices. In earlier work, a greedy scheme that solved the problem by eliminating a largest subset of vertices at each step was described, and an algorithm implementing the scheme in time and space linear in the number of edges of the graph was provided. Here a more efficient greedy scheme, obtained by representing the chordal graph in terms of its maximal cliques, which eliminates a subset of the leaf cliques at each step is described. Several new results about minimal vertex separators in chordal graphs, and in particular the concept of a critical separator of a leaf clique, are employed to prove that the new scheme solves the partitioning problem. We provide an algorithm implementing the scheme in time and space linear in the size of the clique tree.

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

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† IBM Canada Lab, North York, Ontario, Canada.

1.42

PARTITIONING A CHORDAL GRAPH INTO TRANSITIVE SUBGRAPHS FOR PARALLEL SPARSE TRIANGULAR SOLUTION

B. W. Peyton A. Pothen*
X. Yuan[†]

[Abstract of *Linear Algebra and Its Applications* 192, 329 (1993)]

A recent approach for solving sparse triangular systems of equations on massively parallel computers employs a factorization of the triangular coefficient matrix to obtain a representation of its inverse in product form. The number of general communication steps required by this approach is proportional to the number of factors in the factorization. The triangular matrix can be symmetrically permuted to minimize the number of factors over suitable classes of permutations, and thereby the complexity of the parallel algorithm can be minimized. Algorithms for minimizing the number of factors over several classes of permutations have been considered in earlier work. Let $F=L+L^T$ denote the symmetric filled matrix corresponding to a Cholesky factor L , and let G_F denote the adjacency graph of F . We consider the problem of minimizing the number of factors over all permutations which preserve the structure of G_F . The graph model of this problem is to partition the vertices G_F into the fewest transitively closed subgraphs over all perfect elimination orderings while satisfying a certain precedence relationship. The solution to this chordal-graph partitioning problem can be described by a greedy scheme which eliminates a largest permissible subgraph at each step. Further, the subgraph eliminated at each step can

be characterized in terms of lengths of chordless paths in the current elimination graph. This solution relies on several results concerning *transitive perfect elimination orderings* introduced in this paper. We describe a partitioning algorithm with $O(|V| + |\mathcal{E}|)$ time and space complexity.

Research sponsored by Applied Mathematical Sciences Research Program, U.S. DOE Office of Energy Research; by the Pennsylvania State University; by the Canadian Natural Sciences and Engineering Research Council; and by the University of Waterloo.

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1.43

COMPUTING ROW AND COLUMN COUNTS FOR SPARSE QR FACTORIZATION

B. W. Peyton E. Ng
J. Gilbert*

[Abstract of paper presented at the Fifth SIAM Conference on Applied Linear Algebra, Snowbird, UT, June 15-18, 1994; Proc. John G. Lewis, Ed., (1994)]

Some time ago the authors developed a fast algorithm for computing the row and column counts of a sparse Cholesky factor, using only the elimination tree and the structure of the coefficient matrix as input. Here, we modify this algorithm to obtain a fast algorithm for computing row and columns counts for sparse orthogonal factorization, again using only the elimination tree and the structure of the coefficient matrix as input.

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

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Differential Equations

1.44

TOWARD A PARALLEL RECURSIVE SPECTRAL BISECTION MAPPING TOOL

C. A. Leete B. W. Peyton
R. F. Sincovec

[Abstract of paper presented at the Sixth SIAM Conference on Parallel Processing for Scientific Computing Norfolk, VA, March 22-24, 1993; Proc. (1993)]

Recent work has shown that the recursive spectral bisection (RSB) partitioning algorithm results in good load balance and low communica-

tion costs for PDE calculations on a distributed-memory multiprocessor. We have enhanced a recent implementation of the method in the following three ways: We have (1) developed a parallel implementation, (2) used simple "proportional mapping" ideas to handle an arbitrary number of processors, and (3) implemented a more flexible load balancing technique. Our tests indicate that the latter two enhancements are quite effective. We also report timings obtained on an Intel iPSC/860.

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

Visualization

1.45

EQUATE RELATIONSHIPS IN THE IMPROV PROGRAM VISUALIZATION ENVIRONMENT

J. A. Kohl T. L. Casavant*

(Abstract of paper presented at the Workshop on Environments and Tools for Parallel Scientific Computing, Wal-land, TN, May 26-27, 1994)

Graphical views and animation can be useful tools to aid in the design and analysis of parallel programs by presenting both debugging and performance evaluation information. Many existing tools and analysis environments have provided simple but useful visualizations of parallel program behavior. Unfortunately, the construction of more sophisticated views, or even simple, custom, application-specific views, is a tedious and costly process. The IMPROV program visualization en-

vironment, under development for the past two years, serves as a platform for rapidly prototyping animated graphical views of parallel programs. Views are constructed modularly using high-level operations and an interactive, graphical, user interface. One of the advances made in IMPROV is the introduction of the *Equate* as an approach to specifying view functionality. Equates define static relationships among the variables used in constructing a dynamic view. These relationships allow automatic updates of a target *Equate* variable as the dependent variables in its *Equate* expression change. Empirical results have shown that Equates simplify and reduce the size of view specifications, as well as increase the performance of the resulting view implementations.

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

* University of Iowa, Iowa City, IA.

MATHEMATICS

Applied Mathematics

1.46

SOLIDIFICATION MODELING OF IN SITU VITRIFICATION MELTS

V. Alexiades G. K. Jacobs*

[Abstract of book chapter in *Dynamic Systems and Applications - I: Conference Proceedings 1993*, M. Sambandham, Ed. (in press)]

In Situ Vitrification is one of the promising technologies being developed by DOE to treat soil contaminated by heavy metals, radioactive and mixed waste. Contaminated soil is melted in-situ via electrodes to immobilize the contaminants in the igneous rock or glass forming upon cooling. The process creates a lava lake under controlled conditions, resembling natural magmas much better than laboratory scale experiments, and thus it is also of great interest to geologists. A well-instrumented pilot-scale test was conducted at ORNL in May 1991. Some aspects

of the analysis and interpretation of the experimental data and some of the modeling issues will be presented. In particular, a model for the cooling and solidification of the melt, viewed as a two-component magma, will be discussed. The coupled conduction-diffusion model, incorporating and fully consistent with melt thermodynamics, is formulated in a global, weak sense, similar to the enthalpy formulation of the Stefan Problem, whence front-tracking is unnecessary. The discretization is via finite-volumes and explicit in time, but we use super-time-stepping acceleration. It has been implemented in axisymmetric geometry for the Diopside-Anorthite binary, and for a Feldspar-Pyroxene pseudobinary. The simulated cooling curves will be compared with the experimental ones.

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

* Environmental Sciences Division.

1.47

CONSTRAINTS ON MASS BALANCE OF SOIL MOISTURE DURING IN SITU VITRIFICATION

V. Alexiades G. K. Jacobs*
N. W. Dunbare†

[Abstract of *Environmental Geology* 23, 83 (1994)]

In situ vitrification (ISV) is an environmental remediation technology used to melt contaminated soil sites into more stable configurations. The behavior of water and other volatile constituents in the soil-melt system is important to the overall performance of the ISV technology. Mass and volume balance constraints are used to derive a method to indirectly estimate the volume of: (1) soil which dehydrates and releases water vapor to the off-gas, and (2) outside air pulled into the off-gas treatment system. These constraints allow us to speculate on whether some water may remain in the soil rather than being completely transported into the off-gas system. The method is tested with data from a field-scale test. Results suggest that, contrary to previous conceptual models, not all water that is vaporized reaches the surface and captured by the off-gas treatment system. It is probable that some percentage remains within the soil beneath and around the molten ISV mass.

Research sponsored by Applied Mathematical Sciences and the Geosciences Programs, U.S. DOE Office of Basic Energy Sciences and Office of Technology Development.

*Environmental Sciences Division.

†New Mexico Bureau of Mines & Mineral Resources, Socorro, NM.

1.48

EFFICIENT ANALYTICAL INTEGRATION OF SYMMETRIC GALERKIN BOUNDARY INTEGRALS OVER CURVED ELEMENTS THERMAL CONDUCTION FORMULATION

C. Balakrishna* L. J. Gray
J. H. Kane*

[Abstract of *Comput. Methods Appl. Mech. Eng.* 111, 335 (1994)]

Substantial improvements are reported in the computational efficiency of Galerkin boundary element analysis (BEA) employing curved continuous boundary elements. A direct analytical treatment of the singular double integrations involved in Galerkin BEA, adapting a *limit to the boundary* concept used successfully in collocation BEA, is used to obviate significant computation in the determination of the Galerkin coefficient matrices. *Symbolic manipulation* has been strategically employed to aid in the analytical evaluation of the singular contributions to these double integrals. The analytical regularization procedure separates the potentially singular Galerkin integrands into an essentially singular but simple part, plus a regular remainder that can be integrated numerically. The finite contribution from the simplified singular term is then computed analytically. It is shown that the key to containing the explosive growth in the length of the formulae associated with such a hybrid analytical/numerical integration scheme is the strategic timing of *when* to take the limit to the boundary. This regularization also isolates the contribution from the curvature of the boundary element, thus facilitating enhanced computational efficiency in problems with many straight elements. Example problems are presented to quantify the performance of this approach. It is concluded that with these techniques, Galerkin symmetric BEA can be more efficient than its collocation-based counterpart.

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

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1.49

ARE BILINEAR QUADRILATERALS BETTER THAN LINEAR TRIANGLES?

E. F. D'Azevedo

(Abstract of ORNL/TM-12388, August 1993)

This paper compares the theoretical effectiveness of bilinear approximation over quadrilaterals with linear approximation over triangles. Anisotropic mesh transformation is used to generate asymptotically optimally efficient meshes for piecewise linear interpolation over triangles and bilinear interpolation over quadrilaterals. The theory and numerical results suggest triangles may have a slight advantage over quadrilaterals for interpolating convex data function but bilinear approximation may offer a higher order approximation for saddle-shaped functions on a well-designed mesh.

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

1.50

A MATRIX FRAMEWORK FOR CONJUGATE GRADIENT METHODS AND SOME VARIANTS OF CG WITH LESS SYNCHRONIZATION OVERHEAD

E. F. D'Azevedo V. Eijkhout*
C. H. Romine

[Abstract of paper presented at the Sixth SIAM Conference on Parallel Processing for Scientific Computing, Norfolk, VA, March 22-24, 1993; Proc. Vol. II, pp. 644-646 (1993)]

We will present a matrix framework for the conjugate gradient methods, which is expressed in terms of whole vector sequences instead of single vectors or initial parts of sequences. Using this framework, extremely concise derivations of the conjugate gradient method, the Lanczos algorithm, and methods such as GMRES, QMR, CGS, can be given. This framework is then used to present some equivalent forms of computing the inner products in the conjugate gradient and Lanczos algorithms. Such equivalent formulations can perform all inner product calculations of a single iteration simultaneously, thereby making the method more efficient in a parallel computing context.

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

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1.51

A NOTE ON OVERHAUSER ELEMENTS

L. J. Gray

[Abstract of *Boundary Element Communications* 5(2), 62 (1994)]

Overhauser elements provide a C^1 continuous approximation, and are therefore suitable for evaluating hypersingular integrals on smooth surfaces. However, this interpolation does not, in general, satisfy the constraints required for collocating strongly singular equations at a boundary corner. A modified two-dimensional Overhauser element suitable for this purpose is described herein.

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

1.52

SYMBOLIC COMPUTATION OF HYPERSINGULAR BOUNDARY INTEGRALS

L. J. Gray

[Abstract of book chapter in *Advances in Boundary Element Techniques*, Chapter 8, pp. 157-172 (1993)]

Analytical formulas for evaluating hypersingular boundary integrals can be efficiently generated by symbolic computation programs. The singular integrals can be defined in terms of a 'limit-to-the-boundary,' and this limit process can be automated by employing the Taylor-Laurent series expansion capabilities of these programs. As a check on the calculations, the potentially divergent terms which arise in the theory can also be calculated by this method and shown to cancel. The symbolic computation procedure is illustrated for the hypersingular kernels of the two dimensional elastic wave equation.

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

1.53

MORPHOLOGICAL STABILITY OF THIN FILMS

L. J. Gray M. F. Chisholm*
T. Kaplan*

[Abstract of paper presented at the BETECH-93 (Boundary Element Technology) Vilamoura, Portugal, November 9-11, 1993; Proc. Boundary Element Technology VIII, pp. 181-190, H. Pina and C. A. Brebbia, Eds., Computational Mechanics Publications (1993)]

The boundary element method for elastostatics is applied to a thin film stability problem arising in solid state surface science. An aim of this work is to determine the morphology of germanium deposited on a silicon substrate. Nonstandard boundary conditions at the material interface are used to model the epitaxially grown film. In addition to determining the deformed geometry it is also necessary to compute the surface stress tensor. Although the surface displacement at the junction between the interface and the silicon free surface is not differentiable, the hypersingular integral equation for surface stress can still be employed. These techniques will be described, along with results from two-dimensional calculations.

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

*Solid State Division.

1.54

HYPERSINGULAR INTEGRALS AT A CORNER

L. J. Gray L. L. Manne*

[Abstract of paper presented at the BEM (Boundary Element Methods) 15 Conference, Worcester, MA, August 10-12, 1993]

For a smooth boundary, hypersingular integrals can be defined as a limit from the interior, the approach direction being taken, for convenience, normal to the surface. At a boundary corner, the limit process, with a necessarily non-normal approach direction, provides a valid definition of the hypersingular equation, as long as the same direction is employed for all integrations. The terms which are potentially singular in the limit are shown to cancel, provided the function approximations at the corner are consistent.

The analytical formulas for the singular integrals are more complicated than for a smooth surface, but are easily obtained using symbolic computation. These techniques have been employed to accurately solve the "L-shaped domain" potential problem considered by Jaswon and Symm.

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

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1.55

CRACK PROPAGATION MODELING

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E. D. Lutz* P. Wawrzynek*
L. F. Martha* A. R. Ingraffea*

[Abstract of *Mathematical Models and Methods in Applied Science* 4(2), 179 (1994)]

In this paper, we review recent advances in mathematical and computer science techniques for modeling crack propagation in solids. The fracture mechanics aspect of this problem is attacked by boundary integral equation methods, in particular the use of hypersingular integral equations for analyzing crack geometries. Key issues in the development of a software system capable of efficient crack propagation studies are also discussed. As an illustration of these techniques, calculations analyzing crack growth in a fuel door hinge on the Space Shuttle are presented.

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

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1.56

THE APPLICATION OF OPTIMAL CONTROL METHODOLOGY TO BIOREMEDIATION PROCESSES

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A. D. Solomon†

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

An increasingly attractive means of remediating a contaminated site is via in-situ bioremediation (ISB). This is based on the fact that one often finds bacteria indigenous to the site whose metabolic processes result in a breakdown of the

contaminant. In such a case ISB consists of injecting nutrients into the soil at the site, activating the bacterial colonies and raising the rate of contaminant degradation to a level high enough to clean the site. Models of the ISB process are based on differential equations; the level of nutrient is the control variable. We solve the optimal control problem for two specific ISB models.

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

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1.57

ANALYTICAL TREATMENT OF SYMMETRIC GALERKIN BIEs

J. H. Kane* L. J. Gray
C. Balakrishna*

[Abstract of paper presented at the International Symposium on Boundary Element Methods (IABEM-93), University of Braunschweig, Germany, August 23-26, 1993]

At IABEM-92, and later Balakrishna and Kane described a 2D symmetric Galerkin BEA formulation that facilitated the use of curved elements for thermal conduction and elasticity problems. The key to this new formulation was the employment of a regularized (via simple solutions) response and response gradient boundary integral equations (BIEs) and a polar transformation over a doubly integrated intrinsic patch. These works thus demonstrated that Galerkin BEA could be extended to employ curved elements and that such formulations had the potential for computational efficiency in the limit of refined models. However, these five term regularized BIEs were more complex than their unregularized counterparts, and their utilization involved the integration of contributions to near diagonal coefficients from all element pairs. In this paper, an approach that obviates the need for such extra computations is described.

Substantial improvements are reported in the computational efficiency of Galerkin boundary element analysis (BEA) employing curved continuous boundary elements. A direct analytical treatment of the singular double integrations involved in Galerkin BEA, adapting a limit to the boundary concept used successfully in collocation BEA,

is used. Symbolic manipulation has been strategically employed to aid in the analytical evaluation of the singular contributions to these double integrals. The key to containing the explosive growth in the length of the formulae associated with this hybrid analytical/numerical integration scheme is shown to be the strategic timing of when to take the limit to the boundary. This regularization is also shown to isolate the contribution from the curvature of the boundary element, thus facilitating enhanced computational efficiency in problems with many straight elements. Both thermal and elastic formulations are presented. Example problems are presented and it is concluded that with these techniques, Galerkin symmetric BEA can be more efficient than its collocation-based counterpart.

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

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1.58

RESTRICTED APPLICABILITY OF ONSAGER'S RECIPROCITY RELATIONS TO INTERFACE MOTION

T. Kaplan* M. J. Aziz†
L. J. Gray

[Abstract of *Journal of Chemical Physics* (in press)]

Onsager's reciprocity relations have been applied to the motion of a planar interface in a phase transformation in a two-component system, in order to provide a test of kinetic models of alloy solidification. Although applicable to such models in general, Onsager's relations yield no information for a subclass of models in which the thermodynamic driving forces are linearly dependent to first order, as is the case for several models of alloy solidification including the continuous growth model (CGM) of Aziz and Kaplan. As a consequence, experimental tests will likely be required to distinguish between these models. If the CGM is generalized to include diffusion in the growing phase, Onsager's relations are applicable under some circumstances.

Research sponsored by U.S. DOE Division of Materials Sciences.

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1.59

OPTIMAL CONTROL OF A CONVECTIVE-DIFFUSIVE FLUID PROBLEM

S. M. Lenhart

[Abstract of *Quarterly of Mathematical Models and Methods in Applied Sciences* (in press)]

We consider optimal control of a parabolic differential equation, modeling one-dimensional fluid flow through a soil-packed tube in which a contaminant is initially distributed. A fluid is pumped through the tube to remove the contaminant. The convective velocity due to the fluid pumping is the control. The goal is to minimize a performance criterion which is a combination of the total contaminant at the final time and the cost of the control. The optimal control is characterized by an optimality system.

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

1.60

OPTIMAL CONTROL FOR COMPETITIVE - COOPERATIVE SYSTEMS: MODELING FLEXIBLE COALITIONS IN TOMORROW'S COMPETITIVE WORLD

S. M. Lenhart V. Protopopescu

(Abstract of paper presented at the 61st Military Operations Research Society Symposium, Wright-Patterson Air Force Base, Dayton, OH, June 22-24, 1993)

The last years have witnessed a dramatic shift of the world's military, political, and economic paradigm from a bi-polar gridlock to a more fluid, multi-player environment. This change has necessarily been followed by a re-evaluation of the strategic thinking and by a reassessment of mutual positions, options, and decisions. The essential attributes of the new situation are modeled by a system of nonlinear evolution equations with competitive/cooperative interactions. The mathematical setting is quite general to accommodate models related to military confrontation, arms control, economic competition, political negotiations, etc. Irrespective of the specific details, all these situations share a common denominator, namely the presence of various players with differ-

ent and often changing interests and goals. The interests, ranging from conflicting to consensual, are defined in a context of interactions between the players that vary from competitive to cooperative. Players with converging interests tend to build up cooperative coalitions while coalitions with diverging interests usually compete among themselves, but this is not an absolute requirement (namely, one may have groups with converging interests and competitive interactions, and vice-versa). Appurtenance to a coalition may change in time according to the shift in one's perceptions, interests, or obligations. During the time evolution, the players try to modify their strategies as to best achieve their respective goals. An objective functional quantifying the rate of success (payoff) vs. effort (cost) measures the degree of goal attainment for all players involved, thus selecting an optimal strategy based on optimal controls. While the technical details may vary from problem to problem, the general approach described here establishes a standard framework for a host of concrete situations that may arise from tomorrow's "next competition."

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

1.61

OPTIMAL CONTROL FOR COMPETING COALITIONS

S. M. Lenhart V. Protopopescu
A. A. Szpiro*

[Abstract of *Journal of Differential and Integral Equations* (in press)]

We consider the optimal control problem for a game consisting of two competing coalitions that in turn are held together by cooperative interactions. The dynamics are described by a nondegenerate semilinear parabolic system and the controls are the nonhomogeneous terms (sources). Under reasonable assumptions on the interactions we prove the existence and uniqueness of the optimal solution of the game as the saddle point of the associated objective functional. The saddle point can be characterized in terms of the unique solution to an optimality system.

Research sponsored U.S. Department of Energy.

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1.62

MODELING OF THERMAL, ELECTRONIC, HYDRODYNAMIC, AND DYNAMIC DEPOSITION PROCESSES FOR PULSED-LASER DEPOSITION OF THIN FILMS

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R. F. Wood* D. B. Geohegan*
J. M. Donato K. R. Chen†
A. A. Puretzky*

(Abstract of paper presented at the Fall Meeting of the Materials Research Society, Boston, MA, November 28–December 2, 1994)

Various physical processes during laser ablation of solids for pulsed-laser deposition (PLD) are studied using a variety of computational techniques. In the course of our combined theoretical and experimental effort, we have been trying to work on as many aspects of PLD processes as possible, but with special focus on the following areas: (a) the effects of collisional interactions between the particles in the plume and in the background on the evolving flow field and on thin film growth, (b) interactions between the energetic particles and the growing thin films and their effects on film quality, (c) rapid phase transformations through the liquid and vapor phases under possibly nonequilibrium thermodynamic conditions induced by laser-solid interactions, (d) breakdown of the vapor into a plasma in the early stages of ablation through both electronic and photoionization processes, (e) hydrodynamic behavior of the vapor/plasma during and after ablation. The computational techniques used include finite difference (FD) methods, particle-in-cell model, and atomistic simulations using molecular dynamics (MD) techniques.

Research sponsored by U.S. DOE, Division of Materials Sciences.

*Solid State Division.

†Fusion Energy Division.

1.63

ANALYTIC EVALUATION OF SINGULAR BOUNDARY INTEGRALS WITHOUT CPV

E. Lutz* L. J. Gray

[Abstract of *Commun. Numer. Methods in Engineering* 9, 909 (1993)]

Boundary integral equations are generally derived by employing a Cauchy Principal Value definition for the singular integral involving the derivative of the Green's function. As a consequence, evaluation of this integral requires special attention, and computing the associated "solid angle coefficient" can often pose difficulties. As discussed herein, these problems can be avoided by defining the integral directly, in terms of a limit to the boundary. This approach leads to a straightforward evaluation procedure.

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

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1.64

USE OF 'SIMPLE SOLUTIONS' FOR BOUNDARY INTEGRAL METHODS IN ELASTICITY AND FRACTURE ANALYSIS

E. Lutz* A. R. Ingraffea†
L. J. Gray

[Abstract of *Int. J. Numer. Methods Eng.* 35, 1737 (1992)]

The 'simple solutions' or 'indirect' method of analyzing Cauchy and hypersingular integrands in the gradient (flux or traction) boundary integral equation (BIE) is applied to linear elastic fracture analysis. Because of the geometric singularity of the crack surface, application of the simple solutions formulas on the crack face requires integration over a temporary 'closure surface' rather than the remainder of the body. Closure surface constructions are exhibited for crack surfaces, allowing the gradient BIE to be applied as a constraint equation on a crack surface where the primary BIE is degenerate. Computational results are given for two benchmark fracture problems.

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

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1.65

HEAT TRANSFER ANALYSIS OF A FIELD-SCALE MELTING EXPERIMENT

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G. K. Jacobs†

[Abstract of *Int. Comm. Heat Mass Transfer* 20, 793 (1993)]

Heat transfer analysis was used to evaluate conceptual models of processes associated with In Situ Vitrification (ISV). ISV is a phase-change process used to melt contaminated soil sites into more stable configurations for environmental restoration. Using data from a field-scale ISV test we develop relations that allow us to estimate the temperature of the melt from voltage and amperage measurements. The calculated temperatures are in excellent agreement with measured values. A global heat balance calculation is used to account for heats of several processes that occur as soil is heated up and melted during ISV. This analysis yields an efficiency of 33% for the ISV process. Most of the heat is lost from the surface of the melt, and heat transfer concepts confirm that radiative heat transfer is the dominant process.

Research sponsored U.S. DOE Applied Mathematical Sciences and the Geosciences Programs.

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†Environmental Sciences Division.

1.66

POINTWISE ERROR ESTIMATES FOR BOUNDARY ELEMENT CALCULATIONS

V. Zarikian* L. J. Gray
G. H. Paulino†

[Abstract of book chapter in *Boundary Element Technology IX*, Eds., C. A. Brebbia and A. J. Kassab, Computational Mechanics Publications (in press)]

An essential ingredient for all adaptive boundary integral methods is a reliable estimate of the local error. This paper investigates an *a posteriori* error indicator based upon the evaluation of hypersingular equations. Computational experiments were performed for the two dimensional Laplace equations on interior and exterior domains, employing Dirichlet, Neumann, and mixed boundary conditions. The results indicate that the error indicator successfully tracks the form of the exact error curve. Moreover, a reasonable estimate of the magnitude of the error was also obtained.

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

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Numerical Analysis

1.67

IMPLEMENTATION AND PARALLELIZATION OF FAST MATRIX MULTIPLICATION FOR A FAST LEGENDRE TRANSFORM

W. Chen*

(Abstract of ORNL/TM-12285, September 1993)

An algorithm was presented by Alpert and Rokhlin for the rapid evaluation of Legendre transform. The fast algorithm can be expressed as a matrix-vector product followed by a fast cosine transform. Using the Chebyshev expansion to approximate the entries of the matrix and exchange-

ing the order of summations reduced the time complexity of computation from $O(n^2)$ to $O(n \log n)$, where n is the size of the input vector. Our work has been focused on the implementation and the parallelization of the fast algorithm of matrix-vector product. Results have shown the expected performance of the algorithm. Precision problems which arise as n becomes large can be resolved by doubling the precision of the calculation.

Research sponsored jointly by the Great Lake Colleges Association/Associated Colleges of the Midwest and the U.S. Department of Energy CHAMMP Program of the Office of Health and Environmental Research.

*Denison University, Granville, OH.

1.68

ARE BILINEAR QUADRILATERALS BETTER THAN LINEAR TRIANGLES?

E. F. D'Azevedo

[Abstract of *IMA Journal on Numerical Analysis* (in press)]

This paper compares the theoretical effectiveness of bilinear approximation over quadrilaterals with linear approximation over triangles. Anisotropic mesh transformation is used to generate asymptotically optimally efficient meshes for piecewise linear interpolation over triangles and bilinear interpolation over quadrilaterals. The theory and numerical results suggest triangles may have a slight advantage over quadrilaterals for interpolation convex data function but linear approximation may offer a higher order approximation for saddle-shaped functions on a well-designed mesh.

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

1.69

THE FOURIER ANALYSIS TECHNIQUE AND ϵ -PSEUDO-EIGENVALUES

J. M. Donato

[Abstract of *Linear Algebra and Its Applications* (in press); also ORNL/TM-12347, July 1993]

The spectral radii of iteration matrices and the spectra and condition numbers of preconditioned systems are important in forecasting the convergence rates for iterative methods. Unfortunately, the spectra of iteration matrices or preconditioned systems is rarely easily available. The Fourier analysis technique has been shown to be a useful tool in studying the effectiveness of iterative methods by determining approximate expressions for the eigenvalues or condition numbers of matrix systems.

For non-symmetric matrices the eigenvalues may be highly sensitive to perturbations. The spectral radii of nonsymmetric iteration matrices may not give a numerically realistic indication of the convergence of the iterative method. Trefethen and others have presented a theory on the use of ϵ -pseudo-eigenvalues in the study of matrix equations.

For Toeplitz matrices, we show that the theory of ϵ -pseudo-eigenvalues includes the Fourier analysis technique as a limiting case. For non-Toeplitz matrices, the relationship is not clear. We shall examine this relationship for non-Toeplitz matrices that arise when studying preconditioned systems for methods applied to a two-dimensional discretized elliptic differential equation.

Research sponsored by the Applied Mathematical Sciences Research Program, U.S. DOE Office of Energy Research and by the National Aeronautics and Space Administration.

1.70

A COMPARISON OF ITERATIVE METHODS FOR A MODEL COUPLED SYSTEM OF ELLIPTIC EQUATIONS

J. M. Donato

(Abstract of ORNL/TM-12447, August 1993)

Many interesting areas of current industry work deal with non-linear coupled systems of partial differential equations. We examine iterative methods for the solution of a model two-dimensional coupled system based on a linearized form of the two carrier drift-diffusion equations from semiconductor modeling. Discretizing this model system yields a large non-symmetric indefinite sparse matrix.

To solve the model system various point and block methods, including the hybrid iterative method Alternate Block Factorization (ABF), are applied. We also employ GMRES with various preconditioners, including block and point incomplete LU (ILU) factorizations.

The performance of these methods is compared. It is seen that the preferred ordering of the grid variables and the choice of iterative method are independent upon the magnitudes of the coupling parameters. For this model, ABF is the most robust of the non-accelerated iterative methods. Among the preconditioners employed with GMRES, the blocked "by grid point" version of both the ILU and MILU preconditioners are the most robust and the most time efficient over the wide range of parameter values tested. This information may aid in the choice of iterative methods and preconditioners for solving more complicated, yet analogous, coupled systems.

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

1.71

NUMERICAL MODELING OF PLASMA DYNAMICS IN LASER ABLATION PROCESSES

J. M. Donato J.-N. Leboeuf*
C.-L. Liu[†] R. F. Wood[†]

(Abstract of paper presented at the SIAM Annual Conference, San Diego, CA, July 25-29, 1994)

Laser ablation is rapidly becoming the method of choice for thin film deposition of novel materials, such as High-Tc compounds, Diamonds from graphite, and Fullerenes from graphite. We currently model the creation of the plume by laser-materials interactions and the transport of the plume towards the substrate. The equations are similar to the Euler equations for gas dynamics in one-dimension but with laser energy input which varies over time. We present results comparing a first order non-dissipative Rusanov scheme with a first order coupled upwind scheme for the solution of the gas dynamics equations. We are able to detect the creation of the plume and its expansion towards the deposition substrate. Important physical metrics such as the temperature and absorption coefficients are calculated and compared with experimental data. Through the numerical modeling we expect to improve refinements in the laser ablation process by suppressing large particulates and enhancing the uniformity of the deposited film.

Research sponsored by U.S. DOE Office of Fusion Energy.

*Fusion Energy Division.

[†]Solid State Division.

1.72

BOUNDARY ELEMENTS ON DISTRIBUTED MEMORY ARCHITECTURES

R. E. Flanery L. J. Gray
J. B. Drake

[Abstract of *International Journal for Numerical Methods in Engineering* (in press)]

Previous distributed memory parallel algorithms for boundary integral analysis have assigned each processor the task of computing com-

plete rows of the coefficient matrices. This decomposition can lead to load imbalance, and is potentially too coarse grained for massively parallel machines. This paper investigates the performance of a "block oriented" algorithm in which processors are required to compute a particular block of matrix elements. As opposed to the row decomposition approach, the matrix construction phase of the calculations now involves some communication between processors. Computational experiments for two-dimensional elastodynamics problems demonstrate that this algorithm can obtain high efficiencies for large scale calculations.

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

1.73

A NEW KRYLOV-SUBSPACE METHOD FOR SYMMETRIC INDEFINITE LINEAR SYSTEMS

R. W. Freund* N. M. Nachtigal

(Abstract of ORNL/TM-12754, October 1994)

Many important applications involve the solution of large linear systems with symmetric, but indefinite coefficient matrices. For example, such systems arise in incompressible flow computations and as subproblems in optimization algorithms for linear and nonlinear programs. Existing Krylov-subspace iterations for symmetric indefinite systems, such as SYMMLQ and MINRES, require the use of symmetric positive definite preconditioners, which is a rather unnatural restriction when the matrix itself is highly indefinite with both many positive and many negative eigenvalues. In this note, we describe a new Krylov-subspace iteration for solving symmetric indefinite linear systems that can be combined with arbitrary symmetric preconditioners. The algorithm can be interpreted as a special case of the quasi-minimal residual method for general non-Hermitian linear systems, and like the latter, it produces iterates defined by a quasi-minimal residual property. The proposed method has the same work and storage requirements per iteration as SYMMLQ or MINRES, however, it usually converges in considerably fewer iterations. Results of numerical experiments are reported.

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

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1.74

A LOOK-AHEAD VARIANT OF TFQMR

R. W. Freund* N. M. Nachtigal

(Abstract of paper presented at the Colorado Conference on Iterative Methods, Breckenridge, CO, April 5-9, 1994)

Recently, Freund proposed a Krylov subspace iteration, the transpose-free quasi-minimal residual method (TFQMR), for solving general non-singular non-Hermitian linear systems. The algorithm relies on a version of the squared Lanczos process to generate the basis vectors for the underlying Krylov subspace. It then constructs iterates defined by a quasi-minimization property, which leads to a smooth and nearly monotone convergence behavior. We investigate a variant of TFQMR that uses look-ahead to avoid some of the problems associated with breakdowns in the underlying squared Lanczos procedure, and we compare this method to the original algorithm.

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

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1.75

QMRPACK AND APPLICATIONS

R. W. Freund* N. M. Nachtigal

[Abstract of ORNL/TM-12753, October 1994; also paper presented at the Fifth SIAM Conference on Applied Linear Algebra, Snowbird, UT, June 15-18, 1994; Proc. John G. Lewis, Ed., (1994)]

QNIRPACK is a package of quasi-minimal residual algorithms for the iterative solution of linear systems. In this paper, we describe the main features of QMRPACK, comment on the implementations found in the package, and discuss how they would be invoked in a user code. We briefly describe two applications of the codes in the area of simulation of material properties from first principles, and in circuit simulation. We conclude by presenting future directions for QMRPACK.

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

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1.76

QMRPACK USER'S GUIDE

R. W. Freund* N. M. Nachtigal
J. C. Reeb†

(Abstract of ORNL/TM-12807, October 1994)

QMRPACK is a library of FORTRAN 77 sub-routines that may be used to solve linear systems of equations with the quasi-minimal residual (QMR) method and to compute eigenvalue approximations. This User's Guide is designed to be an overview of the codes contained in QMRPACK. Installation information is provided, and the example matrix format is discussed. The relative merits of each algorithm, as well as usage criterion are described. We also provide instructions for making the test drivers, as well as test output from several machines.

Research sponsored by Applied Mathematical Sciences Research Program, U.S. DOE Office of Energy Research and by Research Institute for Advanced Computer Science (RI-ACS).

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1.77

RECENT DEVELOPMENTS IN PARALLEL METHOD OF LINES SOLUTIONS OF PARTIAL DIFFERENTIAL EQUATIONS

W. F. Lawkins E. G. Ng
S. Thompson*

(Abstract of paper presented at the 14th IMACS World Congress on Computation and Applied Math, Georgia Institute of Technology, Atlanta, GA, July 11-15, 1994)

We present a summary of recent and ongoing attempts to exploit parallelism in the numerical solution of method of lines (MOL) problems in partial differential equations (PDEs). MOL is an established technique for solving PDEs. The success of MOL depends in part on the choice of the spatial differentiation scheme(s) used to reduce PDEs to systems or ordinary differential equations (ODEs) and in part on the use of high quality ODE solvers to integrate the resulting systems. There are several such ODE solvers available. Some of the best include DDRIV3, LSODE, and VODE. The primary expense associated with

the use of ODE solvers is the formation of the Jacobian matrix and the linear algebra required to solve the corrector equations. For dense systems, it is not uncommon for these two stages in the solution to account for virtually all of the execution time required to solve a problem in this fashion. Even when problem structure (e.g., sparsity) is exploited, these operations often account for most of the execution time required.

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

*Radford University, Radford, VA.

1.78

BOUNDS FOR EIGENVALUES AND DEPARTURE FROM NORMALITY, WITH APPLICATIONS

S. L. Lee

[Abstract of paper presented at the Fifth SIAM Conference on Applied Linear Algebra, Snowbird, UT, June 15-18, 1994; Proc. John G. Lewis, Ed., pp. 509-511 (1994)]

Bounds for the departure from normality and the Frobenius norm of the eigenvalues of a matrix are given. The important properties of these bounds are also described.

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

1.79

A PRACTICAL UPPER BOUND FOR DEPARTURE FROM NORMALITY

S. L. Lee

[Abstract of *SIAM Journal on Matrix Analysis & Application* (in press); also ORNL/TM-12426, August 1993]

The departure from normality of a matrix is a real scalar that is impractical to compute if a matrix is large and its eigenvalues are unknown. A simple formula is presented for computing an upper bound for departure from normality in the Frobenius norm. This new upper bound is cheaper to compute than the upper bound derived by Henrici [*Numer. Math.* 4, 24-40 (1962)]. Moreover, the new bound is sharp for Hermitian matrices, skew-Hermitian matrices and, in general, any matrix with eigenvalues that are horizon-

tally or vertically aligned in the complex plane. In terms of applications, the new bound can be used in computing bounds for eigenvalue perturbations or bounds for the spectral norm of matrix functions.

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

1.80

A NOTE ON THE TOTAL LEAST SQUARES PROBLEM FOR COPLANAR POINTS

S. L. Lee

(Abstract of ORNL/TM-12852, September 1994)

The Total Least Squares (TLS) fit to the points (x_k, y_k) , $k = 1, \dots, n$, minimizes the sum of the squares of the *perpendicular* distances from the points to the line. This sum is the TLS error, and minimizing its magnitude is appropriate if x_k and y_k are uncertain. A priori formulas for the TLS fit and TLS error to coplanar points were originally derived by Pearson, and they are expressed in terms of the mean, standard deviation and correlation coefficient of the data. In this note, these TLS formulas are derived in a more elementary fashion. The TLS fit is obtained via the ordinary least squares problem and the algebraic properties of complex numbers. The TLS error is formulated in terms of the triangle inequality for complex numbers.

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

1.81

BOUNDS FOR DEPARTURE FROM NORMALITY AND THE FROBENIUS NORM OF MATRIX EIGENVALUES

S. L. Lee

(Abstract of ORNL/TM-12853, December 1994)

New lower and upper bounds for the departure from normality and the Frobenius norm of the eigenvalues of a matrix are given. The significant properties of these bounds are also described. For example, the upper bound for matrix eigenvalues improves upon the one derived by Kress, de Vries,

and Wegmann in *Lin. Alg. Appl.* 8, 109-120 (1974). The upper bound for departure from normality is sharp for any matrix whose eigenvalues are collinear in the complex plane. Moreover, the latter formula is a practical estimate that costs (at most) $2m$ multiplications, where m is the number of nonzeros in the matrix. In terms of applications, the results can be used to bound from above the sensitivity of eigenvalues to matrix perturbations or bound from below the condition number of the eigenbasis of a matrix.

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

1.82

PARALLEL FAST FOURIER TRANSFORMS FOR NON POWER OF TWO DATA

B. D. Semeraro

(Abstract of paper presented at the Intel Users Group Meeting, San Diego, CA, June 26-29, 1994)

This report deals with parallel algorithms for computing discrete Fourier transforms of real sequences of length N not equal to a power of two.

The method described is an extension of existing power of two transforms to sequences with N a product of small primes. In particular, this implementation requires $N = 2^p 3^q 5^r$. The communication required is the same as for a transform of length $N = 2^p$.

The algorithm presented is intended for use in the solution of partial differential equations, or in any situation in which a large number of forward and backward transforms must be performed and in which the Fourier Coefficients need not be ordered. This implementation is a one dimensional FFT but the techniques are applicable to multidimensional transforms as well. The algorithm has been implemented on a 128 node Intel Ipsc/860.

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

Global Climate Modeling

1.83

GRAND CHALLENGE COMPUTING: STATUS AND PROSPECTS FOR CLIMATE MODELING

J. B. Drake

(Abstract of paper presented at the Intel Super Computer User's Group Meeting, St. Louis, MO, March 15, 1993)

A climate modeling project using the Intel Paragon reveals the state of parallel computing and identifies issues yet to be resolved. A brief overview of a parallel version of the NCAR Community Climate Model, CCM2, implemented for MIMD parallel computers using a message-passing programming paradigm is described. Performance

numbers on computationally intensive kernels indicate that the i860 compilers are doing a reasonable job of optimizing code. Coarse grained decompositions using around 100 processors show good parallel performance while the use of a larger number of processors is impeded by low communication speeds and load imbalance. Climate models generate large quantities of data, some as temporary files and some to be archived. The need for high I/O speeds during the execution of a climate model can be partially offset by a large local memory on each node. Other issues remain, however, for the production use of climate models in a highly parallel computing environment.

Research sponsored by U.S. Department of Energy.

1.84

PARALLELIZING THE SPECTRAL TRANSFORM METHOD: A COMPARISON OF ALTERNATIVE PARALLEL IMPLEMENTATIONS

I. T. Foster * P. H. Worley

[Abstract of paper presented at the Sixth SIAM Conference on Parallel Processing for Scientific Computing, Norfolk, VA, March 22-24, 1993; Proc. pp. 100-107 (1993)]

The spectral transform method is a standard numerical technique for solving partial differential equations on the sphere and is widely used in global climate modeling. In this paper, we outline different approaches to parallelizing the method and describe experiments that we are conduct-

ing to evaluate the efficiency of these approaches on parallel computers. The experiments are conducted using a testbed code that solves the nonlinear shallow water equations on a sphere, but are designed to permit evaluation in the context of a global model. They allow us to evaluate the relative merits of the approaches as a function of problem size and number of processors. The results of this study are guiding ongoing work on PCCM2, a parallel implementation of the Community Climate Model developed at the National Center for Atmospheric Research.

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

* Argonne National Laboratory, Argonne, IL.

Computational Distribution Theory

1.85

PARALLEL ALGORITHMS FOR THE SPECTRAL TRANSFORM METHOD

I. T. Foster* P. H. Worley

[Abstract of *SIAM Journal on Scientific Computing* (in press); also ORNL/TM-12507, April 1994]

The spectral transform method is a standard numerical technique for solving partial differential equations on a sphere and is widely used in atmospheric circulation models. Recent research has identified several promising algorithms for implementing this method on massively parallel computers; however, no detailed comparison of the different algorithms has previously been attempted. In this paper, we describe these different parallel algorithms and report on computational experiments that we have conducted to evaluate their efficiency on parallel computers. The experiments used a testbed code that solves the nonlinear shallow water equations on a sphere; considerable care was taken to ensure that the experiments provide a fair comparison of the different algorithms and that the results are relevant to global models. We focus on hypercube- and mesh-connected multicomputers with cut-through routing, such as the Intel iPSC/860, DELTA, and Paragon, and the nCUBE/2, but also indicate how the results extend to other parallel computer architectures.

The results of this study are relevant not only to the spectral transform method but also to multidimensional FFTs and other parallel transforms.

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

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1.86

PARALLEL SPECTRAL TRANSFORM SHALLOW WATER MODEL: A RUNTIME-TUNABLE PARALLEL BENCHMARK CODE

P. H. Worley I. T. Foster*

[Abstract of paper presented at the Scalable High Performance Computing Conference, Knoxville, TN, May 23-25, 1994; Proc. IEEE Computer Society Press, pp. 207-214 (1994)]

Fairness is an important issue when benchmarking parallel computers using application codes. The best parallel algorithm on one platform may not be the best on another. While it is not feasible to reevaluate parallel algorithms and reimplement large codes whenever new machines become available, it is possible to embed algorithmic options into codes that allow them to be "tuned" for a particular machine without requiring code

modifications. In this paper, we describe a code in which such an approach was taken.

PSTSWM was developed for evaluating parallel algorithms for the spectral transform method in atmospheric circulation models. Many levels of runtime-selectable algorithmic options are supported. We discuss these options and our evaluation methodology. We also provide empirical results from a number of parallel machines, indicating the importance of tuning for each platform before making a comparison.

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

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1.87

ALGORITHM COMPARISON AND BENCHMARKING USING A PARALLEL SPECTRAL TRANSFORM SHALLOW WATER MODEL

P. H. Worley I. T. Foster*
B. Toonen*

(Abstract of paper presented at the Sixth Workshop on Parallel Processing in Meteorology, European Center for Medium-Range Weather Forecasting, Reading, United Kingdom, November 21-25, 1994)

In recent years, a number of computer vendors have produced supercomputers based on a massively parallel processing (MPP) architecture.

These computers have been shown to be competitive in performance with conventional vector supercomputers for some applications. As spectral weather and climate models are heavy users of vector supercomputers, it is interesting to determine how these models perform on MPPs, and which MPPs are best suited to the execution of spectral models.

In a recent study, we developed a testbed code called PSTSWM that incorporated a wide range of parallel spectral transform algorithms. Studies with this testbed confirm that the performance of different algorithms can vary significantly from computer to computer, and that there is no single algorithm that is optimal on all platforms and for all problem sizes. Availability of this testbed makes it feasible to perform a comprehensive and fair benchmarking exercise of MPP platforms for spectral transform codes. We report the preliminary results of this exercise in this paper, presenting benchmark results for the Intel Paragon, the Cray T3D, and the IBM SP1.

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

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Materials Science

1.88

ELECTRONIC STRUCTURES OF DISORDERED Ag-Mg ALLOYS

R. G. Jordan* Y. Liu*
S. L. Qiu* E. Bruno†
B. Ginatempo† W. A. Shelton
G. M. Stocks†

[Abstract of *Physical Review B* 50(16), 459 (1994)]

We have calculated the electronic structures of the valence bands in a series of α -phase (disordered fcc) Ag-Mg alloys over the range 0-30 at.% Mg using the Korringa-Kohn-Rostoker method within the coherent potential approxima-

tion (KKR-CPA). We find that the variation of the equilibrium lattice constant with composition is in good agreement with experimental measurements. The bandwidth of the Ag-related d-states decreases with the addition of Mg although the position of the bottom of the band remains roughly fixed in energy with respect to the Fermi level; an observation that is consistent with photoemission measurements. The electronic spectral densities are very sharply peaked at the Fermi energy with widths that are $<1\%$ of the Brillouin zone dimension and so the Fermi surfaces of the alloys are well-defined throughout the zone. The radius of the neck at the L -point and the belly radii in the ΓX and ΓK direction increase approximately linearly with increasing Mg content. Taking into

account some previous work on the origin of short range order in Ag-rich alloys, we conclude that the LDA-KKR-CPA method provides a realistic description of the electronic structure in α -phase Ag-Mg alloys.

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

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‡Metals and Ceramics Division.

1.89

THE ORIGIN OF SHORT RANGE ORDER IN AG-MG ALLOYS

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S. L. Qiu* G. M. Stocks†
W. A. Shelton B. Ginatempo‡

[Abstract of *Acta Metallurgica* (in press)]

We have calculated the Fermi surfaces in a number of α -phase Ag-Mg solid solution alloys. We find that there are well-defined, parallel regions of surface in the $\langle 110 \rangle$ directions that give rise to the formation of concentration waves, resulting in satellite peaks in the electron diffuse scattering. The positions of the intensity maxima are directly related to the vector spanning such parallel regions and we show that the calculated variation of the peak separation with Mg concentration is in excellent agreement with the experimentally measured values. Thus, we provide strong evidence that the short-range-order in α -phase Ag-Mg is Fermi surface driven.

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

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1.90

STATIONARITY OF THE DENSITY FUNCTIONAL FREE ENERGY: APPLICATION TO ACCELERATED MULTIPLE SCATTERING CALCULATIONS

D. M. C. Nicholson* G. M. Stocks†
Y. Wang† W. A. Shelton
Z. Szotek† W. M. Temmerman†

[Abstract of *Rapid Communications* (in press)]

The density functional theory free energy can be written in such a form that it is stationary with respect to many of the variables that parameterize it. This stationarity beckons us to search for approximate values, that can act as *stand-ins* for their exact counterparts. We propose a set of stand-ins that perform almost as well as the exact values and can be systematically improved. They greatly increase the computational speed with which the energy of large systems can be calculated. The major players are: first, an electron density at each site that is based on exact solution of the Poisson equation combined with a solution of the multiple scattering problem in which only scattering from a small cluster of sites surrounding the site in question is retained; second, an approximate occupation function having a finite number of poles.

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

*Computing Applications Division.

†Metals and Ceramics Division.

1.91

APPROXIMATE FERMI FUNCTIONS FOR ACCELERATING DENSITY FUNCTIONAL CALCULATIONS

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 G. M. Stocks[†] Y. Wang[†]
 W. A. Shelton Z. Szotek[†]
 W. M. Temmerman[‡]

(Abstract of paper presented at the March Meeting of the American Physical Society, Pittsburgh, PA, March 21-25, 1994)

The free energy can be written in a form that is stationary with respect to variations about the Fermi occupation function, f_F . It is possible to use separate occupation functions for various contributions to the electronic density, and maintain stationarity with respect to the individual occupation functions. For example the single site contribution to the free energy can be calculated with f_F , while the multiple scattering part is evaluated with an approximate f . There are many choices for f which maintain better than mRy accuracy but require calculation of the electronic Green function at only a handful of energies. Examples of different choices for f will be presented for Cu, Mo, and NiAl.

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

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1.92

TOTAL ENERGY OF ORDERED AND DISORDERED CuAu

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 W. A. Shelton G. M. Stocks[†]
 D. D. Johnson[‡]

(Abstract of paper presented at the March Meeting of the American Physical Society, Pittsburgh, PA, March 21-25, 1994)

The total energy of CuAu is calculated using the self-consistent-field, multiple-atoms-per-unit-cell, Korringa-Kohn-Rostocker, screened coherent potential approximation (SCF-KKR-scr.CPA). The scr.CPA includes charge correla-

tion via shifts in the potentials, which reflect the effects of the average screening charges. We show how the scr.CPA can be extended to handle several atoms per unit cell. We have calculated the total energy for this alloy as a function of the long-range order parameter.

Research sponsored by the Ohio Supercomputer Center and Cray Research Inc. and by U.S. DOE Office of Basic Energy Sciences, Division of Materials Science.

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1.93

TOTAL ENERGY OF ORDERED AND DISORDERED Cu_cAu_{1-c} ALLOYS

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 D. D. Johnson[‡]

(Abstract of paper presented at the American Physical Society 1993 Annual Meeting, Seattle, WA, March 22, 1993)

We have calculated the total energy of the stoichiometric Cu_cAu_{1-c} alloy system as a function of the long range order parameter. These calculations were performed using the local-density-approximation (LDA) based first principles, multi-atom per unit cell, scalar-relativistic, self-consistent-field, Korringa-Kohn-Rostoker, coherent potential approximation (SCF-KKR-CPA). The LDA is used to treat the effects of electron correlation and exchange while the CPA is used to handle the effects of substitutional disorder on the electronic structure within the multiple scattering formalism of the Green function based KKR method. The relativistic effects of the mass-velocity and Darwin terms are treated within the scalar-relativistic approximation whilst the spin orbit term is omitted. Using this approach we are able to make a precise determination of the mixing energy.

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

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1.94

FIRST PRINCIPLES SIMULATION OF MATERIALS PROPERTIES

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 L. Qui[†] D. D. Johnson[‡]
 F. J. Pinski[§] J. B. Staunton[#]
 B. Ginatempo^{**}

(Abstract of paper presented at the Scalable High Performance Computing Conference, Knoxville, TN, March 28, 1994)

We have developed a hybrid, parallel computer code for calculating the electronic structure of both ordered and substitutionally disordered materials. By using PVM3.3, we can integrate into our local computer environment multiple parallel and vector supercomputers as well as high performance workstations. Without this approach, calculations of materials properties of large systems would be otherwise untenable due to a lack of computer resources. For example, we have determined the short-range order intensity and its electronic origin for the Ag-Mg alloy system, including an estimate of the order-disorder (spinodal) temperature.

Research sponsored by the Applied Mathematical Sciences Research Program, U.S. DOE Office of Energy Research; by the National Science Foundation; by the Southeastern Universities Research Association; and by U.S. DOE Basic Energy Sciences, Division of Materials Science under a New Initiative at Sandia.

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1.95

ALLOY CALCULATIONS ON MASSIVELY PARALLEL COMPUTERS

G. M. Stocks* D. M. C. Nicholson*
 Y. Wang* W. A. Shelton
 W. M. Temmerman[†] Z. Szotek[‡]
 B. Ginatempo[†]

[Abstract of book chapter in *Metallic Alloys: Experimental and Theoretical Perspectives*, J. S. Faulkner and R. G. Jordan, Eds. (in press); also paper presented at the NATO Advanced Research Workshop on Metallic Alloys: Experimental and Theoretical Perspectives, Boca Raton, FL, July 16-21, 1993]

We discuss ways that first principles LDA methods can be adapted to take advantage of the computational power of massively parallel supercomputers. We discuss the need for new theoretical and computational strategies that circumvent the N^3 problem associated with standard LDA implementations limiting their extension to large systems. We propose a new, spatially local, multiple scattering theory algorithm that offers that possibility of producing a scalable $O(N)$ method. As a first step, we use the method to calculate the self-consistent charge density for a large system.

Research sponsored by Division of Materials Science, Applied Mathematical Sciences Research Program, U.S. DOE Office of Energy Research and by Consiglio Nazionale Delle Ricerche, Italy.

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1.96

TOWARDS SCALABLE ELECTRONIC CALCULATIONS FOR ALLOYS

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 Y. Wang* W. A. Shelton
 Z. Szotek[‡] W. M. Temmerman[†]

[Abstract of paper presented at the Society for Computer Simulation (SCS), Simulation Multiconference (SMC) '94, LaJolla, CA, April 11-13, 1994]

A new approach to calculating the properties of large systems within the local density approximation (LDA) that offers the promise of scalability on the massively parallel supercomputers

is outlined. The electronic structure problem is formulated in real space using multiple scattering theory. The standard LDA algorithm is divided into two parts. Firstly, finding the self-consistent field (SCF) electron density. Secondly, calculating the energy corresponding to the SCF density. We show, at least for metals and alloys, that the former problem is easily solved using real space methods. For the second we take advantage of the variational properties of a generalized Harris-Foulkes free energy functional, a new conduction band Fermi function, and a fictitious finite electron temperature that again allow us to use real-space methods. Using a *compute-node* $\Rightarrow$ *atom* equivalence the new method is naturally highly parallel and leads to $O(N)$ scaling where N is the number of atoms making up the system. We show scaling data gathered on the Intel XP/S 35 Paragon for systems up to 512-atoms/simulation cell. To demonstrate that we can achieve *metallurgical*-precision, we apply the new method to the calculation the energies of disordered $\text{Cu}_{0.5}\text{Zn}_{0.5}$ alloys using a large *random* sample.

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

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1.97

TOWARDS A SCALABLE LDA MULTIPLE SCATTERING METHOD FOR LARGE SYSTEMS

G. M. Stocks* D. M. C. Nicholson†
Y. Wang* W. A. Shelton
Z. Szotek‡ W. M. Temmerman†

(Abstract of paper presented at the March Meeting of the American Physical Society, Pittsburgh, PA, March 21-25, 1994)

We outline a new approach to performing LDA calculations on large systems that circumvents the N^3 problem associated with the matrix diagonalization/inversion step in conventional band structure methods. We formulate the electronic structure problem in real space using mul-

tipple scattering theory and show that, by taking advantage of the variational properties of a generalized Harris-Foulkes free-energy functional, it is possible to calculate energetics using entirely real-space methods. Furthermore, the real-space algorithms lend themselves naturally to parallel computing architectures and lead to $O(N)$ scaling. We show results obtained using the Intel *Paragon* massively parallel supercomputer that demonstrate both convergence and scaling.

Research sponsored by Division of Materials Science and Applied Mathematical Sciences Research Program, U.S. DOE Office of Energy Research.

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1.98

TOWARDS SCALABLE, PARALLEL, MULTIPLE SCATTERING THEORY, ALGORITHMS FOR LARGE METALLIC SYSTEMS

G. M. Stocks* W. A. Shelton
D. M. Nicholson* Z. Szotek†
W. M. Temmerman†

(Abstract of paper presented at the Sanibel Symposium, Gainesville, FL, March 13-20, 1993)

The advent of massively parallel supercomputers has the potential to make an impact on our ability to calculate the properties of metals and alloys at least as large as that afforded by the vector machines of the 80's. One area that offers promise is the application of first principles LDA based methods to situations where it is necessary to treat, quantum mechanically, the interactions between large numbers of atoms (alloy phase stability, dislocation core structure etc). However, in order to exploit this potential, new scalable methods will have to be developed that to some degree avoid the so called N -cubed problem associated with conventional applications of LDA methods in condensed matter physics. This presentation is divided into two parts. Firstly, I will outline the methods that we employed and the performance that we obtained during the parallelization of a standard pre-existing electronic structure code: the LDA-KKR-CPA method for

calculating the electronic structure and energetics of disordered solid solution alloys. I will show performance figures for a number of different parallel computing paradigms (Cray YMP, 128-node Intel iPSC/860 and Parallel Virtual Machine). Whilst this work was very successful, in that we were able to obtain record setting execution rates, it also served to point out that straight forward parallelization strategies do not lead to scalable codes. Consequently, in the second part of this presentation, I will outline a new approach based on multiple scattering theory and spatially local view of the electronic structure that offers the promise of scalability and can thereby take advantage of the next generation of massively parallel machines such as the 1048-processor Intel Paragon that is being installed at Oak Ridge.

Research sponsored by Basic Energy Sciences, Division of Materials Science, and Applied Mathematical Sciences Research Program, U.S. DOE Office of Energy Research.

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1.99

SPIN-POLARIZED KKR-CPA CALCULATIONS FOR FERROMAGNETIC CuNi ALLOYS

Y. Wang* G. M. Stocks*
D. M. C. Nicholson† W. A. Shelton

(Abstract of paper presented at the TMS Symposium on Alloy Modeling and Design, Pittsburgh, PA, October 17, 1993)

Ab initio electronic structure calculations of ferromagnetic copper-nickel alloys are carried out using the self-consistent-field Korringa-Kohn-Rostoker coherent potential approximation (SCF-KKR-CPA) method. The calculated lattice constants and magnetic moments of the alloy are in good agreement with the experimental results. It is also shown that the calculation is scalable with respect to the energy mesh and can be efficiently implemented on a massively parallel supercomputer.

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

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†Computing Applications Division.

1.100

SCALABLE LARGE SYSTEM MULTIPLE SCATTERING METHOD: APPLICATION TO CuZn ALLOYS

Y. Wang* G. M. Stocks*
D. M. C. Nicholson† W. A. Shelton
X. Y. Liu† Z. Szotek§
W. M. Temmerman§

(Abstract of paper presented at the March Meeting of the American Physical Society, Pittsburgh, PA, March 21-25, 1994)

A local density approximation Large System Multiple Scattering (LSMS) method has been developed for solving alloy problems where it is necessary to treat, quantum mechanically, the interactions between large numbers of atoms. It is shown that the method is completely scalable and can be implemented on a massively parallel supercomputer. The LSMS method is applied to the calculation of the energetics, as a function of both long and short range order parameters, of disordered CuZn systems in a large cell model involving hundreds of atoms. For the homogeneously disordered alloy, the results of this large scale simulation are compared with the results of both standard and charge correlated LDA-KKR-CPA calculations.

Research sponsored by Division of Materials Science and Applied Mathematical Sciences Research Program, U.S. DOE Office of Energy Research.

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STATISTICS

Research in General Statistical Methods

1.101

**COMMENTS ON "USE OF
CONDITIONAL SIMULATION
IN NUCLEAR WASTE SITE
PERFORMANCE ASSESSMENT"
BY CAROL GOTWAY**

D. J. Downing

[Abstract of paper presented at the 1993 Joint Statistical Meetings, San Francisco, CA, August 7-12, 1993; *Technometrics* 36(2), 147 (1994)]

This paper discusses Carol Gotway's paper, "The Use of Conditional Simulation in Nuclear Waste Site Performance Assessment." The paper centers on the use of conditional simulation and the use of geostatistical methods to simulate an entire field of values for subsequent use in a complex computer model. The issues of sampling designs for geostatistics, semivariogram estimation and anisotropy, turning bands method for random field generation, and estimation of the cumulative distribution function are brought out.

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

1.102

**ROLE OF LOW-PASS FILTERING
IN THE PROCESS OF ATTRACTOR
RECONSTRUCTION FROM
EXPERIMENTAL CHAOTIC
TIME SERIES**

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

[Abstract of *Phys. Rev. E* 47(4), 2520 (1993)]

We discuss issues concerning the reconstruction of attractors from experimental chaotic time-series data using Taken's method of delays [in *Proceedings of the Warwick Symposium, 1981*, edited by D. A. Rand and L. S. Young (Springer, New York, 1981)]. The focus of this paper is on the selection of appropriate lag-time and embedding-dimension values with an emphasis on the re-

lationship between those parameters and data-measurement considerations. We are particularly interested in the effect that low-pass filtering has on the appearance and measured properties of reconstructed attractors. Empirical results are presented using data measured from a laboratory fluidized bed and from data generated by integrating the Lorenz [J. Atmospheric Sci. 20, 130 (1963)] and Franceschini [Physica 6D, 285 (1983)] and Franceschini models of chaotic dynamic systems.

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

*Engineering Technology Division.

†Instrumentation and Controls Division.

1.103

**RESPONSE TO THE LETTER OF
S. A. ROBERTS AND J. H. HENDRY**

M. D. Morris T. D. Jones*

[Abstract of *Radiation Research* 138(2), 303 (1994)]

Almost without question, compensatory hematopoiesis depends on daughter cells that proliferate and mature from pluripotent stem cells. Replacement therapy has shown that hematopoiesis can, in precisely conditioned animals, be restored by infusion of only one or a few such stem cells. However, those cells cannot act alone; hematopoietic processes of proliferation and maturation also require a functional marrow stroma and stromal mediated growth factors or cytokines. Our analysis has indicated that, at least with respect to 30-day animal mortality, the stromal tissues appear to be the weakest link in the chain.

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

*Health and Safety Research Division.

1.104

**RESPONSE TO THE LETTER OF
A. C. C. RUIFORK AND
H. D. THAMES**

M. D. Morris T. D. Jones*

[Abstract of *Experimental Hematology* 22, 536 (1994)]

Ruifrok and Thames have criticized our papers and, claiming that our methods do not sufficiently account for cellular heterogeneity, and that as a result we have underestimated the ra-

diosensitivity of the "critical pool" of marrow cells. Briefly, their hypothesis of cellular variability seems unwarranted based on current biological knowledge of normal marrow cells. Even if such variability were present, it would not lead to the biasing phenomenon they claim. This is more fully explained below, but we shall first respond to secondary points raised in their letter.

Research sponsored by Defense Nuclear Agency and Applied Mathematical Sciences Research Program, U.S. DOE Office of Energy Research.

*Health and Safety Research Division.

Applications of Statistical Methods

1.105

**APPLICATION OF CANONICAL
VARIATE ANALYSIS IN THE
EVALUATION AND PRESENTATION
OF MULTIVARIATE BIOLOGICAL
RESPONSE DATA**

**S. M. Adams* K. D. Ham†
J. J. Beauchamp**

[Abstract of *Environmental Toxicology and Chemistry* 13(10), 1673 (1994)]

We have applied canonical variate analysis procedures for evaluating multivariate responses of fish populations to various contaminant stressors. Using examples of fish populations experiencing high levels of PCBs in a reservoir and mixed contaminants in a stream, the significance of integrated stress responses among sample populations was compared statistically and graphically using two- and three-dimensional data presentations. For fish from both systems, the most powerful axis of discrimination among sample populations was correlated with the activity of the detoxification enzyme, EROD (7-ethoxyresorufin O-deethylase). Indicators of organ dysfunction were the variables most correlated with the second axis of discrimination among sites in the PCB-contaminated reservoir study. Indicators of lipid metabolism were the variables most correlated with the second and third axes of discrimination among stream fish. Canonical variate analysis procedures are useful for evaluating multivariate response data because they take into account the interrelations and asso-

ciations among response variables and reveal the integrated nature of organism responses to stress. Using this procedure, the significance of integrated stress responses among different sample populations can be graphically compared and evaluated using two- or three-dimensional data presentations. These types of graphical displays help provide an understanding of the relationships among sample populations that may not be evident from tabular or other types of data summaries. In addition, this approach can be useful in helping to identify factors such as toxicants or other environmental stressors which impair the health of aquatic ecosystems.

Research sponsored by U.S. DOE Department of Environmental Management, Health Safety, Environmental, and Accounting Division.

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1.106

STATISTICAL METHODS FOR THE ANALYSIS OF A SCREENING TEST FOR CHRONIC BERYLLIUM DISEASE

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S. P. Colyer*

(Abstract of ORNL-6818, October 1994)

The lymphocyte proliferation test (LPT) is a noninvasive screening procedure used to identify persons who may have chronic beryllium disease. A practical problem in the analysis of LPT well counts is the occurrence of outlying data values (approximately 7% of the time). A log-linear regression model is used to describe the expected well counts for each set of test conditions. The variance of the well counts is proportional to the square of the expected counts, and two resistant regression methods are used to estimate the parameters of interest. The first approach uses least absolute values (LAV) on the log of the well counts to estimate beryllium stimulation indices (SIs) and the coefficient of variation. The second approach uses a resistant regression version of maximum quasi-likelihood estimation. A major advantage of the resistant regression methods is that it is not necessary to identify and delete outliers. These two new methods for the statistical analysis of the LPT data and the outlier rejection method that is currently being used are applied to 173 LPT assays. We strongly recommend the LAV method for routine analysis of the LPT.

Outliers are also important when trying to identify individuals with beryllium hypersensitivity, since these individuals have large positive values for the SIs. A new method for identifying large SIs using combined data from the not exposed group and the beryllium workers is proposed. The log(SIs) are described with a Gaussian distribution with location and scale parameters estimated using resistant methods. This approach is applied to the test data and results are compared with those obtained from the current method.

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

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1.107

COMPARISON OF TWO FRESHWATER TURTLE SPECIES AS MONITORS OF RADIONUCLIDE AND CHEMICAL CONTAMINATION: DNA DAMAGE AND RESIDUE ANALYSIS

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J. J. Beauchamp B. T. Walton†

[Abstract of *Environmental Toxicology and Chemistry* 12, 1487 (1993)]

Two species of turtles that occupy different ecological niches were compared for their usefulness as monitors of freshwater ecosystems where both low-level radioactive and nonradioactive contaminants are present. The pond slider (*Trachemys scripta*) and common snapping turtle (*Chelydra serpentina*) were analyzed for the presence of ^{90}Sr , ^{137}Cs , ^{60}Co , and Hg, radionuclides and chemicals known to be present at the contaminated site, and single-strand breaks in liver DNA. The integrity of the DNA was examined by the alkaline unwinding assay, a technique that detects strand breaks as a biological marker of possible exposure to genotoxic agents. This measure of DNA damage was significantly increased in both species of turtles at the contaminated site compared with turtles of the same species at a reference site, and shows that contaminant-exposed populations were under more severe genotoxic stress than those at the reference site. The level of strand breaks observed at the contaminated site was high and in the range reported for other aquatic species exposed to deleterious concentrations of genotoxic agents such as chemicals and ionizing radiation. Statistically significantly higher concentrations of radionuclides and Hg were detected in the turtles from the contaminated area. Mercury concentrations were significantly higher in the more carnivorous snapping turtle compared with the slider; however, both species were effective monitors of the contaminants.

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

*University of Tennessee, Knoxville, TN.

†Environmental Sciences Division.

1.108

DEVELOPMENT OF RELATIONSHIP BETWEEN TRUCK ACCIDENTS AND GEOMETRIC DESIGN: PHASE I

S.-P. Miaou* P. S. Hu*
T. Wright S. C. Davis*
A. K. Rathi*

[Abstract of Federal Highway Administration Technical Report #RD-91-124 (August 1993)]

The purpose of this study was to establish empirical relationships between truck accidents and highway geometric design. First, statistical frameworks based on Poisson and negative binomial regression models were proposed. Preliminary models were then developed using accidents and road inventory data from the Highway Safety Information System (HSIS). Three roadway classes were considered in the model development: rural Interstate, urban Interstate and freeway, and rural two-lane undivided arterial. The maximum likelihood method was used to estimation of model parameters. Information criterion, asymptotic t-statistic, and goodness-of-fit test statistics were employed to evaluate the estimated models. The model results based on data from one of the HSIS States—Utah, were used for analysis and for suggesting areas in which the quality and quantity of the existing HSIS data can be enhanced to improve the developed models.

Despite the limitations in existing Utah data, some encouraging preliminary relationships were developed for horizontal curvature, length of curve, vertical grade, length of grade, shoulder width, number of lanes, and annual average daily traffic (AADT) per lane (a surrogate measure for vehicle flow density). Goodness-of-fit test statistics indicated that extra variations (or overdispersion) existed in the data over the developed Poisson models for all three roadway classes. Subsequent analyses suggested that a future study can be performed to enhance the predictive power of these preliminary models by including detailed truck exposure information, e.g., time-of-day, truck type, and weather conditions, by considering more explanatory variables, such as roadside design and superelevation, and by reducing the sampling errors of vehicle exposure data (both AADT and truck percentages).

Research sponsored by Office of Safety and Traffic Operations R&D, Federal Highway Administration and U.S. Department of Energy.

*Energy Division.

1.109

STATISTICAL SIMULATION AND THREE-DIMENSIONAL VISUALIZATION FOR ANALYSIS AND INTERPRETATION OF SOIL VOC DATA SETS

T. J. Mitchell O. R. West*
R. L. Siegrist*

(Abstract of paper presented at the National Symposium on Measuring and Interpreting VOCs in Soils, Las Vegas, NV, January 12–14, 1993)

The characterization of a VOC-contaminated soil region typically consists of two parts: (1) measurement of soil VOC concentrations at discrete points within a three-dimensional soil region, and (2) interpretation of the VOC distribution including the development of an empirical spatial model for the three-dimensional soil VOC dataset. This empirical modeling can be very simple, such as two-dimensional contouring of VOC concentrations within fixed depth strata. Alternatively, empirical spatial modeling can involve a more rigorous application of statistical and numerical procedures to determine a three-dimensional interpolating or smoothing function that estimates the "true" VOC concentration as a function of location within three dimensional space. The appropriate interpolating or smoothing function is chosen to be consistent with the VOC measurements and with some prior assumptions about the smoothness of the "true" VOC concentration function.

Research sponsored by U.S. Department of Energy.

*Environmental Sciences Division.

1.110

SOIL SORPTION OF VOLATILE AND SEMIVOLATILE ORGANIC COMPOUNDS IN A MIXTURE

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T. A. Anderson† W. H. Griest†
R. Merriweather† J. J. Beauchamp
C. W. Francis*

[Abstract of *J. Environ. Qual.* 21(4), 552 (1992)]

Studies were conducted to evaluate lipophilicity as a predictor of sorption for a mixture of organic compounds with high vapor pressures commonly present at hazardous waste sites. Sorption partition coefficients (K_p) for the mixture of 16 volatile and semivolatile organic compounds

were measured on a Captina silt loam (Typic Fragiudult) and a McLaurin sandy loam (Typic Paleudults) using a zero headspace extractor. The experimental K_p was determined for acrylonitrile, furan, methyl ethyl ketone, tetrahydrofuran, benzene, toluene, *p*-xylene, chlorobenzene, chloroform, nitrobenzene, 1,2-dichlorobenzene, 1,2,3-trichloropropane, carbon tetrachloride, ethylene dibromide, 1,2,4,5-tetrachlorobenzene, and hexachlorobenzene on each of the two soils. The K_p values were generally lower in the McLaurin sandy loam, which had a lower organic C content ($0.66 \pm 0.04\%$) than the Captina silt loam (organic C content = $1.49 \pm 0.06\%$). Sorption was normalized to soil organic C content of the soil by converting K_p for each compound and soil to K_{oc} . Weighted regression analyses of K_{oc} observed for the compounds in the mixture on K_{oc} predicted from the *n*-octanol/water partition coefficient (K_{ow}) for individual compounds yielded a pooled, weighted regression of K_{oc} observed = $1.084 + 0.457 K_{oc}$ predicted, $n = 29$, $r = 0.88$. Statistical analysis indicated that the slope of 0.457 ± 0.046 (estimated standard error) was significantly less than 1.00, indicating that soil sorption of nonionic organic compounds differed from that predicted for the same individual compounds based on K_{ow} . The results indicate that predictive equations for sorption of individual organic compounds can be applied to mixtures of volatile and semivolatile organic compounds in soils when log K_{ow} are in a range from approximately 1 to 3; however, outside this range a correction factor may be needed.

Research sponsored by U.S. DOE and USEPA.

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‡Analytical Chemistry Division.

1.111

RECENT GROWTH INCREASES IN OLD-GROWTH LONGLEAF PINE

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M. L. Tharp‡	J. J. Beauchamp
W. J. Platt§	D. J. Downing

[Abstract of *Can. J. For. Res.* 23, 846 (1993)]

Longleaf pine (*Pinus palustris* Mill.) tree-ring data were obtained from an old-growth stand located in Thomas County, Georgia. The tree-ring chronology from the pine stand is composed of a collection of cores extracted from 26 trees ranging in age from approximately 100 to 400 years. These cores were prepared, dated, and measured, and the resulting data were examined with dendrochronological and statistical techniques. Beginning in approximately 1950 and continuing to the present, annual increments of all age classes examined in this study have increased, resulting in an average annual ring increment approximately 40% greater in 1987 than in 1950. When compared with expected annual increment, the increase for 100- to 150-year-old trees is approximately 45%, while the increase for 200- to 400-year-old trees is approximately 35%. In terms of stand-level aboveground biomass accumulation, the increased growth has resulted in approximately 5% more biomass than expected. The increased growth cannot be explained by disturbance; stand history; or trends in precipitation, temperature, or Palmer drought severity index over the last 57 years. Increased atmospheric CO_2 is a possible explanation for initiation of the observed trend, while SO_x and NO_x may be augmenting continuation of this phenomenon.

Research sponsored by the Carbon Dioxide Research Division, Office of Energy Research, U.S. DOE and by the National Science Foundation's Ecosystem Studies Program.

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†U.S. Fish and Wildlife Service, Lafayette, LA.

‡Computing Applications Division.

§Louisiana State University, Baton Rouge, LA.

1.112

THE 1990 NATIONWIDE TRUCK ACTIVITY AND COMMODITY SURVEY SUMMARY REPORT

P. S. Hu* S. Davis*
T. Wright

(Abstract of ORNL/TM-12361, June 1993)

The **Truck Inventory and Use Survey (TIUS)** is the oldest national, vehicle-based survey of freight transportation. The TIUS is performed by the U.S. Bureau of the Census as part of its quinquennial Census of Transportation, and collects extensive information on the typical and year-long use of trucks, vans, and mini-vans. While the 1987 TIUS nationwide sample of approximately 105,000 vehicles provides critical information on the typical use of the nation's trucking fleet, it does not provide a detailed picture

of the temporal and geographic variation in truck use. To provide this detailed picture, a subsample known as the **Nationwide Truck Activity and Commodity Survey (NTACS)** was conducted by the U.S. Bureau of the Census for the U.S. Department of Transportation over a 12-month period that ended in 1990. The NTACS measured detailed trip characteristics and other information for a large sample of TIUS respondents on randomly sampled days. The complex nature of the survey, resulted in a low response rate, and required special analysis and imputations by ORNL's Center for Transportation Analysis. A public use file was developed and documented in 1992. The purpose of this summary report is to provide selected tables based on the public use file.

Research sponsored by U.S. Department of Energy.

*Energy Division.

Design of Experiments

1.113

ASYMPTOTIC BAYES CRITERIA FOR NONPARAMETRIC RESPONSE SURFACE DESIGN

T. Mitchell J. Sacks*
D. Ylvisaker†

[Abstract of *Annals of Statistics* (in press)]

The paper deals with Bayesian design for response surface prediction when the prior may be finite or infinite dimensional, the design space arbitrary. In order that the resulting problems be manageable, we resort to asymptotic versions of D-, G-, and A-optimality. Here the asymptotics stem from allowing the error variance to be large. The problems thus elicited have strong game-like characteristics. Examples of theoretical solutions are brought forward, especially when the priors are stationary processes on an interval, and we give numerical evidence that the asymptotics work well in the finite domain.

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

*National Institute of Statistical Sciences.

†University of California, Los Angeles, CA.

1.114

DESIGN AND ANALYSIS FOR AN INVERSE PROBLEM ARISING FROM AN ADVECTION - DISPERSION PROCESS

M. D. Morris A. D. Solomon*

[Abstract of *Technometrics* (in press)]

We consider a process of one-dimensional fluid flow through a soil-packed tube in which a contaminant is initially distributed. The contaminant concentration, as a function of location in the tube and time after flushing begins, is classically modeled as the solution of a linear second-order partial differential equation. Here, we consider the related issues of how contaminant concentration measured at some location-time combinations can be used to approximate concentration at other locations and times, and how the sampled location-time combinations can be most effectively selected for this purpose (i.e. experimental design). The method is demonstrated for the case in which initial concentrations are approximated based on data collected only at the down-stream end of the tube. Finally, the effect of misspecify-

ing one of the model parameters is discussed, and alternative designs are developed for instances in which that parameter must be estimated from the data.

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

*Omer, Israel.

Statistical Sampling Theory

1.115

AN APPROACH TO DETERMINING AN OPTIMAL SAMPLING FREQUENCY FOR MEASURING TEMPORAL CHANGES IN WATER QUALITY

G. R. Moline* J. J. Beauchamp
T. Wright

[Abstract of *Ground Water* (in press)]

In the Data Quality Objectives (DQO) process, statistical methods are used to determine an optimal sampling and analysis plan. Often, the process is geared toward the uncertainty inherent in the analytical methods and the variability at a single monitoring location in order to determine whether or not contaminant concentrations exceed regulatory limits. When the DQO decision rule for instituting remedial actions is based on a critical change in water quality, the monitoring program design must ensure that this change can be detected and measured with a specified confidence. Thus, a more challenging problem is that of measuring overall changes for a small region over time, where both spatial and temporal variability exist and where the uncertainty associated with these variations far exceeds measurement error. Historical water quality data can be used to quantify the statistical parameters necessary for establishing initial sampling frequencies or for determining the minimum change that can be declared statistically significant if a sampling design has already been established. This information can then be used to guide refinement of the sampling program as additional data are obtained. Statistical methods are developed for testing the statistical sig-

nificance of a linear trend and an annual change compared to a baseline year for a group of water quality wells, and are demonstrated by application to a waste disposal site in Oak Ridge, Tennessee.

Research sponsored by U.S. Department of Energy.

*Environmental Sciences Division.

1.116

RARE ATTRIBUTES IN FINITE UNIVERSES: HYPOTHESES TESTING SPECIFICATION AND EXACT RANDOMIZED UPPER CONFIDENCE BOUNDS

T. Wright

(Abstract of ORNL/TM-12269, March 1993)

When attributes are rare and few or none are observed in the selected sample from a finite universe, sampling statisticians are increasingly being challenged to use whatever methods are available to declare with high probability or confidence that the universe is near or completely attribute-free. This is especially true when the attribute is undesirable. Approximations such as those based on normal theory are frequently inadequate with rare attributes. For simple random sampling without replacement, an appropriate probability distribution for statistical inference is the hypergeometric distribution. But even with the hypergeometric distribution, the investigator is limited from making claims of attribute-free with high confidence unless the sample size is quite large using nonrandomized techniques. In the hypergeometric setting with rare attributes, exact randomized tests

of hypothesis are investigated to determine the effect on power of how one specifies the null hypothesis. In particular, specifying the null hypothesis as zero attributes does not always yield maximum possible power. We also consider the hypothesis specification question under complex sampling designs including stratified random sampling and two-stage cluster sampling (one case involves random selection at first stage and another case involves probability proportional to size without replacement selection at first stage). Also under simple random sampling, this article defines and presents a simple algorithm for the construction of exact "randomized" upper confidence bounds which permit one to possibly report tighter bounds than those exact bounds obtained using "nonrandomized" methods.

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

1.117

PREDICTION AND STANDARD ERROR ESTIMATION FOR A FINITE UNIVERSE TOTAL WHEN A STRATUM IS NOT SAMPLED

T. Wright

(Abstract of ORNL/TM-12379, January 1994; also paper presented at the 1994 Joint Statistical Meetings, Toronto, Canada, August 14-18, 1994)

In the context of a universe of trucks operating in the United States in 1990, this paper presents statistical methodology for estimating a finite universe total on a second occasion when a part of the universe is sampled and the remainder of the universe is not sampled. Prediction is used to compensate for the lack of data from the unsampled portion of the universe. The sample is assumed to be a subsample of an earlier sample where stratification is used on both occasions before sample selection. Accounting for births and deaths in the universe between the two points in time, the detailed sampling plan, estimator, standard error, and optimal sample allocation, are presented with a focus on the second occasion. If prior auxiliary information is available, the methodology is also applicable to a first occasion.

Research sponsored by the Federal Highway Administration, U.S. Department of Transportation, U.S. DOE.

Estimation Theory

1.118

A METHOD FOR ESTIMATING OCCUPATIONAL RADIATION DOSE TO INDIVIDUALS, USING WEEKLY DOSIMETRY DATA

T. J. Mitchell* **G. Ostrouchov**
E. L. Frome **G. D. Kerr†**

[Abstract of *Health Physics* (in press); also ORNL-6778, December 1993; also paper presented at the 1994 ASA Conference on Radiation and Health, Nantucket, MA, June 26-July 1, 1994]

Statistical analyses of data from epidemiologic studies of workers exposed to radiation have been based on recorded annual radiation doses. It is usually assumed that the annual dose val-

ues are known exactly, although it is generally recognized that the data contain uncertainty due to measurement error and bias. We propose the use of a probability distribution to describe an individual's dose during a specific period of time. Statistical methods for estimating this dose distribution are developed. The methods take into account the "measurement error" that is produced by the dosimetry system, and the bias that was introduced by policies that lead to right censoring of small doses as zero. The method is applied to a sample of dose histories obtained from hard copy dosimetry records at Oak Ridge National Laboratory (ORNL). The result of this evaluation raises serious questions about the validity of the historical personnel dosimetry data that is currently being used in low-dose studies of nuclear industry

workers. In particular, it appears that there was a systematic underestimation of doses for ORNL workers. This could result in biased estimates of dose-response coefficients and their standard errors.

Research sponsored by U.S. Office of Energy Research, Office of Epidemiology and Health Surveillance, Environment, Safety and Health.

*Deceased.

†Health Sciences Research Division.

Computational Distribution Theory

1.119

DISCRETING THE PEARSON AND JOHNSON SYSTEM OF CURVES

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

[Abstract of *Biometrics* (in press)]

The frequency with which sister chromatid exchanges (SCR) occur in the nucleus of a normal human cell is noticeably larger (7-8 per cell) than chromosomal aberrations which occur, spontaneously, with very low frequency (1 in 100 cells). In a recent paper, Bender *et al.* (1992) present SCE counts made up of 200 peripheral blood lymphocytes from each of 393 normal human subjects. A total of 19,650 SCE's were counted with the number per cell ranging from 0 to 32. We characterize the resulting frequency distributions as Pearson-type and Johnson translation system distributions that have been discretized and fitted by the method of moments.

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

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1.120

THE EVALUATION OF MOMENTS FOR FITTING MULTIPARAMETER SINUSOIDAL MODELS

K. O. Bowman M. K. Miller*
L. R. Shenton†

[Abstract of *Applied Surface Science* (in press)]

Moment methods have been applied to several different models of decomposition observed in atom probe random area analysis data such as (1)

$\{p = a_0 + a_1 \sin \theta, p = a_0 + a_1 \cos \theta\}$ [2 moments], (2) $p = a_0 + a_1 \sin \theta + a_2 \cos \theta$ [3 moments], (3) $p = a_0 + a_1 \sin \theta + a_2 \sin(2\theta)$ [3 moments], (4) $p = a_0 + a_1 \sin \theta + a_2 \sin^2 \theta$ [3 moments], (5) $p = a_0 + a_1 \sin \theta + a_2 \sin^3 \theta$ [3 moments] and (6) $\{p = a_0 + a_1 \sin \theta + a_2 \cos \theta + a_3 \sin(2\theta), p = a_0 + a_1 \sin \theta + a_2 \cos \theta + a_3 \cos(2\theta)\}$ [4 moments] and $a_0 + a_1 \sin \theta + a_2 \cos \theta + a_3 \sin(2\theta) + a_4 \cos(2\theta)$ [5 moments]. A comparison of the best fits for these various models to experimental atom probe data from spinodally decomposed iron-chromium alloys showed that in most cases where solutions were found, the periodic binomial distributions used here with only a few moments seem to result in a moderate improvement over previous models.

Research sponsored by U.S. DOE Division of Materials Sciences.

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1.121

CONTRIBUTION TO THE DISCUSSION ON THE PAPER BY R. C. H. CHENG AND I. TAYLOR ON "NON-REGULAR MAXIMUM LIKELIHOOD PROBLEMS" ON 19 JANUARY, 1994

K. O. Bowman L. R. Shenton*

[Abstract of *Journal of Royal Statistical Society* (in press)]

It was pointed out that previous work of Bowman and Shenton (1987, 1988) discussed in some detail the three parameter gamma model (threshold parameter, shape parameter and scale parameter), three parameters being estimated both by maximum likelihood and moment method. Four moments were found by simulation method and approximate distribution set up.

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

*University of Georgia, Athens, GA.

1.122

**ADDITIONAL BOWMAN-SHENTON
APPROXIMATE PERCENTAGE
POINTS FOR PEARSON
DISTRIBUTIONS BASED
ON PEARSON TYPE VI**

K. O. Bowman L. R. Shenton*

[Abstract of *Commun. Statist.-Simula.* 23(3), 583 (1994)]

The Bowman and Shenton approximate percentage points for Pearson distributions are extended to include some cases for which the skewness β_1 exceeds four. Use is made of the reciprocity property existing between the Pearson Type VI distribution and the Type I distribution.

Research sponsored by Applied Mathematical Sciences Research Program, U.S. DOE Office of Energy Research and by the Center for Indoor Air Research.

*University of Georgia, Athens, GA.

1.123

**MOMENT SOLUTION TO
AN URN MODEL**

L. R. Shenton* K. O. Bowman

[Abstract of *The Annals of the ISM* (in press)]

A subset of Bernard's RD-model (replenishment-depletion) is considered from the viewpoint of the calculus of finite differences.

The most general case is considered and includes urn with balls of many colors, each color being replenished either deterministically or stochastically. Factorial moment generating functions (fmgf) are employed to define probability generating function (with probabilities) when the replenishments are positive valued random variables with given factorial moments.

This result involves beta integral transforms defining manifold of discrete distributions. Particular cases relate to hypergeometric discrete distributions.

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

*University of Georgia, Athens, GA.

Section 2

NUCLEAR DATA MEASUREMENT AND EVALUATION

2.0. INTRODUCTION

D. C. Larson

Activities in the Nuclear Data Measurement and Evaluation Section centered around measurements of neutron cross sections and related quantities performed using the Oak Ridge Electron Linear Accelerator (ORELA). Both basic research and work of interest to applications of nuclear physics are performed. In addition to measurement work, complete neutron cross section evaluations are produced, and model codes which support the evaluation work are developed and improved. As noted in the previous report, DOE funding for applied nuclear data work was rapidly decreasing, and in FY96 the measurement component of the nuclear data program will be dropped. As a result of changes in DOE program directions and the desire to keep ORELA available, this section was transferred to the Physics Division at ORNL, with a mission in nuclear astrophysics and fundamental interactions. Future work at ORELA will be reported in Physics Division Information Meetings and Annual Reports.

Since its inception, over 550 publications and several hundred reports have been written to describe ORELA-based research. Capture cross sections for over 180 nuclides have been measured to meet applied needs and for astrophysics studies, and total, fission, elastic and inelastic cross sections, as well as neutron and gamma-ray production cross sections, have been measured. ORELA data have impacted over 80% of the evaluations in the U.S. Evaluated Nuclear Data File (ENDF/B), used worldwide for nuclear technology development.

ORELA staff member J. K. Dickens was selected as General Chairman of the 1994 International Conference on Nuclear Data for Science and Technology, held in Gatlinburg in May. This was the next in a series of conferences previously held in Knoxville (1979), Antwerp (1982), Santa Fe (1985), Mito (1988) and Julich (1991). The program included a wide range of interdisciplinary studies dealing with measurement, calculation, evaluation, application and use of nuclear data. Both energy and non-energy related data was treated with emphasis on application-oriented numerical data. Special attention was given to new applications (technology transfer) of nuclear data. The conference had national and international sponsorship, and over 300 experts in the nuclear data field from 30 countries participated.

Several members of our section are also involved in a NEA Working Group on International Evaluation Cooperation. The purpose of this activity is to identify and eliminate cross section discrepancies among the four major evaluated data libraries in the world. As the work continues, the libraries are expected to converge into one library for world-wide use.

Nuclear model and analysis codes continue to be improved and be used around the world. The resonance parameter code SAMMY developed in our section by N. M. Larson (CAD) can now analyze differential elastic scattering data, including corrections for finite size samples, and capture cross section data, correcting the data for finite size and multiple scattering effects. These developments will keep it unique and at the front of resonance parameter analysis code development. The nuclear model code TNG, developed by C. Y. Fu, continues to broaden its capabilities and improve its physics content through improvements to the level density. It is the workhorse of cross section evaluation work for the MeV region in our section.

EXPERIMENTAL RESULTS AND THEIR ANALYSIS

2.1

MEASUREMENT AND ANALYSIS OF THE NITROGEN TOTAL AND DIFFERENTIAL SCATTERING CROSS SECTIONS IN THE RESONANCE REGION

C. O. Beasley, Jr. N. M. Larson*
J. A. Harvey D. C. Larson
G. M. Hale[†]

[Abstract of paper presented at the Eighth ASTM-EURATOM Symposium on Reactor Dosimetry, Vail, CO, August 29–September 3, 1993; Proc. Harry Farrar IV, E. Parvin Lippincott, J. G. Williams, and D. W. Vehar, Eds., pp. 737–743 (1994)]

High-resolution neutron transmission and differential elastic scattering measurements have been made on samples of nitrogen from 0.5 eV to 10 MeV at the Oak Ridge Electron Linear Accelerator (ORELA). For the transmission measurement several different detectors were used at various flight path lengths, with high-purity nitrogen gas samples. The data have been corrected for the dead time of the time digitizer and for several small backgrounds. For the scattering measurements six detectors were placed at various angles inside an evacuated scattering chamber at 200 meters from the neutron producing target. The sample was silicon nitride held in a thin graphite container. Scattering from carbon and silicon samples was also measured to correct for these materials and calibrate the relative efficiencies of the scattering detectors. The data have been corrected for dead time and for a constant background. A preliminary analysis has been completed to obtain parameters of the resonances up to 4.8 MeV.

Research sponsored by U.S. DOE Office of Energy Research, Division of Nuclear Energy.

*Computing Applications Division.

[†]Los Alamos National Laboratory, Los Alamos, NM.

2.2

PRECISION MEASUREMENT OF THE ^{56}Fe CROSS SECTION FOR THE $E_\gamma=846\text{-keV}$ TRANSITION AND FOR E_n BETWEEN THRESHOLD AND 4 MeV

J. K. Dickens

(Abstract of paper presented at the IAEA First Research Coordination Meeting on Measurement, Calculation and Evaluation of Photon Production Data, Bologna, Italy, November 14–17, 1994)

An experimental system is described which is designed to provide accurate cross-section measurements of the production of the 846-keV gamma-ray due to inelastic neutron scattering by ^{56}Fe . Six aspects of the measurement are considered: (a) precision determination of the incident neutron flux; (b) gamma-ray detection resolution; (c) incident neutron-energy determination; (d) interacting neutron-energy resolution; (e) counting rates; and (f) multiple-scattering and attenuation corrections. For precision determination of the incident neutron flux, a simultaneous measurement of the 478-keV gamma ray from the $^{10}\text{B}(n,\alpha_1)^7\text{Li}$ reaction is proposed, since this reaction cross section has been recently determined to a precision of $\approx 2\%$ for incident neutrons up to 4 MeV. A large-volume intrinsic Ge detector is proposed for gamma-ray detection; the Oak Ridge Electron Linear Accelerator will provide a pulsed neutron beam. Measurements under actual operating conditions will be necessary to optimize counting rates and incident neutron-energy resolution. Multiple-scattering and attenuation corrections will be determined using a modification of the documented Monte-Carlo code SCINFUL; needed cross sections will be taken from evaluation, or in the case of the cross section for the $^{10}\text{B}(n,\alpha\gamma)^7\text{Li}$ monitor reaction, from recent experimental results.

Research sponsored by U.S. DOE Office of Energy Research, Division of Nuclear Energy.

2.3

**IN-BEAM GAMMA-RAY
SPECTROMETRIC
MEASUREMENTS OF
MULTI-BODY BREAKUP
REACTIONS FOR E_n
BETWEEN THRESHOLD
AND 40 MeV**

J. K. Dickens D. C. Larson

(Abstract of paper presented at the Specialists' Meeting on Measurement, Calculation and Evaluation of Photon Production Data, Bologna, Italy, November 8–11, 1994)

A system for in-beam gamma-ray spectrometric measurements to study inelastic neutron scattering has been extended to increasing incident neutron energies to study multi-body breakup reactions on light and medium-weight elements. The $(n, 2n\gamma)$ cross sections are generally the largest; however, reactions of the types $(n, \alpha\gamma)$, $(n, np\gamma)$ and $(n, 3n\gamma)$ have been observed. In addition to improved understanding of reaction channels studied by other techniques, this method provides data for some reactions, e.g. $^{56}\text{Fe}(n, 3n)^{54}\text{Fe}$, which have not been observed previously.

Research sponsored by U.S. DOE Office of Energy Research, Division of Nuclear Energy.

2.4

**NEUTRON CAPTURE AND TOTAL
CROSS SECTIONS OF ^{144}Sm**

R. L. Macklin N. W. Hill*
J. A. Harvey G. L. Tweed†

[Abstract of *Phys. Rev. C.* **48**(3), 1120 (1993)]

Neutron capture and transmission measurements have been made from 0.5 eV to 500 keV and have been analyzed to give parameters of resonances up to ~ 100 keV. The average resonance spacing for s-wave resonances was determined to be 670 ± 60 eV and the s-wave strength function $(3.6 \pm 0.8) \times 10^{-4}$. The average radiation width for s-wave resonances was 74 ± 5 meV and that for p-wave resonances somewhat larger ~ 89 meV. The Maxwellian average capture cross section at a stellar temperature of 30 keV was 92 ± 6 mb. The capture resonance integral of 1.7 ± 0.1 b calculated from the resonance parameters and the thermal

cross section is smaller than the recently measured value of 2.38 ± 0.17 b.

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

*Instrumentation and Controls Division.

†Systematic Management Services, Inc., Oak Ridge, TN.

2.5

**NEUTRON RESONANCE PARAMETERS
AND THERMAL-NEUTRON CAPTURE
BY ^{43}Ca**

M. C. Moxon* J. A. Harvey
S. Raman† J. E. Lynn‡
W. Ratynski§

[Abstract of *Phys. Rev. C.* **48**(2), 553 (1993)]

Neutron transmission measurements have been carried out on a small sample (205.9 mg) of CaCO_3 with a ^{43}Ca enrichment of 49.1%. The parameters (spins and neutron widths) of eight resonances below the neutron energy of 20 keV have been determined. This information was combined with a previously measured thermal-neutron coherent scattering length to deduce the separate scattering lengths for the two spin states present in s-wave scattering. These values were used to calculate the direct (potential + valence) capture cross sections of the primary electric-dipole gamma transitions in ^{44}Ca using optical-model potentials with physically realistic parameters. For those states below 6.2 MeV for which the $\ell=1$ (d, p) spectroscopic factors are known, the experimental cross sections are consistent with our current understanding of the direct and compound-nuclear capture processes. The processes leading to states above 6.2 MeV require further experimental and theoretical studies.

Research sponsored by U.S. Department of Energy.

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2.6

A RELATIVE MEASUREMENT OF THE $^{10}\text{B}(n, \alpha_1 \gamma)^7\text{Li}$ CROSS SECTION BETWEEN 0.2 AND 4.0 MeV

R. A. Schrack* O. A. Wasson*
D. C. Larson J. K. Dickens
J. H. Todd†

[Abstract of *Nucl. Sci. Eng.* 114, 352 (1993)]

Relative cross-section measurements for the $^{10}\text{B}(n, \alpha_1 \gamma)^7\text{Li}$ reaction were made using the Oak Ridge Electron Linear Accelerator Laboratory neutron source. The cross sections were measured by observing the 478-keV photon using an intrinsic germanium detector. The neutron flux was monitored with a high-efficiency plastic scintillator. Monte Carlo calculations were used to provide multiple-scattering and neutron-attenuation corrections to the data. The measured cross sections differ as much as 40% from the ENDF/B-VI evaluation for incident neutron energies greater than 1.5 MeV.

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

*National Institute of Standards and Technology, Gaithersburg, MD.

†Instrumentation and Controls Division.

2.7

THE ORNL NEUTRON-CAPTURE CROSS SECTION FACILITY

R. R. Spencer J. H. Todd*
N. M. Larson† L. W. Weston*

(Abstract of paper presented at the International Conference on Nuclear Data for Science and Technology, Gatlinburg, TN, May 9-13, 1994)

In order to meet the cross section needs required by astrophysical calculations within recent cosmological models, the neutron-capture cross section facility at the Oak Ridge Electron Linear Accelerator (ORELA) has been improved and restored to operation. Changes to the system include replacement of the C_6F_6 scintillation detectors with C_6D_6 , reduction of the structural mass near and around the detectors, and incorporation of a new IBM PS/2-based data handler. Preliminary measurements on natural iron samples yield

$\Gamma_n = 61.6 \pm 1.8$ meV for the 1.15-keV resonance, using a fixed $\Gamma_\gamma = 574$ meV from transmission, compared to the value $\Gamma_n = 61.7 \pm 0.9$ meV obtained from the transmission measurements.

Research sponsored by U.S. DOE Office of Energy Research, Division of Nuclear Energy.

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†Computing Applications Division.

2.8

NORMALIZATION AND MINIMUM VALUES OF THE ^{239}Pu FISSION CROSS SECTION

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

[Abstract of *Nucl. Sci. Eng.* 115, 164 (1993)]

Measurements were carried out to accurately determine the shape of the fission cross section of ^{239}Pu down to 0.025 eV in order to determine a more accurate normalization for previously reported fission cross-section measurements from Oak Ridge National Laboratory at higher neutron energies. Also, experimental backgrounds were carefully studied to verify the cross section between resonances. Results indicate a 3.0% higher normalization should have been used previously, and the low cross sections between resonances reported earlier were correct. New differential cross-section data were obtained from 0.002 to 100 eV.

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

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CROSS SECTION EVALUATION AND NUCLEAR MODELING

2.9

NEUTRON EMISSION SPECTRA CALCULATED WITH EXCITON LEVEL DENSITIES BASED ON ONE AND TWO KINDS OF FERMIONS

C. Y. Fu

(Abstract of paper presented at the International Conference on Nuclear Data for Science and Technology, Gatlinburg, TN, May 9-13, 1994)

Recent calculations show that ratios of exciton level densities in one- and two-fermion formulations vary with both excitation energy U and exciton number n . This means that the exciton level density in the two-fermion formulation, which is the correct one, cannot be simulated by a normalization of its one-fermion counterpart to the total level density in the two-fermion formulation, which is only a function of U . Such a normalization has been adopted in several unified Hauser-Feshbach and pre-equilibrium codes. Some of the resulting problems are studied and clarified in this paper. It is shown that all three exciton level densities (one fermion, two fermion, and normalization) lead to very different cross sections and neutron emission spectra if a fixed set of model parameters are used. However, close agreements of calculated neutron emission spectra with data for all three options can be obtained by adjusting a parameter that controls the pre-equilibrium strength. A fourth option of an exciton level density that contains only bound final states in the two-fermion formulation yields the best results for incident energies lower than 15 MeV.

Research sponsored by U.S. DOE Office of Energy Research, Division of Nuclear Energy.

2.10

TNG CALCULATIONS AND EVALUATIONS OF PHOTON PRODUCTION DATA FOR SOME ENDF/B-VI MATERIALS

C. Y. Fu

(Abstract of paper presented at the OECD NEANSC Specialists' Meeting on Measurement, Calculation and Evaluation of Photon Production Data, Bologna, Italy, November 8-11, 1994)

Among the new evaluations in the ENDF/B-VI general purpose files, 25 were based on calculations using TNG, a consistent Hauser-Feshbach pre-equilibrium nuclear model code. The photon production cross sections and spectra were calculated simultaneously with the particle emission cross sections and spectra, assuring energy balance for each reaction. The theories used in TNG for these calculations are summarized. Several examples of photon production data, taken from the ENDF/B-VI files, are compared with the available experimental data.

Research sponsored by U.S. DOE Office of Energy Research, Division of Nuclear Energy.

2.11

STATUS OF NUCLEAR DATA FOR ITER APPLICATIONS

D. C. Larson E. T. Cheng*
F. M. Mann† G. Saji‡

(Abstract of paper presented at the International Conference on Nuclear Data for Science and Technology, Gatlinburg, TN, May 9-13, 1994)

As the development of a near-term fusion reactor, such as the International Thermonuclear Experimental Reactor (ITER), enters the engineering design activity phase, one of the essential elements leading to the successful design, construction and operation of such a reactor is nuclear data. High quality nuclear data for all reactor materials relevant to ITER will be required in order to assess the nuclear performance, radiation damage, and safety and environmental aspects of all reactor components. In this paper we review the

current ITER design, noting which materials and associated nuclear data are important in the various reactor components. We also review the contents of the Fusion Evaluated Nuclear Data Library (FENDL) accepted for use by ITER, and identify materials for which nuclear data improvements are required.

Research sponsored by U.S. DOE Office of Energy Research, Division of Nuclear Energy.

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†Westinghouse Hanford Corporation, Hanford, WA.

‡ITER San Diego Co-Center, La Jolla, CA.

2.12

ANALYSIS OF $\text{Fe}(n, x\gamma)$ CROSS SECTIONS USING THE TNG NUCLEAR REACTIONS MODEL CODE

K. J. McCollam*

(Abstract of ORNL/TM-12358, April 1993)

Theoretical gamma-ray cross sections have been calculated using a nuclear reaction model code. These are compared to experimental gamma-ray production cross sections obtained from neutron interactions with ^{56}Fe at incident neutron energies of 1 to 40 MeV. The optical model and nuclear level density parameters in the code have been varied to affect a close agreement between calculations and the data. Present analyses, which focus on incident neutron energies between 17 and 40 MeV, display somewhat better agreement than those previously reported.

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

*University of Minnesota, St. Paul, MN.

2.13

COMMENTS ON THE ENDF/B-VI EVALUATIONS FOR ^{235}U IN THE NEUTRON ENERGY REGION FROM 1 TO 20 eV

M. C. Moxon*

(Abstract of ORNL/TM-12304, February 1993)

A discrepancy of $\sim 6\%$ has been reported between the measured capture resonance integral of ^{235}U and that calculated from the resonance parameters in ENDF/B-VI. This discrepancy may be due to the use of a value for the average radiation width which is too small. The possibility that small resonances whose widths are primarily capture were missed experimentally due to their proximity to resonances with large fission widths was also considered, but dismissed. Since accurate values of neutron widths, Γ_n , and total widths, Γ_T , of resonances can be determined from transmission data and are not dependent on any normalization factors, an interim solution might be to assume an average radiation width Γ_γ and calculate the fission width Γ_f for each resonance from the relation $\Gamma_T = \Gamma_n + \Gamma_\gamma$. The ratio of the partial fission widths of the two fission channels for each resonance would be kept the same as in ENDF/B-VI data files. The average value of the radiation width selected should also be consistent with differential and integral measurements.

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

*A.E.A. Technology, Harwell.

2.14

COMPILATION OF REQUESTS FOR NUCLEAR DATA

L. W. Weston D. C. Larson

(Abstract of ORNL/TM-12291, February 1993)

This compilation represents the current needs for nuclear data measurements and evaluations as expressed by interested fission and fusion reactor designers, medical users of nuclear data, nuclear data evaluators, CSEWG members and other interested parties. The requests and justifications

are reviewed by the Data Request and Status Subcommittee of CSEWG as well as most of the general CSEWG membership.

The basic format and computer programs for the Request List were produced by the National Nuclear Data Center (NNDC) at Brookhaven National Laboratory. The NNDC produced the Request List for many years. The Request List is compiled from a computerized data file.

This is a working document in that it will change with time. New requests or comments may be submitted to the editors or a regular CSEWG member at any time.

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

Section 3

INTELLIGENT SYSTEMS

3.0. INTRODUCTION

R. C. Mann

Research activities in the Intelligent Systems Section (ISS) concentrate on 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 Dynamic Systems and Intelligent Sensory Control Group, the Informatics Group and the Cognitive Systems and Human Factors Group. The Center for Engineering Systems Advanced Research (CESAR), sponsored 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 systems. Other DOE sponsors include the Office of Health and Environmental Research, Office of Fossil Energy, Office of Nonproliferation and National Security, Office of Environmental Restoration and Waste Management, and the Technology Transfer Program of Energy Research. Other sponsors include the Office of Naval Research, the National Highway Transportation Safety Administration, the Federal Highway Administration, the Federal Aviation Administration, and the Nuclear Regulatory Commission.

During this reporting period the section experienced growth in a number of exciting research areas. The Human Factors Group grew due to new work on human-machine interface problems in advanced transportation systems, including intelligent vehicle/highway systems. The Informatics Group grew due to expanding work on biomedical applications, leveraging the success of GRAIL and related systems, and due to new work in information processing in collaboration with the integrated U.S. Textile Industry as part of the AMTEXTM partnership. The CESAR program successfully passed its fourth on-site peer-review. Under the new leadership of Dr. Jacob Barhen, the Center is rapidly moving to seize new leveraging opportunities for the research thrusts of the Center in intelligent systems and analysis of complex systems.

The Omnidirectional Holonomic Platform developed by Francois Pin and Steve Killough, based on an orthogonal wheel design, won a 1993 RD100 Award. For the second year in a row (GRAIL in 1992), a development by researchers in the section was recognized by a RD100 Award for one of the 100 most technologically significant products of the year.

ROBOTICS AND INTELLIGENT SYSTEMS

3.1

**A NEW SOLUTION METHOD FOR
THE INVERSE KINEMATIC
JOINT VELOCITY CALCULATIONS
OF REDUNDANT MANIPULATORS**

F. G. Pin* P. F. R. Belmans[†]
J.-C. Culioli[‡] D. D. Carlson[§]
F. A. Tulloch[#]

[Abstract of 1994 IEEE International Conference on Robotics and Automation, San Diego, CA, May 8-13, 1994; Proc. pp. 96-102 (1994)]

A new analytical method to resolve underspecified systems of algebraic equations is presented. The method is referred to as the Full Space Parameterization (FSP) method and utilizes easily-calculated projected solution vectors to generate the entire space of solutions of the underspecified system. Analytic parameterizations for both the space of solutions and the nullspace of the system reduce the determination of a task-requirement-based single solution to a $m-n$ dimensional problem, where $m-n$ is the degree of underspecification, or degree of redundancy, of the system. An analytical solution is presented to directly calculate the least-norm solution from the parameterized space and the results are compared to solutions of the standard pseudo-inverse algorithm which embodies the (least-norm) Moore-Penrose generalized inverse. Application of the new solution method to a variety of systems and task requirements are discussed, and sample results using four-link planar manipulators with one or two degrees of redundancy and a seven degree-of-freedom manipulator with one or four degrees of redundancy are presented to illustrate the efficiency of the new FSP method and algorithm.

Research sponsored by U.S. DOE Office of Technology Support Programs and Oak Ridge Associated Universities.

*Transferred to ORNL Robotics and Process Systems Division after publication of this work.

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3.2

**A NEW TECHNIQUE FOR DYNAMIC
LOAD DISTRIBUTION WHEN TWO
MANIPULATORS MUTUALLY LIFT
A RIGID OBJECT - PART 1:
THE PROPOSED TECHNIQUE**

M. A. Unseren

[Abstract of paper presented at the International Symposium on Robotics and Manufacturing (ISRAM '94), Wailea, Maui, HI, August 14-18, 1994; Proc. Intelligent Automation and Soft Computing Trends in Research, Development, and Applications, Vol. 2, pp. 359-366 (1994)]

A general framework for solving the dynamic load distribution when two manipulators hold a rigid object is proposed. The underspecified problem of solving for the contact forces and torques based on the object's equations of motion is transformed into a well specified problem. This is accomplished by augmenting the object's equations of motion with additional equations which relate a new vector variable quantifying the internal contact force and torque degrees of freedom (DOF) as a linear function of the contact forces and torques. The resulting augmented system yield a well specified solution for the contact forces and torques in which they are separated into their motion inducing and internal components. A particular solution is suggested which enables the designer to conveniently specify what portion of the payload's mass each manipulator is to bear. It is also shown that the results of the previous work are just a special case of the general load distribution framework described here.

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

3.3

**A NEW TECHNIQUE FOR DYNAMIC
LOAD DISTRIBUTION WHEN TWO
MANIPULATORS MUTUALLY LIFT
A RIGID OBJECT - PART 2:
DERIVATION OF ENTIRE SYSTEM
MODEL AND CONTROL
ARCHITECTURE**

M. A. Unseren

[Abstract of paper presented at the International Symposium on Robotics and Manufacturing (ISRAM '94), Wailea, Maui, HI, August 14-18, 1994; Proc. Intelligent Automation and Soft Computing Trends in Research, Development, and Applications, Vol. 2, pp. 367-372 (1994)]

A rigid body model for the entire system which accounts for the load distribution scheme proposed in Part 1 as well as for the dynamics of the manipulators and the kinematic constraints is derived in the joint space. Direct application of the method is to obtain the model results in an inertia matrix for the entire system which is not symmetrical. A technique is presented for expressing the object dynamics in terms of the joint variables of both manipulators which leads to a positive definite and symmetric inertia matrix. The model is then transformed to obtain reduced order equations of motion and a separate set of equations which govern the behavior of the internal contact forces. The control architecture proposed is applied to the model which results in the explicit decoupling of the position and internal contact force-controlled degrees of freedom (DOF).

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

3.4

**DERIVATION OF THREE CLOSED
LOOP KINEMATIC VELOCITY
MODELS USING NORMALIZED
QUATERNION FEEDBACK FOR AN
AUTONOMOUS REDUNDANT
MANIPULATOR WITH APPLICATION
TO INVERSE KINEMATICS**

M. A. Unseren

(Abstract of ORNL/TM-12288, April 1993)

The report discusses the orientation tracking control problem for a kinematically redundant, autonomous manipulator moving in a three dimen-

sional workspace. The orientation error is derived using the normalized quaternion error method of Ickes; the Luh, Walker, and Paul error method, and a method suggested here utilizing the Rodrigues parameters, all of which are expressed in terms of normalized quaternions. The analytical time derivatives of the orientation errors are determined. The latter, along with the translational velocity error, form a closed loop kinematic velocity model of the manipulator using normalized quaternion and translational position feedback. An analysis of the singularities associated with expressing the models in a form suitable for solving the inverse kinematics problem is given. Two redundancy resolution algorithms originally developed using an open loop kinematic velocity model of the manipulator are extended to properly take into account the orientation tracking control problem. This report furnishes the necessary mathematical framework required prior to experimental implementation of the orientation tracking control schemes on the seven axis CESArm research manipulator or on the seven-axis Robotics Research K1207i dexterous manipulator, the latter of which is to be delivered to the Oak Ridge National Laboratory in 1993.

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

3.5

**USING MINIMAX APPROACH TO PLAN
OPTIMAL TASK COMMUTATION
CONFIGURATIONS FOR COMBINED
MOBILE PLATFORM-MANIPULATOR
SYSTEMS**

**F. G. Pin* J.-C. Culicli†
D. B. Reister**

[Abstract of *IEEE Transactions on Robotics and Automation* 10(1), 44 (1994)]

An important characteristic of mobile manipulators is their particular kinematic redundancy created by the addition of the degrees of freedom of the platform and those of the manipulator. This kinematic redundancy is very desirable since it allows mobile manipulators to operate under many modes of motion and to perform a wide variety of tasks. On the other hand, it also significantly complicates the problem of planning a series of sequential tasks, in particular for the critical times at

which the system needs to "switch" from one task to the other (task commutation), with changes in mode of motion, task requirement, and task constraints. This paper focuses on the problem of planning the positions and configurations in which the system needs to be at task commutation in order to assure that it can properly initiate the next task to be performed. The concept of and need for "commutation configurations" in sequences of mobile manipulator tasks is introduced, and an optimization approach is proposed for their calculation during the task sequence planning phase. A variety of optimization criteria were previously investigated to optimize the task commutation configurations of the system when task requirements involve obstacle avoidance, reach, maneuverability, and optimization of strength. In this paper, we show that a "minimax" approach is particularly adapted for most of these requirements. We develop the corresponding criteria and discuss solution algorithms to solve the "minimax" optimization problems. An implementation of the algorithms for our HERMIES-III mobile manipulator is then described and sample results are presented and discussed.

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

*Transferred to ORNL Robotics and Process Systems Division after publication of this work.

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3.6

OMNIDIRECTIONAL HOLONOMIC PLATFORMS

F. G. Pin* S. M. Killough†

[Abstract of paper presented at the Twelfth Symposium on Energy Engineering Sciences, Argonne, IL, April 27-29, 1994; Proc. 169-176 (1994)]

This paper presents the concepts for a new family of wheeled platforms which feature full omnidirectionality with simultaneous and independently controlled rotational and translational motion capabilities. We first present the "orthogonal-wheels" concept and the two major wheel assemblies on which these platforms are based. We then describe how a combination of these assemblies with appropriate control can be used to generate an omnidirectional capability for mobile robot

platforms. The design and control of two prototype platforms are then presented and their respective characteristics with respect to rotational and translational motion control are discussed.

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

*Transferred to ORNL Robotics and Process Systems Division after publication of this work.

†Robotics and Process Systems Division.

3.7

A NEW FAMILY OF OMNIDIRECTIONAL AND HOLONOMIC WHEELED PLATFORMS FOR MOBILE ROBOTS

F. G. Pin* S. Killough†

[Abstract of *IEEE Transactions on Robotics and Automation* 10(4), 480 (1994)]

This paper presents the concepts for a new family of holonomic wheeled platforms which feature full omnidirectionality with simultaneous and independent rotational and translational motion capabilities. We first present the "orthogonal-wheels" concept and the two major wheel assemblies on which these platforms are based. We then describe how a combination of these assemblies with appropriate control can be used to generate an omnidirectional capability for mobile robot platforms. Several alternative designs are considered, and their respective characteristics with respect to rotational and translational motion control are discussed. The design and control of a prototype platform developed to test and demonstrate the proposed concepts is then described, and experimental results illustrating the full omnidirectionality of the platform with decoupled rotational and translational degrees of freedom are presented.

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

*Transferred to ORNL Robotics and Process Systems Division after publication of this work.

†Robotics and Process Systems Division.

3.8

USING A MIN-MAX OF TORQUE TO RESOLVE REDUNDANCY FOR A MOBILE MANIPULATOR

D. B. Reister

(Abstract of ORNL/TM-12489, November 1993)

We have considered the problem of determining the time trajectories of the joint variables of a mobile manipulator with many redundant degrees of freedom that will minimize the maximum value of the torque during a large scale motion by the manipulator. To create a well defined problem, we will divide the problem into two components: path planner and surveyor. The path planner will choose a path (between two points in Cartesian space) that will minimize the maximum value of the torque along the path. The input to the path planner is a network of path segments with the maximum value of the torque on each segment. The surveyor will find the points in joint space that are local minimums for the maximum value of the torque at each Cartesian position and define the network of path segments. In this paper, our focus will be on the surveyor and not on the path planner.

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

3.9

TIME OPTIMAL PATHS FOR HIGH SPEED MANEUVERING

D. B. Reister S. M. Lenhart

[Abstract of *International Journal of Robotics Research* (in press); also ORNL/TM-12289, January 1993]

Recent theoretical results have completely solved the problem of determining the minimum length path for a vehicle moving from an initial configuration to a final configuration. Time optimal paths for a constant speed vehicle are a subset of the minimum length paths. This paper uses the Pontryagin maximum principle to find time optimal paths for a constant speed vehicle. The time optimal paths consist of sequences of arcs of circles and straight lines. The maximum principle introduces concepts (dual variables, bang-bang solutions, singular solutions, and transversality con-

ditions) that provide important insight into the nature of the time optimal paths. We explore the properties of the optimal paths and present some experimental results for a mobile robot following an optimal path.

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

3.10

PLANNING A TIME-MINIMAL MOTION AMONG MOVING OBSTACLES

K. Fujimura H. Samet*

[Abstract of *Algorithmica* (in press)]

Motion planning for a point robot is studied in a time-varying environment. Each obstacle is a convex polygon that moves in a fixed direction at a constant speed. The point to be reached (referred to as the destination point) also moves along a known trajectory. The concept of 'accessibility' from a point to a moving object is introduced, and is used to define a graph on a set of moving obstacles. If the point robot is able to move faster than any of the obstacles, then the graph exhibits an important property: a time-minimal motion is given as a sequence of edges in the graph. An algorithm is described for generating a time-minimal motion and its execution time is analyzed.

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

*University of Maryland, College Park, MD.

3.11

**POSITION AND CONSTRAINT
FORCE CONTROL OF A
VEHICLE WITH TWO OR
MORE STEERABLE
DRIVE WHEELS**

D. B. Reister M. A. Unseren

[Abstract of *IEEE Transactions on Robotics and Automation* 9(6), 723 (1993)]

Since a vehicle with two or more steerable drive wheels is always traveling in a circle about an instantaneous center of rotation, the motion of the wheels is constrained. The wheel translational velocity divided by the radius to the center of rotation must be the same for all wheels. When the drive wheels are controlled independently using position control, the motion of the wheels may violate the constraints and the wheels may slip. Consequently, substantial errors can occur in the position and orientation of the vehicle. A vehicle with N steerable drive wheels has N holonomic constraints on the steering angles, $(N-1)$ nonholonomic constraints on the wheel velocities, and one degree of freedom. We have developed a new approach to the control of a vehicle with N steerable drive wheels. The novel aspect of our approach is the introduction of variables to control the constraint forces. To control the vehicle, we have one variable to control motion and (N_1) variables that can control the constraint forces to reduce errors. Recently, Kankaanranta and Koivo developed a control architecture that allows the control variables for force and position to be decoupled. In the work of Kankaanranta and Koivo the control variables for force are an exogenous input. We have made the control variables for force endogenous by defining them in terms of the errors in satisfying the nonholonomic constraints. We have applied the control architecture to the HERMIES-III robot and have measured a dramatic reduction in error (more than a factor of 20) compared to motions without constraint force control.

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

3.12

**TERRAIN FOLLOWING AND MAPPING
OF ARBITRARY SURFACES USING
HIGH PRECISION PROXIMITY DATA**

J. E. Baker

[Abstract of *Optical Engineering* 32(5), 1117 (1993)]

Many robotic operations, e.g., mapping, scanning, feature following, etc., require accurate surface following or arbitrary targets. This paper presents a versatile surface following and mapping system designed to promote hardware, software and application independence, modular development, and upward expandability. These goals are met by: a full, *a priori* specification of the hardware and software interfaces; a modular system architecture; and a hierarchical surface-data analysis method, permitting application specific tuning at each conceptual level of topological abstraction. This surface following system was fully designed and implemented independently of any specific robotic host, then successfully integrated with and demonstrated on a completely *a priori* unknown, real-time robotic system.

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

3.13

**EXPERIMENTAL INVESTIGATIONS
OF SENSOR-BASED SURFACE
FOLLOWING PERFORMED BY A
MOBILE MANIPULATOR**

**D. B. Reister M. A. Unseren
J. E. Baker F. G. Pin***

(Abstract of ORNL/TM-12864, October 1994)

We discuss a series of surface following experiments using a range finder mounted on the end of an arm that is mounted on a vehicle. The goal is to keep the range finder at a fixed distance from an unknown surface and to keep the orientation of the range finder perpendicular to the surface.

During the experiments, the vehicle moves along a predefined trajectory while planning software determines the position and orientation of the arm. To keep the range finder perpendicular to the surface, the planning software calculates the surface normal for the unknown surface. We assume that the unknown surface is a cylinder (the surface depends on x and y but does not depend on z). To calculate the surface normal, the planning software must calculate the locations (x , y) of points on the surface in world coordinates. The calculation requires data on the position and orientation of the vehicle, the position and orientation of the arm, and the distance from the range finder to the surface.

We discuss four series of experiments. During the first series of experiments, the calculated surface normal values had large high frequency random variations. A filter was used to produce an average value for the surface normal and we limited the rate of change in the yaw angle target for the arm. We performed the experiment for a variety of concave and convex surfaces. While the experiments were qualitative successes, the measured distance to the surface was significantly different than the target. The distance errors were systematic, low frequency, and had magnitudes up to 25 mm.

During the second series of experiments, we reduced the variations in the calculated surface normal values. While reviewing the data collected while following the surface of a barrel, we found that the radius of the calculated surface was significantly different than the measured radius of the barrel. We performed a third series of experiments with the arm in a fixed position and determined that the position and orientation errors in the dead reckoning system for the vehicle was the source of the radii errors.

Our objective during the fourth series of experiments was to reduce the distance errors. Although we introduced a correction term, we were unable to significantly reduce the distance errors.

We concluded that the experiment must be redesigned to reduce the errors in the calculations of points on the unknown surface.

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

*Transferred to ORNL Robotics and Process Systems Division after publication of this work.

3.14

EXPERIMENTAL INVESTIGATIONS OF SENSOR-BASED SURFACE FOLLOWING TASKS BY A MOBILE MANIPULATOR

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[Abstract of paper presented at the International Symposium on Experimental Robotics, Kyoto, Japan, October 27-29, 1993; Proc. pp. 110-114 (1993); also book chapter in *Control and Information Sciences: Experimental Robotics III*, pp. 514-527, T. Yoshikawa and F. Miyazaki, Eds., Springer-Verlag (1993)]

This paper discusses experimental investigations of the feasibility and requirements of simultaneous external-sensor-based-control of the wheeled platform and the manipulator of a mobile robot. The experiments involve 3-D arbitrary surface following by the manipulator while the platform moves along a predefined trajectory.

A variety of concave and convex surfaces were used in the experiments, during which target and measured values of the platform and arm positions and orientations, together with the surface absolute location and normal estimates, were logged at 10 Hz. For all experiments, the data logs showed significant noise, at high frequency, in the calculated surface normal values despite smooth tracking of their target values by the arm and the platform, with typical closed loop delays between target and achieved values of the order of 100 msec. This high-frequency noise in the calculated values is conjectured to result mainly from the arm's transmission cables compliance and backlash in

the spherical wrist gears. On the other hand, the end-effector distance to the surface showed some low frequency errors of the order of $\pm 20\%$. The two major sources of these low frequency errors appeared to reside respectively in the low values of the velocity bound and gain parameters utilized to filter the high frequency noise in the calculated normal values prior to using them as input to the arm control, and in the rolling contact of the platform's rubber-coated wheels on the ground where significant errors in the platform's positions and orientations can accumulate.

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

*Transferred to ORNL Robotics and Process Systems Division after publication of this work.

3.15

ON APPROXIMATE REASONING AND MINIMAL MODELS FOR THE DEVELOPMENT OF ROBUST OUTDOOR VEHICLE NAVIGATION SCHEMES

F. G. Pin*

[Abstract of paper presented at the ICAR '93, The Sixth International Conference on Advanced Robotics, Tokyo, Japan, November 1-2, 1993; Proc. pp. 257-262 (1993)]

Outdoor sensor-based operation of autonomous robots has revealed to be an extremely challenging problem, mainly because of the difficulties encountered when attempting to represent the many uncertainties which are always present in the real world. These uncertainties are primarily due to sensor imprecisions and unpredictability of the environment, i.e., lack of full knowledge of the environment characteristics and dynamics. Two basic principles, or philosophies, and their associated methodologies are proposed in an attempt to remedy some of these difficulties. The first principle is based on the concept of "minimal model" for accomplishing given tasks and proposes to utilize only the minimum level of information and precision necessary to accomplish elemental functions of complex tasks. This approach diverges completely from the direction taken by most artificial vision studies which conventionally call for crisp and detailed analysis of every available component in the perception data. The paper will first review the basic concepts of this approach and will discuss

its pragmatic feasibility when embodied in a behaviorist framework. The second principle which is proposed deals with implicit representation of uncertainties using Fuzzy Set Theory-based approximations and approximate reasoning, rather than explicit (crisp) representation through calculation and conventional propagation techniques. A framework which merges these principles and approaches is presented, and its application to the problem of sensor-based outdoor navigation of a mobile robot is discussed. Results of navigation experiments with a real car in actual outdoor environments are also discussed to illustrate the feasibility of the overall concept.

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

*Transferred to ORNL Robotics and Process Systems Division after publication of this work.

3.16

AUTOMATIC GENERATION OF FUZZY RULES FOR THE SENSOR-BASED NAVIGATION OF A MOBILE ROBOT

F. G. Pin* Y. Watanabe†

[Abstract of paper presented at the International Symposium on Robotics and Manufacturing (ISRAM '94), Wailea, Maui, HI, August 14-18, 1994; Proc. Intelligent Automation and Soft Computing Trends in Research, Development, and Applications (1994)]

A system for automatic generation of fuzzy rules is proposed which is based on a new approach, called "Fuzzy Behaviorist," and on its associated formalism for rule base development in behavior-based robot control systems. The automated generator of fuzzy rules automatically constructs the set of rules and the associated membership functions that implement reasoning schemes that have been expressed in qualitative terms. The system also checks for completeness of the rule base and independence and/or redundancy of the rules to ensure that the requirements of the formalism are satisfied. Examples of the automatic generation of fuzzy rules for cases involving suppression and/or inhibition of fuzzy behaviors are given and discussed. Experimental results obtained with the automated fuzzy rule generator applied to the domain of sensor-based navigation in *a priori* unknown environments using one

of our autonomous test-bed robots are then presented and discussed to illustrate the feasibility of large-scale automatic fuzzy rule generation using our proposed "Fuzzy Behaviorist" approach.

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

*Transferred to ORNL Robotics and Process Systems Division after publication of this work.

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3.17

SENSOR-BASED NAVIGATION OF A MOBILE ROBOT USING AUTOMATICALLY CONSTRUCTED FUZZY RULES

Y. Watanabe* F. G. Pin†

[Abstract of paper presented at ICAR '93, The Sixth International Conference on Advanced Robotics, Tokyo, Japan, November 1-2, 1993; Proc. 81-87 (1993)]

A system for automatic generation of fuzzy rules is proposed which is based on a new approach, called "Fuzzy Behaviorist," and on its associated formalism for rule base development in behavior-based robot control systems. The automated generator of fuzzy rules automatically constructs the set of rules and the associated membership functions that implement reasoning schemes that have been expressed in qualitative terms. The system also checks for completeness of the rule base and independence and/or redundancy of the rules to ensure that the requirements of the formalism are satisfied. Examples of the automatic generation of fuzzy rules for cases involving suppression and/or inhibition of fuzzy behaviors are given and discussed. Experimental results obtained with the automated fuzzy rule generator applied to the domain of sensor-based navigation in a priori unknown environments using one of our autonomous test-bed robots are then presented and discussed to illustrate the feasibility of large-scale automatic fuzzy rule generation using our proposed "Fuzzy Behaviorist" approach.

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

*Hitachi Construction Machinery Co., Tsuchiura, Japan.

†Transferred to ORNL Robotics and Process Systems Division after publication of this work.

3.18

USING FUZZY BEHAVIORS FOR THE OUTDOOR NAVIGATION OF A CAR WITH LOW-RESOLUTION SENSORS

F. G. Pin* Y. Watanabe†

[Abstract of paper presented at the 1993 IEEE International Conference on Robotics and Automation, Atlanta, GA, May 2-6, 1993; Proc. Vol. 1, pp. 548-553 (1993)]

Vehicle control in a priori unknown, unpredictable, and dynamic environments requires many calculational and reasoning schemes to operate on the basis of very imprecise, incomplete, or unreliable data. For such systems, in which all the uncertainties can not be engineered away, approximate reasoning may provide an alternative to the complexity and computational requirements of conventional uncertainty analysis and propagation techniques. A proposed approach using superposition of elemental fuzzy behaviors to emulate human-like qualitative reasoning schemes is first discussed. We then describe how a previously developed navigation scheme implemented on custom-designed VLSI fuzzy inferencing boards for indoor navigation of a small laboratory-type robot was progressively enhanced to investigate two control modes for driving a car in a priori unknown environments on the basis of sparse and imprecise sensor data. In the first mode, the car navigates fully autonomously, while in the second mode, the system acts as a driver's aid providing the driver with linguistic (fuzzy) commands to turn left or right and speed up or slow down depending on the obstacles perceived by the sensors. Experiments with both modes of control are described in which the system uses only three acoustic range (sonar) sensor channels to perceive the environment. Simulation results as well as indoors and outdoors experiments are presented and discussed to illustrate the feasibility of outdoor navigation using fuzzy behaviors operating on possibly very inaccurate sensor data.

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

*Transferred to ORNL Robotics and Process Systems Division after publication of this work.

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3.19

DRIVING A CAR USING REFLEXIVE FUZZY BEHAVIORS

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[Abstract of paper presented at the Second IEEE International Conference on Fuzzy Systems, San Francisco, CA, March 28–April 1, 1993; Proc. pp. 1425–1430 (1993)]

Vehicle control in *a-priori* unknown, unpredictable, and dynamic environments requires many calculational and reasoning schemes to operate on the basis of very imprecise, incomplete, or unreliable data. For such systems, in which all the uncertainties can not be engineered away, approximate reasoning may provide an alternative to the complexity and computational requirements of conventional uncertainty analysis and propagation techniques. Two types of computer boards including custom-designed VLSI chips have been developed to add a fuzzy inferencing capability to real-time control systems. All inferencing rules on a chip are processed in parallel, allowing execution of the entire rule base in about 30 μ sec (i.e., at rates much faster than sensor data acquisition), and therefore, making control of “reflex-type” of motions envisionable. The use of these boards and the approach using superposition of elemental sensor-based behaviors for the development of qualitative reasoning schemes emulating human-like navigation in *a-priori* unknown environments are first discussed. We then describe how the human-like navigation scheme implemented on one of the qualitative inferencing boards was installed on a test-bed platform to investigate two control mode for driving a car in *a-priori* unknown environments on the basis of sparse and imprecise sensor data. In the first mode, the car navigates fully autonomously, while in the second mode, the system acts as a driver’s aid providing the driver with linguistic (fuzzy) commands to turn left or right and speed up or slow down depending on the obstacles perceived by the sensors. Experiments with both modes of control are described in which the system uses only three acoustic range (sonar) sensor channels to perceive the environment. Simulation results as well as indoors and outdoors experiments are presented and discussed to illustrate the feasibility and robustness of autonomous navigation and/or safety enhancing driver’s aid using the new fuzzy

inferencing hardware system and some human-like reasoning schemes which may include as little as six elemental behaviors embodied in fourteen qualitative rules.

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

*Transferred to ORNL Robotics and Process Systems Division after publication of this work.

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3.20

DRIVING A CAR WITH SPARSE AND IMPRECISE SENSOR DATA USING VLSI FUZZY INFERENCING CHIPS AND BOARDS

F. G. Pin* Y. Watanabe†

[Abstract of paper presented at the 12th International Federation of Automatic Control World Congress, Sydney, Australia, July 19–23, 1993; Proc. Vol. 5, pp. 561–564 (1993)]

Two types of computer boards which incorporate custom-designed VLSI fuzzy inferencing chips have been developed to add a qualitative reasoning capability to real-time control systems. The design and operation of these boards are first described and a proposed approach which merges the Fuzzy Set and Behavior Theories to emulate human-like perception-based reasoning is presented. This approach is then applied to the development of qualitative reasoning schemes for human-like driving and navigation in *a-priori* unknown environments. We show that the superposition of elemental sensor-based behaviors which our proposed approach allows, results in easy development and testing of the inferencing rule base, while providing for progressive addition of behaviors to resolve situations of increasing complexity.

The human-like navigation scheme implemented on one of the qualitative inferencing boards was first tested on a simulation system and then installed on a test-bed platform. The investigation focussed on developing and demonstrating two control modes for the driving of a car in *a-priori* unknown environments on the basis of sparse and imprecise data. In the first mode, the car navigates fully autonomously, while in the second mode, the system acts as a driver’s aid providing the driver with linguistic (fuzzy) commands to

turn left or right and speed up or slow down depending on the obstacles perceived by the sensors. Experiments with both modes of control are presented in which the system uses only three channels of acoustic range (sonar) sensors to perceive the environment. Sample results in both simulated and actual indoors and outdoors environments are discussed to illustrate the feasibility and robustness of the proposed fuzzy behaviors approach for sensor-based functions such as autonomous navigation and/or driver's aid for safety enhancement.

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

*Transferred to ORNL Robotics and Process Systems Division after publication of this work.

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3.21

STEPS TOWARD SENSOR-BASED VEHICLE NAVIGATION IN OUTDOOR ENVIRONMENTS USING A FUZZY BEHAVIORIST APPROACH

F. G. Pin* Y. Watanabe†

[Abstract of *Journal of Intelligent and Fuzzy Systems* 1, 95 (1993)]

Because outdoor environments are typically dynamic and not fully predictable, real-time vehicle control in such environments requires many calculational and reasoning schemes to operate on the basis of incomplete, unreliable, and/or imprecise information. For such systems, in which all the uncertainties cannot be engineered away, approximate reasoning may provide an alternative to the complexity and computational requirements of conventional uncertainty analysis and propagation techniques. Two types of computer boards including custom-designed VLSI fuzzy inferencing chips have been developed to add an approximate reasoning capability to real-time control systems. All inferencing rules on a chip are processed in parallel, allowing execution of the entire rule base in about 30 μ s (i.e., at rates much faster than typical sensor sampling rates) and therefore making control of "reflex-type" motions envisionable. The use of these boards and a proposed approach using superposition of sensor-based fuzzy behaviors for the development of qualitative reasoning schemes are first discussed. We then describe how

a fuzzy behavior-based navigation scheme emulating human-like navigation in *a priori* unknown environments was implemented on one of the fuzzy inferencing boards and installed on a test-bed platform to investigate two control modes for driving a car on the basis of sparse and imprecise sensor data. In the first mode, the car navigates fully autonomously, while in the second mode, the system acts as a driver's aid providing the driver with linguistic-type (fuzzy) commands to turn left or right, and speed up, slow down, or back up depending on the obstacles perceived by the sensors. Experiments with both modes of control are described in which the system uses only three acoustic-range (sonar) sensor channels to perceive the environment. Simulation results as well as indoor and outdoor experiments are presented and discussed to illustrate the feasibility and robustness of the proposed approach for sensor-based functions such as autonomous navigation and/or safety-enhancing driver's aid.

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

*Transferred to ORNL Robotics and Process Systems Division after publication of this work.

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3.22

MOBILE ROBOT NAVIGATION USING QUALITATIVE REASONING

F. G. Pin* Y. Watanabe†

[Abstract of paper presented at the American Nuclear Society Fifth Topical Meeting on Robotics and Remote Handling, Knoxville, TN, April 26-29, 1993; Proc. pp. 523-530 (1993)]

Vehicle control in a priori unknown, unpredictable, and dynamic environments requires many calculational and reasoning schemes to operate on the basis of very imprecise, incomplete, or unreliable data. For such systems, in which all the uncertainties cannot be engineered away, approximate reasoning may provide an alternative to the complexity and computational requirements of conventional uncertainty analysis and propagation techniques. Two types of computer boards including custom-designed VLSI chips have been developed to add a fuzzy inferencing capability to real-time control systems. The use of these

boards and an approach using superposition of elemental sensor-based behaviors for the development of qualitative reasoning schemes emulating human-like navigation are first discussed. We then describe how the human-like navigation schemes were implemented on a test-bed platform to investigate two control modes for driving a car in a priori unknown environments on the basis of sparse and imprecise sensor data. In the first mode, the car navigates fully autonomously, while in the second mode, the system acts as a driver's aid providing the driver with linguistic (fuzzy) commands to turn left or right and speed up or slow down depending on the obstacles perceived by the sensors. Experiments with both modes of control are described in which the system uses only three acoustic range (sonar) sensor channels to perceive the environment. Simulation results as well as indoors and outdoors experiments are presented and discussed to illustrate the feasibility and robustness of autonomous navigation and/or safety enhancing driver's aid using the new fuzzy inferencing hardware system and methodologies.

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

*Transferred to ORNL Robotics and Process Systems Division after publication of this work.

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3.23

ROBOT NAVIGATION IN UNKNOWN TERRAINS: INTRODUCTORY SURVEY OF NON-HEURISTIC ALGORITHMS

N. S. V. Rao S. Kareti*
W. Shi* S. S. Iyengar†

[Abstract of *ACM Computing Surveys* (in press); also ORNL/TM-12410, July 1993]

A formal framework for navigating a robot in a geometric terrain populated by an unknown set of obstacles is considered. Here the terrain model is not a priori known, but the robot is equipped with a sensor system (vision or touch) employed for the purpose of navigation. Our focus is restricted to the *non-heuristic algorithms* which can be theoretically shown to be correct within a given framework of models for the robot, terrain and sensor system. These formulations, although abstract and simplified compared to real-life scenar-

ios, provide foundations for practical systems by highlighting the underlying critical issues. First, we consider the algorithms that are shown to navigate correctly without much consideration given to the performance parameters such as distance traversed, etc. Second, we consider non-heuristic algorithms that guarantee bounds on the distance traversed or the ratio of the distance traversed to the shortest path length (computed if the terrain model is known). Then we consider the navigation of robots with very limited computational capabilities such as finite automata, etc.

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

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3.24

UNKNOWN-TERRAINS NAVIGATION OF A MOBILE ROBOT USING AN ARRAY OF SONARS

N. S. V. Rao

(Abstract of paper presented at the International Dedicated Conference on Robotics Motion and Machine Vision, Aachen, Germany, October 31–November 4, 1994)

A mobile robot equipped with an array of sonars is required to navigate to a destination through a planar terrain populated by polygonal obstacles whose locations and shapes are unknown. A navigation method is proposed based on a trapezoidal decomposition of the terrain for an abstract formulation, where elementary navigational steps consist of following the obstacle edges and turning around the corners. The convergence of an abstract version of the algorithm is first analytically established. Then experimental results on implementing the algorithm on an experimental mobile robot are reported.

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

3.25

EXPERIMENTS IN MOBILE ROBOT NAVIGATION AND RANGE IMAGING

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 H. M. Nielsen† E. Sorensen†
 J. J. Sorensen† H. I. Christensen†

(Abstract of paper presented at the Eighth Scandinavian Conference on Image Analysis, Tromsø, Norway, May 25-28, 1993)

This paper describes some experiments in sensor-based mobile robot navigation conducted at Oak Ridge National Laboratory over the past several years. Two implemented systems are described. One uses a laser range camera as the sole sensor. The other uses, in addition, an array of sonars and a stereo vision system. We discuss a communication system for heterogeneous LAN-connected multiprocessor systems, useful in reasonably large development projects such as these. We also describe some work on the estimation of curvature in range images which introduces a new variational principle motivated by minimization of the change of curvature. Application of this principle is shown to produce results which are more desirable in some respects than those obtained using standard quadratic variation.

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

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3.26

ON FAST PLANNING OF SUB-OPTIMAL PATHS AMIDST POLYGONAL OBSTACLES IN PLANE

N. S. V. Rao

[Abstract of *Theoretical Computer Science* (in press)]

The problem of planning a path for a point robot from a source point s to a destination point d so as to avoid a set of polygonal obstacles in plane is considered. Using well-known methods, a shortest path from s to d can be computed with

a time complexity of $O(n^2)$ where n is the total number of obstacle vertices. The focus here is in (a) planning paths faster at the expense of settling for sub-optimal path lengths, and (b) performance analysis of simple and/or well-known sub-optimal methods. A method that enables a hierarchical implementation of any path planning algorithm with no increase in the worst-case time complexity, is presented; this implementation enables fast planning of simple paths. Then methods are presented based on the Voronoi diagrams, trapezoidal decomposition and triangulation, which compute (sub-optimal) paths in $O(n \sqrt{\log n})$ time with the preprocessing costs of $O(n \log n)$, $O(n^2)$ and $O(n \log n)$ respectively. Using existing navigational algorithms for unknown terrains, algorithms that run in $O(n \log n)$ time (after preprocessing) and yield sub-optimal paths, are presented. For all these algorithms, upper bounds on the path lengths are estimated in terms of the shortest path length, and parameters such as the maximum clearance, perimeters of the obstacles, etc.

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

3.27

ROBOT NAVIGATION IN UNKNOWN GENERALIZED POLYGONAL TERRAINS USING VISION SENSORS

N. S. V. Rao

[Abstract of *IEEE Transactions on Systems, Man and Cybernetics* (in press)]

The problem of navigating a point robot R in an unknown two-dimensional terrain populated by disjoint generalized polygonal obstacles is considered. A *generalized polygon* consists of a connected sequence of circular arcs and straight-line segments. The terrain model is not known a priori, but the robot R is equipped with a vision sensor. A *discrete vision sensor* detects all visible (from a single position) portions of the obstacle boundaries in a single scale operation. The *navigation problem* deals with moving R through the terrain from a source position to a destination position, and the *terrain model acquisition* problem deals with autonomously building a model of the terrain. A complete solution to either problem is shown to require an infinite number of scan opera-

tions in critical regions form a pair of convex and concave obstacle edges. Every problem is considered solved with a precision ϵ if the points that have not been scanned are those in a critical region with a clearance less than ϵ from two obstacle edges. Three methods are proposed to solve both problems with a precision ϵ based on extensions of the generalized visibility graph, the generalized Voronoi diagram, and the trapezoidal decomposition. Then simplified versions of these structures are proposed to exactly solve the navigation and terrain model acquisition problems using a *continuous vision sensor* that detects all visible obstacle boundaries as the robot navigates along a path.

Research sponsored by U.S. DOE Office of Basic Energy Sciences; by National Science Foundation; and by Old Dominion University.

3.28

LEARNING SEPARATIONS BY BOOLEAN COMBINATIONS OF HALF-SPACES

N. S. V. Rao E. M. Oblow
C. W. Glover

[Abstract of *IEEE Transactions on Pattern Analysis and Machine Intelligence* 16(7), 765 (1994)]

Given two subsets S_1 and S_2 (not necessarily finite) of $\mathcal{R}^d$ separable by a Boolean combination of *learning* halfspaces, we consider the problem of (in the sense of Valiant) the separation function from a finite set of examples, i.e., we produce with a high probability a function close to the actual separating function. Our solution consists of a system of N perceptrons and a single consolidator which combines the outputs of the individual perceptrons. We show that an off-line version of this problem, where the examples are given in a batch, can be solved in time polynomial in the number of examples. We also provide an on-line learning algorithm that incrementally solves the problem by suitably training a system of N perceptrons much in the spirit of the classical perceptron learning algorithm.

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

3.29

MAJORITY AND LOCATION-BASED FUSERS FOR SYSTEMS OF PAC CONCEPT LEARNERS

N. S. V. Rao E. M. Oblow

[Abstract of *IEEE Transactions on Systems, Man, and Cybernetics* 24(5), 713-727 (1994)]

A system of probably and approximately correct learners of Valiant type that infer concepts from a sample is considered. Each learner had been trained by a sample using the methods of minimizing the empirical error, and no examples are available to the fuser. A majority fuser is known to make the composite system better than the best of the learners in terms of normalized confidence (that corresponds to the same precision value). An analysis of general majority fusers is carried out to obtain bounds on actual and expected errors. Conditions under which the r of N fuser performs better, in terms of normalized confidence or precision, than best of the individual learners are obtained. For a special class of statistically independent learners, slightly weaker conditions are obtained. Two fusers that use the location information of a test point are proposed, and are shown to be better than a learner with least empirical error.

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

3.30

N-LEARNERS PROBLEM: FUSION OF CONCEPTS

N. S. V. Rao E. M. Oblow
C. W. Glover G. E. Liepins*

[Abstract of *IEEE Transactions on Systems, Man and Cybernetics* 24(2), 319 (1994)]

Given N learners each capable of learning concepts (subsets) in the sense of Valiant, we are interested in combining them using a single *fuser*. We consider two cases. In *open fusion* the fuser is given the sample and the hypotheses of the individual learners; we show that a fusion rule can be obtained by formulating this problem as another learning problem. We show sufficiency conditions that ensure the composite system to be

better than the best of the individual. Second, in *closed fusion* the fuser does not have an access to either the training sample or the hypotheses of the individual learners. By using a linear threshold fusion function (of the outputs of individual learners) we show that the composite system can be made better than the best of the statistically independent learners.

Research sponsored by U.S. DOE Office of Basic Energy Sciences; by National Science Foundation; and by Old Dominion University.

*Deceased.

3.31

N-LEARNERS PROBLEM: SYSTEM OF PAC LEARNERS

N. S. V. Rao E. M. Oblow

[Abstract of book chapter in *Computational Learning and Machine Learning*, Ed., R. Grenier, MIT Press (in press); also paper presented at the Computational Learning and Machine Learning Workshop, Provincetown, MA, September 10-12, 1993]

A system of N probably and approximately correct learners (of Valiant kind) is given where each learner had produced its hypothesis based on a sample. When no further examples are available, the question of combining the learners to form a composite system is addressed. It is shown that the outputs of these learners can be combined using a fuser that approaches an optimal Bayesian fuser within a specified confidence. Also conditions under which the composite system is better than the best of the individual learners are obtained.

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

3.32

ON STOCHASTIC APPROXIMATION ALGORITHMS FOR CLASSES OF PAC LEARNING PROBLEMS

N. S. V. Rao V. R. R. Uppuluri*
E. M. Oblow

[Abstract of *IEEE Trans. on Systems, Man, and Cybernetics* (in press); also IEEE World Congress on Computational Intelligence, Orlando, FL, June 26-July 2, 1994; Proc. IEEE International Conference on Neural Networks Vol. 2, pp. 791-796 (1994)]

The classical stochastic approximation methods are shown to yield algorithms to solve several formulations of the PAC learning problem defined on the domain $[0,1]^d$. Under some assumptions on differentiability of the probability measure functions, simple algorithms to solve some PAC learning problems are proposed based on networks of non-polynomial units (e.g. artificial neural networks). Conditions on the sizes of the samples required to ensure the error bounds are derived using martingale inequalities.

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

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3.33

LEARNING ALGORITHMS FOR FEEDFORWARD NETWORKS BASED ON FINITE SAMPLES

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R. C. Mann E. M. Oblow
S. S. Iyengar*

(Abstract of ORNL/TM-12819, September 1994)

Two classes of convergent algorithms for learning continuous functions (and also regression functions) that are represented by feedforward networks, are discussed. The first class of algorithms, applicable to networks with unknown weights located only in the output layer, is obtained by utilizing the potential function methods of Aizerman et al. The second class, applicable to general feedforward networks, is obtained by utilizing the classical Robbins-Monro style stochastic approximation methods. Conditions relating the sample sizes to the error bounds are derived for both classes of algorithms using martingale-

type inequalities. For concreteness, the discussion is presented in terms of neural networks, but the results are applicable to general feed-forward networks, in particular to wavelet networks. The algorithms can be directly adapted to concept learning problems.

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

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3.34

FUSION RULE ESTIMATION IN MULTIPLE SENSOR SYSTEMS WITH UNKNOWN NOISE DISTRIBUTIONS

N. S. V. Rao

(Abstract of paper presented at the Indo-U.S. Workshop on Distributed and Parallel Signal and Image Integration, Pune, India, December 16-18, 1993)

A system of N sensors $S_1, S_2, \dots, S_N$ is considered; corresponding to an object with parameter $x \in \mathcal{R}^d$, sensor S_i yields output $y^{(i)} \in \mathcal{R}^d$ according to an unknown probability distribution $p_i(y^{(i)}|x)$. A training l -sample $(x_1, y_1), (x_2, y_2), \dots, (x_l, y_l)$ is given where $y_i = (y_i^{(1)}, y_i^{(2)}, \dots, y_i^{(N)})$ and $y_i^{(j)}$ is the output of S_j in response to input x_i . The problem is to estimate a fusion rule $f: \mathcal{R}^{Nd} \mapsto \mathcal{R}^d$, based on the sample, to minimize $I(f)$ which is the expected value of $[x - (y_i^{(1)}, y_i^{(2)}, \dots, y_i^{(N)})]^2$. Let $f_* \in \Lambda$ minimize $I(\cdot)$. Using Vapnik's empirical risk minimization method, we show that if Λ has finite capacity then under bounded error, for sufficiently large sample we can obtain an estimate f_{emp} of f_* such that $P[I(f_{emp}) - I(f_*) > \epsilon] < \delta$ for arbitrarily specified $\epsilon > 0$ and $\delta, 0 < \delta < 1$.

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

3.35

STOCHASTIC APPROXIMATION METHODS FOR FUSION-RULE ESTIMATION IN MULTIPLE SENSOR SYSTEMS

N. S. V. Rao

(Abstract of paper presented at the Twelfth Symposium on Energy Engineering Sciences, Argonne, IL, April 27-29, 1994; Proc. pp. 161-168 (1994))

A system of N sensors $S_1, S_2, \dots, S_N$ is considered; corresponding to an object with parameter $x \in \mathcal{R}^d$, sensor S_i yields output $y^{(i)} \in \mathcal{R}^d$ according to an unknown probability distribution $p_i(y^{(i)}|x)$. A training l -sample $(x_1, y_1), (x_2, y_2), \dots, (x_l, y_l)$ is given where $y_i = (y_i^{(1)}, y_i^{(2)}, \dots, y_i^{(N)})$ and $y_i^{(j)}$ is the output of S_j in response to input x_i . The problem is to estimate a fusion rule $f: \mathcal{R}^{Nd} \mapsto \mathcal{R}^d$, based on the sample, such that the expected square error $I(f) = \int [x - f(y^{(1)}, y^{(2)}, \dots, y^{(N)})]^2 p(y^{(1)}, y^{(2)}, \dots, y^{(N)}|x) p(x) dy^{(1)} dy^{(2)} \dots dy^{(N)} dx$ is to be minimized over a family of fusion rules Λ based on the given l -sample. Let $f_* \in \Lambda$ minimize $I(f)$. Three stochastic approximation methods are presented to compute $\hat{f}$, such that under suitable conditions, for sufficiently large sample, $P[I(\hat{f}) - I(f_*) > \epsilon] < \delta$ for arbitrarily specified $\epsilon > 0$ and $\delta, 0 < \delta < 1$.

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

3.36

FUSION RULE ESTIMATION IN MULTIPLE SENSOR SYSTEMS USING LEARNING

N. S. V. Rao

(Abstract of paper presented at the Dagstuhl Seminar on Environment Modeling and Motion Planning, Dagstuhl, Germany, October 24-28, 1994)

A formal framework for estimating fusion rules for a system of N sensors, based on a set of examples, is presented. No knowledge about the probability densities of sensor errors is assumed. Given an input vector $x \in \mathcal{R}^d$, the sensor S_i , i

$= 1, 2, \dots, N$, generates output $y_i \in \mathcal{R}^d$ according to an unknown density $p_i(y_i|x)$. For a fusion rule $f: \mathcal{R}^{Nd} \mapsto R$, is to be chosen from a family Λ , such that the expected error $I(f)$ is minimized. Given a sample $(x^{(1)}, y^{(1)}), (x^{(2)}, y^{(2)}), \dots, (x_N^{(l)}, y_N^{(l)})$ where $y^j = (y_1^{(j)}, y_2^{(j)}, \dots, y_N^{(j)})$ corresponds to the input $x^{(j)}$, we consider the conditions under which an estimator $\hat{f} \in \Lambda$ can be computed such that $P[I(\hat{f}) - I(f^*) > \epsilon] < \delta$ for sufficiently large l , where $I(f^*) = \min_{f \in \Lambda} I(f)$. We present

three algorithmic methods based on (i) stochastic approximation, (ii) empirical estimation and potential functions, and (iii) regression estimation. Two experimental scenarios involving (a) identification of glassware in a structured environment, and (b) recognition of a narrow doorway by a mobile robot equipped with an array of ultrasonic and infrared sensors, are described to illustrate the applicability of the proposed methods.

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

3.37

IMAGE ACCURACY AND REPRESENTATIONAL ENHANCEMENT THROUGH LOW-LEVEL, MULTI-SENSOR INTEGRATION TECHNIQUES

J. E. Baker

(Abstract of paper presented at the Conference on Sensor Fusion and Aerospace Applications, Optical Engineering/Aerospace Science and Sensing, Orlando, FL, April 12-16, 1993, Proc. Vol. 1956 (1993); also ORNL/TM-12218, May 1993)

Multi-Sensor Integration (MSI) is the combining of data and information from more than one source in order to generate a more reliable and consistent representation of the environment. The need for MSI derives largely from basic ambiguities inherent in our current sensor imaging technologies. These ambiguities exist as long as the mapping from reality to image is not 1-to-1. That is, if different "realities" lead to identical images, a single image cannot reveal the particular reality which was the truth. MSI techniques attempt to resolve some of these ambiguities by appropriately coupling complementary images to eliminate pos-

sible inverse mappings. What constitutes the best MSI technique is dependent on the given application domain, available sensors, and task requirements.

The "data enhancement" algorithms developed include general-purpose, sensitivity enhancement techniques and specific sensor anomaly detection and remediation techniques. These techniques are evaluated on actual multi-modal sensor data obtained from a laser range camera, i.e., range and reflectance images. A suite of over thirty conceptual enhancement techniques are developed, evaluated and compared on this sensor domain. For objective analysis, each algorithm's performance is optimized by Genetic Algorithms, a machine learning technique, for a predefined level of detail. However, the general applicability of these techniques is empirically verified by applying the laser range camera optimized results to different sensor domains, e.g., ground conductivity data including quadrature and in-phase strength images. The overall result is a general-purpose. MSI conceptual enhancement approach which can be efficiently implemented and used to supply input to a variety of high-level processes, including: object recognition, path planning and object avoidance systems.

Research sponsored by U.S. DOE Engineering Research Program, Office of Basic Energy Sciences and by the Office of Technology Development.

3.38

ADAPTIVE LEARNING OF MULTI-SENSOR INTEGRATION TECHNIQUES WITH GENETIC ALGORITHMS

J. E. Baker

[Abstract of paper presented at the International Symposium on Robotics and Manufacturing (ISRAM '94), Wailea, Maui, HI, August 14-18, 1994; Proc. Intelligent Automation and Soft Computing Trends in Research, Development, and Applications, Vol. 2 (1994)]

This research focuses on automating the time-consuming process of developing and optimizing multisensor integration techniques. Our approach is currently based on adaptively learning how to exploit low-level image properties to correctly cluster pixels so as to yield the desired level of image detail. Although this system is specifically

designed to be both sensor and application domain independent, an empirical validation with actual multi-modal sensor data is presented.

Research sponsored by U.S. DOE Engineering Research Program, Office of Basic Energy Sciences and by the Naval Air Warfare Center Aircraft Division Lakehurst.

3.39

AUTOMATIC CALIBRATION OF LASER RANGE CAMERAS USING ARBITRARY PLANAR SURFACES

J. E. Baker

[Abstract of paper presented at the Conference on Sensor Fusion and Aerospace Applications II, Opto-Electronics/Aerospace Sensing, SPIE, Orlando, FL, April 5-8, 1994; Proc. Vol. 2234, pp. 38-48 (1994)]

Laser Range Cameras (LRCs) are powerful tools for many robotic/computer perception activities. They can provide accurate range images and perfectly registered reflectance images of the target scene, useful for constructing reliably detailed 3-D world maps and target characterizations. An LRC's output is an array of distances obtained by scanning a laser over the scene. To accurately interpret this data, the angular definition of each pixel, i.e., the 3-D direction corresponding to each distance measurement, must be known. This angular definition is a function of the camera's intrinsic design and unique implementation characteristics, e.g., actual mirror positions, axes of rotation, angular velocities, etc. Typically, the range data is converted to Cartesian coordinates by calibration-parameterized, non-linear transformation equations. Unfortunately, typical LRC calibration techniques are manual, intensive, and inaccurate. Common techniques involve imaging carefully orchestrated artificial targets and manually measuring actual distances and relative angles to infer the correct calibration parameter values.

This paper presents an automated method which uses Genetic Algorithms to search for calibration parameter values and possible transformation equations which combine to maximize the planarity of user-specified sub-regions of the image(s). This method permits calibration to be based on an arbitrary plane, without precise knowledge of the LRC's mechanical precision, intrinsic design, or its relative positioning to the target. Furthermore, this method permits rapid, remote, and on-line

recalibration - important capabilities for many robotic systems. Empirical validation of this system has been performed using two different LRC systems and has led to significant improvement in image accuracy while reducing the calibration time by orders of magnitude.

Research sponsored by U.S. DOE Engineering Research Program, Office of Basic Energy Sciences and by the Naval Air Warfare Center Aircraft Division Lakehurst.

3.40

CALIBRATION AND CONTROL FOR RANGE IMAGING IN MOBILE ROBOT NAVIGATION

O. H. Dorum* A. Hoover†
J. P. Jones

[Abstract of book chapter in *Vision Interface C*, Archibald, Ed., World Scientific Press (in press); also paper presented at the Vision Interface '94, Banff, Alberta, Canada, May 18-20, 1994]

This paper addresses some issues in the development of sensor-based systems for mobile robot navigation which use range imaging sensors as the primary source for geometric information about the environment. In particular, we describe a model of scanning laser range cameras which takes into account the properties of the mechanical system responsible for image formation and a calibration procedure which yields improved accuracy over previous models. In addition, we describe an algorithm which takes the limitations of these sensors into account in path planning and path execution. In particular, range imaging sensors are characterized by a limited field of view and a standoff distance - a minimum distance nearer than which surfaces cannot be sensed. These limitations can be addressed by enriching the concept of configuration space to include information about what can be sensed from a given configuration, and using this information to guide path planning and path following.

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

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†University of South Florida, Tampa, FL.

3.41

LASER RANGE CAMERA DATA FUSION

M. Beckerman F. J. Sweeney

[Abstract of paper presented at the American Nuclear Society Fifth Topical Meeting on Robotics and Remote Handling, Knoxville, TN, April 26-29, 1993; Proc. (1993)]

In this paper we present results of an investigation of the fusion of image data from amplitude-modulated CW laser radar. The goal of the study is the design of an algorithm for simultaneously recovering the underlying surfaces and discontinuities in a manner which is free from errors and artifacts. To accomplish this goal we model the images as a set of coupled Markov random fields. These fields, defined within a Bayesian framework, describe the smooth-surface, discontinuity and noise properties of the images. As a result of the Markovian property simulated annealing can be used to find the global minimum.

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

3.42

SEGMENTATION AND COOPERATIVE FUSION OF LASER RADAR IMAGE DATA

M. Beckerman F. J. Sweeney

[Abstract of paper presented at the Conference on Sensor Fusion and Aerospace Applications II, Opto-Electronics/Aerospace Sensing, SPIE, Orlando, FL, April 5-8, 1994; Proc. Vol. 2233, pp. 88-98 (1994)]

In segmentation, the goal is to partition a given 2D image into regions corresponding to the meaningful surfaces in the underlying physical scene. Segmentation is frequently a crucial step in analyzing and interpreting image data acquired by a variety of automated systems ranging from indoor robots to orbital satellites. In this paper, we present results of a study of segmentation by means of cooperative fusion of registered range and intensity images acquired using a prototype amplitude-modulated CW laser radar. In our approach, we consider three modalities - depth, reflectance and surface orientation. These modalities are modeled as sets of coupled Markov random fields for pixel and line processes. Bayesian infer-

encing is used to impose constraints of smoothness on the pixel process and linearity on the line process. The latter constraint is modeled using an Ising Hamiltonian. We solve the constrained optimization problem using a form of simulated annealing termed quenched annealing. The resulting model is illustrated in this paper in the rapid quenched, or iterated conditional mode, limit for several laboratory scenes.

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

3.43

DATA FUSION THROUGH SIMULATED ANNEALING OF REGISTERED RANGE AND REFLECTANCE IMAGES

M. Beckerman F. J. Sweeney

[Abstract of paper presented at the Conference on Sensor Fusion and Aerospace Applications, Optical Engineering/Aerospace Science and Sensing, Orlando, FL, April 12-16, 1993; Proc. Vol. 1956, pp. 200-211 (1993)]

In this paper we present results of a study of registered range and reflectance images acquired using a prototype amplitude-modulated CW laser radar. Ranging devices such as laser radars represent new technologies which are being applied in aerospace, nuclear and other hazardous environments where remote inspections, 3D identifications and measurements are required. However, data acquired using devices of this type may contain non-stationary, signal-dependent noise, range-reflectance crosstalk and low-reflectance range artifacts. Low level fusion algorithms play an essential role in achieving reliable performance by handling the complex noise, systematic errors and artifacts. The objective of our study is the development of a stochastic fusion algorithm which takes as its input the registered image pair and produces as its output a reliable description of the underlying physical scene in terms of locally smooth surfaces separated by well-defined depth discontinuities. To construct the algorithm we model each image as a set of coupled Markov random fields representing pixel and several orders of line processes. Within this framework we (i) impose local smoothness constraints, introducing a simple linearity property in place of the usual sums over clique potentials; (ii) fuse the range and reflectance images through line pro-

cess couplings, and (iii) use nonstationary, signal-dependent variances, adaptive thresholding, and a form of Markov natural selection. We show that the resulting algorithm yields reliable results even in worst-case scenarios.

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

3.44

FUSION OF VISUAL AND ULTRASOUND SENSOR DATA USING BAYES-MAXIMUM ENTROPY METHODS

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

[Abstract of *IEEE Trans. on Robotics and Automation* (in press)]

In this work we present a Bayes-Maximum Entropy methodology for the fusion of ultrasound and visual sensor data as acquired by a mobile robot. In our approach the principle of maximum entropy is applied to the construction of the prior probabilities and the likelihoods from the data. The data representations used in the fusion process include Maximum Entropy maps and dual visual - ultrasound images. Gibbs distributions of distances between ultrasound and visual feature points are used in the dual image representation to test appropriately chosen null hypotheses. The objective of our Bayesian methodology is the reduction of systematic errors which arise in the processing of the data in the individual sensor domains. The systematic errors treated in this work include ultrasound distortions in size, and visual ambiguities in discriminating depth discontinuities from intensity gradients (edges) generated by other details in the image. However, our methodology is in no way limited to these classes of errors or to the particular visual feature points chosen.

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

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3.45

A LEARNING-BASED METHOD TO RECOGNIZE AND LOCALIZE GLASSWARE USING LASER RANGE IMAGES

S. Toemoe* N. S. V. Rao
R. C. Mann

[Abstract of *Image and Vision Computing* (in press)]

A system that can be trained to recognize and localize glassware located on a workbench using laser range images is described. The training data consists of laser range images of objects of known classification. The image is preprocessed to isolate a box of pixels corresponding to the object, and then the box is given as an input to a neural network. The range readings form the laser range system deviate significantly from the actual distances to the glassware, and consequently a surface fit to the readings has very little resemblance to the actual glassware surface. Thus, the straightforward method of fitting a surface to the images and matching it with the surface of known glassware is not feasible. A first version of the system has been developed based on a system of perceptrons, and the tests have been successful on the images taken by PERCEPTRON P5000 laser range finder.

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

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3.46

REAL-TIME CONSTRUCTION OF THREE-DIMENSIONAL OCCUPANCY MAPS

J. P. Jones

[Abstract of paper presented at the 1993 IEEE International Conference on Robotics and Automation, Atlanta, GA, May 2-6, 1993; Proc. Vol. 1, pp. 52-57 (1993)]

This paper describes a preliminary sensory system for real-time sensor-based navigation in a three-dimensional, dynamic environment. Data from a laser range camera are processed on an iWarp parallel computer to create a 3D occupancy map. This map is rendered using raytracing. The construction and rendering consume less than 800 milliseconds.

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

3.47

REAL-TIME CONSTRUCTION AND RENDERING OF THREE-DIMENSIONAL OCCUPANCY MAPS

J. P. Jones

[Abstract of paper presented at the SPIE Applications of Artificial Intelligence XI Conference, Orlando, FL, April 12-16, 1993; Proc. Vol. 1964, pp. 249-256 (1993)]

This paper describes a preliminary sensory system for real-time sensor-based navigation in a three-dimensional, dynamic environment. Data from a laser range camera are processed on an iWarp parallel computer to create a 3D occupancy map. This map is rendered using raytracing. The construction and rendering consume less than 800 milliseconds.

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

3.48

PARALLEL AND DISTRIBUTED SIGNAL AND IMAGE INTEGRATION PROBLEMS

R. N. Madan* N. S. V. Rao
V. P. Bhatkar† L. M. Patnaik‡
Editors

(Abstract of Parallel and Distributed Signal and Image Integration Problems; Proc. of the Indo-US Workshop, Pune, India, December 16-18, 1993)

The next generation of engineering and computing systems will be both complex and distributed in functionality due to a variety of information sources needed for their operation. Successful development and deployment of these systems critically depends on the mechanisms for acquisition, coordination, communication and integration of information from various components. This collection of papers addresses various aspects in the area of signal and image integration with a specific emphasis on parallel and distributed solutions. A wide spectrum of issues including image and signal processing, parallel architectures/algorithms, sensor integration/fusion, and neural networks/fuzzy systems, are addressed in various papers.

Research sponsored by U.S. Department of Energy.

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3.49

HYBRID PATTERN RECOGNITION SYSTEM CAPABLE OF SELF-MODIFICATION

C. W. Glover N. S. V. Rao
E. M. Oblow

(Abstract of paper presented at the Second International Conference on Information and Knowledge Management, Washington, DC, May 1-5, 1993)

Systems capable of recognizing and learning two-dimensional patterns can be used in imaging systems and robotic perception systems. The symbolic and neuromorphic methods for pattern processing problems of this type are complemen-

tary in character. We present a hybrid system that utilizes components of symbolic and neuro-morphic type; we employ two hybrid components that simultaneously operate up on the same data to produce hypotheses about the data. To resolve the potential conflicts in these hypotheses, we propose a method that learns a combination rule based on a set of examples. We employ the method of empirical risk minimization and does not require knowledge about the error probability distributions of the modules. We are building a prototype system to recognize control panels using a vision system.

Research sponsored by U.S. DOE Office of Basic Energy Sciences and Laboratory Director R&D Fund.

3.50

ON POLYNOMIAL-TIME TESTABLE COMBINATIONAL CIRCUITS

N. S. V. Rao S. Toida*

[Abstract of *IEEE Transactions on Computers* 43(11), 1298 (1994)]

The problems of identifying several nontrivial classes of Polynomial-Time Testable (PTT) circuits are shown to be NP-complete or harder. First, PTT classes obtained by using circuit decompositions proposed by Fujiwara and Chakradhar et al. are considered. Another type of decompositions, based on fanout-reconvergent ($f-r$) pairs, which also lead to PTT classes are proposed. The problems of obtaining these decompositions, and also some structurally similar general graph decompositions, are shown to be NP-complete or harder. Then, the problems of recognizing PTT classes formed by the Boolean formulae belonging to the weakly positive, weakly negative, bijnunctive and affine classes (proposed by Schaefer) are shown to be NP-complete.

Research sponsored by U.S. DOE Office of Basic Energy Sciences; by National Science Foundation; and by Old Dominion University.

*Old Dominion University, Norfolk, VA.

3.51

ON SIMILARITY OF POLYNOMIAL CONFIGURATIONS

N. S. V. Rao C. Luo*

[Abstract of *Information Processing Letters* 47(5), 231 (1993)]

The problem of checking the equivalence of two sets of polynomial curves (in plane), each set of total degree n , under the affine transformations of translation, rotation, scaling and mirror reflection is studied. An optimal $\theta(n \log n)$ time algorithm for this problem is presented. This algorithm is based on efficient computation of Bezier polygons by using some polynomial manipulations that employ FFT methods.

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

*Old Dominion University, Norfolk, VA.

3.52

PROCEEDINGS OF THE SEVENTH INTERNATIONAL SYMPOSIUM ON METHODOLOGIES FOR INTELLIGENT SYSTEMS (POSTER SESSION)

K. S. Harber (Editor)

(Abstract of ORNL/TM-12375, May 1993)

This volume contains papers which were selected for presentation at the Poster Session of the Seventh International Symposium on Methodologies for Intelligent Systems - ISMIS '93, held in Trondheim, Norway, June 15-18, 1993. The symposium was hosted by the Norwegian Institute of Technology and sponsored by the University of Trondheim, NFR/NTNF - The Norwegian Research Council, UNC-Charlotte, Office of Naval Research, Oak Ridge National Laboratory and ES-PRIT BRA Compulog Network of Excellence.

ISMIS is a conference series that was started in 1986 in Knoxville, Tennessee. It has since then been held in Charlotte, North Carolina, once in Knoxville, and once in Torino, Italy.

The major areas for ISMIS '93 are: (1) Approximate Reasoning, (2) Constraint Programming, (3) Expert Systems, (4) Intelligent

Databases, (5) Knowledge Representation, (6) Learning and Adaptive Systems, (7) Manufacturing, and (8) Methodologies.

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

3.53

ROBOTICS AND ARTIFICIAL INTELLIGENCE FOR HAZARDOUS ENVIRONMENTS

P. F. Spelt

(Abstract of paper presented at the XVII Congreso de Investigación Científica Universidad Interamericana de Puerto Rico, San Juan, Puerto Rico, February 11-12, 1993)

In our technological society, hazardous materials including toxic chemicals, flammable, explosive, and radioactive substances, and biological agents, are used and handled routinely. Each year, many workers who handle these substances are accidentally contaminated, in some cases resulting in injury, death, or chronic disabilities. If these hazardous materials could be handled remotely, either with a teleoperated robot (operated by a worker in a safe location) or by an autonomous robot, then human suffering and economic costs of accidental exposures could be dramatically reduced. At present, it is still difficult for commercial robotic technology to completely replace humans involved in performing complex work tasks in hazardous environments. The robotics efforts at the Center for Engineering Systems Advanced Research represent a significant effort at contributing to the advancement of robotics for use in hazardous environments. While this effort is very broad-based, ranging from dexterous manipulation to mobility and integrated sensing, the technical portion of this paper will focus on machine learning and the high-level decision making needed for autonomous robotics.

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

3.54

RESEARCH AND APPLICATIONS OF COOPERATING MOBILE ROBOTS

A. L. Bangs

[Abstract of paper presented at the 1993 IEEE International Conference on Robotics and Automation, Atlanta, GA, May 2-6, 1993; Proc. Vol. 1 (1993)]

As envisioned robotics applications expand, there are certain motivations to use solutions that involve multiple robots. These include redundancy, speeding completion of tasks, and manipulating large objects. Current research in cooperating mobile robotics is focussed in several areas: motion planning, modular robotics, cellular or swarm robotics, task planning, and communication. This talk will present an overview of these areas, give examples of research being performed in these areas, and present a taxonomy for evaluating cooperation research.

In addition, applications for cooperating mobile robots are examined, and a set of criteria for examining applications is given. These criteria are useful for evaluating the research technologies and how they would apply to certain applications.

Finally, work in progress at CESAR in cooperating mobile robots is discussed, including the CESAR focus in cooperation, the application paradigms we have chosen, and current work to date.

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

3.55

SUPPORTING ROBOTICS TECHNOLOGY REQUIREMENTS THROUGH RESEARCH IN INTELLIGENT MACHINES

R. C. Mann

(Abstract of paper presented at the Robotics Industry Forum and Annual Meeting, Orlando, FL, November 2-4, 1994)

"Safer, better, cheaper" are recurring themes in many robot development efforts. Significant improvements are being accomplished with existing technology, but basic research sets the foundations for future improvements and breakthrough discoveries. Advanced robots represent systems that integrate the three basic functions of sensing, rea-

soning, and acting (locomotion and manipulation) into one functional unit. Depending on the application requirements, some of these functions are implemented at a more or less advanced level than others. For example, some navigation tasks can be accomplished with purely reactive control and do not require sophisticated reasoning and planning methodologies.

Robotics work at the Oak Ridge National Laboratory (ORNL) spans the spectrum from basic research to application-specific development and rapid prototyping of systems. This presentation summarizes recent highlights of the robotics research activities at ORNL.

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

3.56

ALLIANCE: AN ARCHITECTURE FOR FAULT TOLERANT, COOPERATIVE CONTROL OF HETEROGENEOUS MOBILE ROBOTS

L. E. Parker

(Abstract of paper presented at the IROS '94, IEEE/RSJ/GI International Conference on Intelligent Robots and Systems, Munich, Germany, September 12-16, 1994)

This research addresses the problem of achieving fault tolerant cooperation within small-to medium-sized teams of heterogeneous mobile robots. We describe a novel behavior-based, fully distributed architecture, called ALLIANCE, that utilizes adaptive action selection to achieve fault tolerant cooperative control in robot missions involving loosely coupled, largely independent tasks. The robots in this architecture possess a variety of high-level functions that they can perform during a mission, and must at all times select an appropriate action based on the requirements of the mission, the activities of other robots, the current environmental conditions, and their own internal states. Since such cooperative teams often work in dynamic and unpredictable environments, the software architecture allows the team members to respond robustly and reliably to unexpected environmental changes and modifications in the robot team that may occur due to mechanical failure, the learning of new skills or the addition or removal of robots from the team by human intervention. After presenting ALLIANCE, we describe in detail our experimental results of an implemen-

tation of this architecture on a team of physical mobile robots performing a cooperative box pushing demonstration. These experiments illustrate the ability of ALLIANCE to achieve adaptive, fault-tolerant cooperative control amidst dynamic changes in the capabilities of the robot team.

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

3.57

A MODULAR CONTROL ARCHITECTURE FOR REAL-TIME SYNCHRONOUS AND ASYNCHRONOUS SYSTEMS

P. L. Butler* **J. P. Jones**

[Abstract of book chapter in *Experimental Environments in Computer Vision and Image Processing*, H. I. Christensen and J. L. Crowley, Eds., Vol. 18, pp. 157-182 World Scientific Press, Singapore (1994)]

This paper describes a control architecture for real-time control of complex robotic systems. The Modular Integrated Control Architecture (MICA), which is actually two complementary control systems, recognizes and exploits the differences between asynchronous and synchronous control. The asynchronous control system simulates shared memory on a heterogeneous network. For control information, a portable event scheme is utilized. This scheme provides consistent interprocess coordination among multiple tasks on any number of distributed systems. The machines in the network can vary with respect to their native operating systems and the internal representation of numbers they employ. The synchronous control system is needed for tight real-time control over complex electromechanical systems such as robot manipulators and utilizes multiple processors at a specified rate. Both the synchronous and asynchronous portions of MICA have been developed to be extremely modular. MICA presents a simple programming model to code developers and also considers the needs of system integrators and maintainers. MICA has been used successfully in a complex robotics project involving a mobile 7-degree-of-freedom manipulator in a heterogeneous network with a body of software totaling over 100,000 lines of code.

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

*Robotics and Process Systems Division.

3.58

AUTOMATIC CODE GENERATION FOR DISTRIBUTED ROBOTIC SYSTEMS

J. P. Jones

[Abstract of paper presented at the American Nuclear Society Fifth Topical Meeting on Robotics and Remote Systems, Knoxville, TN, April 26-29, 1993; Proc. (1993)]

Hetero Helix is a software environment which supports relatively large robotic system development projects. The environment supports a heterogeneous set of message-passing LAN-connected common-bus multiprocessors, but the "programming model" seen by software developers is a simple shared memory. The conceptual simplicity of shared memory makes it an extremely attractive programming model, especially in large projects where coordinating people can itself become a significant source of complexity. We present results from five system development efforts. Each of these efforts used automatic software generation in Hetero Helix to create 10 to 20 percent of the system.

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

3.59

ROBOTICS APPLICATION FOR IN-SERVICE INSPECTION OF THE ALMR

**W. Kwant* N. L. Ramsour*
F. J. Sweeney**

(Abstract of paper presented at the Second International Conference on Nuclear Engineering, San Francisco, CA, March 21-24, 1993)

The U.S. Advanced Liquid Metal Reactor (ALMR) Program is developing and licensing a reactor system that is compact for factory fabrication and modular construction. The design includes provisions for in-service inspection to verify performance and safety capabilities throughout the life of the plant. A DOE sponsored robotics team, comprised of members from the universities of Florida, Michigan, Tennessee, Texas and from Oak Ridge National Laboratory, is developing advanced inspection equipment using robotics for nuclear application. This equipment is compact and

remotely operated and particularly suited for inspection of the ALMR. Extensive 3D simulations are used to refine and demonstrate the inspection methods.

This paper focuses on inspection methods for the reactor vessel and the reactor vessel auxiliary cooling system (RVACS). Inspection capabilities are included for visual inspection of the reactor vessel outer surface and volumetric inspection of the welds. The robotics team is devising a compact crawler design with the capabilities to perform these inspections. Similarly, various robot concepts are being evaluated for accomplishing the RVACS visual inspection and cleaning procedures.

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

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3.60

DESIGNS FOR REMOTE INSPECTION OF THE ALMR REACTOR VESSEL AUXILIARY COOLING SYSTEM (RVACS)

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[Abstract of paper presented at the American Nuclear Society Fifth Topical Meeting on Robotics and Remote Handling, Knoxville, TN, April 26-29, 1993; Proc. Vol. 1, pp. 431-438 (1993)]

One of the most important safety systems in General Electric's (GE) Advanced Liquid Metal Reactor (ALMR) is the Reactor Vessel Auxiliary Cooling System (RVACS). Because of high temperature, radiation, and restricted space conditions, GE desired methods to remotely inspect the RVACS, emissive coatings, and reactor vessel welds during normal refueling operations. The DOE/NE Robotics for Advanced Reactors program formed a team with GE to evaluate the ALMR design for remote inspection of the RVACS. Conceptual designs for robots to perform the required inspection tasks were developed by the team. Design criteria for these remote systems included robot deployment, power supply, navigation, environmental hardening of components, tether management, communication with an oper-

ator, sensing, and failure recovery. The operation of the remote inspection concepts were tested utilizing 3-D simulation models of the ALMR. In addition, the team performed an extensive technology review of robot components that could survive the environmental conditions in the RVACS.

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

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3.61

DESIGN OF THE REACTOR VESSEL INSPECTION ROBOT FOR THE ADVANCED LIQUID METAL REACTOR

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[Abstract of paper presented at the International Symposium on Robotics and Manufacturing (ISRAM '94), Wailea, Maui, HI, August 14-18, 1994; Proc. Intelligent Automation and Soft Computing Trends in Research, Development, and Applications, Vol. 2 (1994)]

A consortium of four universities and Oak Ridge National Laboratory designed a prototype wall-crawling robot to perform weld inspection in an advanced nuclear reactor. The restrictions of the inspection environment presented major challenges to the team. These challenges were met in the prototype, which has been tested in a mock nonhostile environment and shown to perform as expected.

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

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3.62

A WALL-CRAWLING ROBOT FOR REACTOR VESSEL INSPECTION IN ADVANCED REACTORS

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(Abstract of paper presented at the AIR '94, Application of Artificial Intelligence and Robotics to Nuclear Plants, Tokai-mura, Naka-gun, Ibaraki, Japan, May 29-June 2, 1994)

A consortium of four universities and the Center for Engineering Systems Advanced Research of the Oak Ridge National Laboratory has designed a prototype wall-crawling robot to perform weld inspection in advanced nuclear reactors. Design efforts for the reactor vessel inspection robot (RVIR) concentrated on the Advanced Liquid Metal Reactor because it presents the most demanding environment in which such a robot must operate. The RVIR consists of a chassis containing two sets of suction cups that can alternately grasp the side of the vessel being inspected, providing both locomotion and steering functions. Sensors include three CCD cameras and a weld inspection device based on new shear-wave technology. The restrictions of the inspection environment presented major challenges to the team. These challenges were met in the prototype, which has been tested in a non-radiation, room-temperature mockup of the robot work environment and shown to perform as expected.

Research sponsored by the Office of Nuclear Energy, Office of Technology Support Programs, U.S. DOE.

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3.63

ENABLING GENETIC ALGORITHMS TO EXHIBIT IMPLICIT PARALLELISM: CORRECTION OF ITS STOCHASTIC SAMPLING ROUTINE

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[Abstract of *IEEE Transactions on Systems, Man, and Cybernetics* (in press)]

Genetic Algorithms, GAs, are extremely powerful adaptive global search techniques derived from natural population genetics. Although GAs cannot guarantee discovery of the optimal solution, they have proven themselves as powerful global search techniques. The power of the GA has long been associated with the implicit parallelism of its allocation of trials to the search space's genetic hyperplanes, i.e., regions sharing identical genetic material. It has recently been proven that for GAs to exhibit pure implicit parallelism, it is both necessary and sufficient to have an accurate sampling algorithm. To function properly, GAs must sample from a pool of candidates according to some predefined probability distribution. Unfortunately no acceptable sampling algorithm was available prior to this research. To be acceptable, the GA's sampling algorithm must be: (1) functional - obtain a predefined number of samples from the available pool; (2) accurate - ensure each sample is selected according to its own selection probability; (3) consistent - ensure that each sample's actual selection frequency is as close to its selection probability as is theoretically possible, given N ; and (4) efficient - be of time complexity. All previously available sampling algorithms are inefficient and fail to provide both accurate and consistent sampling. This paper reviews and empirically analyzes various sampling algorithms and offers two, time-efficient, maximally consistent algorithms: a highly accurate, partially parallel algorithm and a completely accurate, sequential algorithm. Its use enables GAs, for the first time, to perform according to its theoretical specifications and actually achieve implicit parallelism.

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

3.64

AVERAGE WAITING TIME PROFILES OF UNIFORM DQDB MODEL

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(Abstract of paper presented at the IEEE Infocom '94: 13th Joint Conference on IEEE Computer and Communication Societies, Toronto, Canada, June 12-16, 1994)

The Distributed Queue Dual Bus (DQDB) system consists of a linear arrangement of N nodes that communicate with each other using two contra-flowing buses; the nodes use an extremely simple protocol to send messages on these buses. This simple, but elegant, system has been found to be very challenging to analyze. We consider a simple and uniform abstraction of this model to highlight the fairness issues in terms of average waiting time. We introduce a new approximation method to analyze the performance of DQDB system in terms of the average waiting time of a node expressed as a function of its position. Our approach abstracts the intimate relationship between the load of the system and its fairness characteristics, and explains all basic behavior profiles of DQDB observed in previous simulation. For the uniform DQDB with equal distance between adjacent nodes, we show that the system operates under three basic behavior profiles and a finite number of their combinations that depend on the load of the network. Consequently, the system is not fair at any load in terms of the average waiting times. In the vicinity of a critical load of $1-4N$, the uniform network runs into a state akin to chaos, where its behavior fluctuates from one extreme to the other with a load variation of $2/N$. Our analysis is supported by simulation results. We also show that the main theme of the analysis carries over to the general (non-uniform) DQDB; by suitably choosing the inter-node distances, the DQDB can be made fair around some loads, but such systems will become unfair as the load changes.

Research sponsored by U.S. DOE Office of Basic Energy Sciences; by Sun Microsystems, Inc.; by Virginia's Center for Innovative Technology; and by Taurus Technologies, Inc.

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3.65

AN EVALUATION OF INTEGRATION OF THE TRACE ASSERTION METHOD WITH THE BOX STRUCTURE METHOD FOR CODING IN C++

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(Abstract of ORNL/TM-12439, August 1993)

The Trace Assertion Method, originated by David Parnas, is a method for developing specifications for software modules. The nature of the method allows verification of consistency and completeness of the specification, and provides a rigid structure to the designer. This method is extended to work with object-oriented designs for a C++ system involving a user interface. A number of object-oriented concepts which are not present in the original Trace Assertion Method are incorporated into the method and demonstrated on two completely specified increments of the system being developed. In addition, the method is incorporated into a system wide view beyond the original modular scope of the method. Advantages of the adapted method and its problems are discussed.

Research sponsored by U.S. Department of Energy.

3.66

A METHOD FOR OBTAINING A LEAST SQUARES FIT OF A HYPERPLANE TO UNCERTAIN DATA

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(Abstract of ORNL/TM-12686, May 1994)

For many least squares problems, the uncertainty is in one of the variables [for example, $y=f(x)$ or $z=f(x,y)$]. However, for some problems, the uncertainty is in the geometric transformation from measured data to Cartesian coordinates and all of the calculated variables are uncertain.

When we seek the best least squares fit of a hyperplane to the data, we obtain an over determined system (we have $n+1$ equations to determine n unknowns). By neglecting one of the equations at a time, we can obtain $n+1$ different solutions for the unknown parameters. However, we cannot average the $n+1$ hyperplanes to obtain a single best estimate. To obtain a solution with-

out neglecting any of the equations, we solve an eigenvalue problem and use the eigenvector associated with the smallest eigenvalue to determine the unknown parameters. We have performed numerical experiments that compare our eigenvalue method to the approach of neglecting one equation at a time.

Research sponsored by U.S. DOE Engineering Research Program, Office of Basic Energy Sciences and by the Naval Air Warfare Center Aircraft Division/API Group, Technology and Development Office.

3.67

ERRATA SHEET FOR HERBERT GOLDSTEIN'S CLASSICAL MECHANICS, SECOND EDITION

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[Abstract of *American Journal of Physics* (in press); also ORNL/TM-12176, January 1993]

An errata sheet for Herbert Goldstein's textbook *Classical Mechanics*, Second Edition (Copyright 1980, ISBN 0-201-02918-9) is presented. Some of the errors in current printings of the text were corrected in the second printing; however, after communicating with Addison Wesley, the publisher for *Classical Mechanics*, it was discovered that the corrected galley proofs had been lost by the printer and that no one had complained of any errors in the eleven years since the second printing. The errata sheet corrects errors from all printings of the second edition.

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

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INFORMATICS

3.68

**CORRECTING SEQUENCING ERRORS
IN DNA CODING REGIONS USING
A DYNAMIC PROGRAMMING
APPROACH**

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E. C. Uberbacher

[Abstract of ORNL/TM-12821, December 1994; also *Computer Applications in the Biosciences* (in press)]

This paper presents an algorithm for detecting and "correcting" sequencing errors that occur in DNA coding regions. The types of sequencing error addressed include insertions and deletions (*indels*) of DNA bases. The goal is to provide a capability which makes single-pass or low-redundancy sequence data more informative, reducing the need for high-redundancy sequencing for gene identification and characterization purposes. This would permit improved sequencing efficiency and reduce genome sequencing costs. The algorithm detects sequencing errors by discovering changes in the statistically preferred reading frame within a putative coding region and then inserts a number of "neutral" bases at a perceived reading frame transition point to make the putative exon candidate frame consistent. We have implemented the algorithm as a front-end subsystem of the GRAIL DNA sequence analysis system to construct a version which is very error tolerant and also intend to use this as a testbed for further development of sequencing error-correction technology. Preliminary test results have shown the usefulness of this algorithm and also exhibited some of its weakness, providing possible directions for further improvement. On a test set consisting of 68 Human DNA sequences with 1% randomly generated indels in coding regions, the algorithm detected and corrected 76% of the indels. The average distance between the position of an indel and the predicted one was 9.4 bases. With this subsystem in place, GRAIL correctly predicted 89% of the coding messages with 10% false message on the "corrected" sequences, compared to 69% correctly predicted coding messages and 11% falsely predicted messages on the "corrupted" sequences using standard GRAIL II method (version 1.2).

The method uses a dynamic programming algorithm, and runs in time and space linear to the size of the input sequence.

Research sponsored by the Office of Health and Environmental Research U.S. DOE and by the Laboratory Directed Research and Development Programs.

*Biology Division.

3.69

**GENE RECOGNITION AND
ASSEMBLY IN GRAIL SYSTEM**

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R. J. Mural*

(Abstract of paper presented at the Third Contractor-Grantee Workshop for the DOE Human Genome Program, Santa Fe, NM, February 4-7, 1993)

GRAIL is a modular expert system being constructed to analyze and characterize the genetic structure of DNA sequences. Sufficient components of GRAIL have been constructed to allow the evaluation of the basic methodology for the recognition and modeling of genes, and to provide the basis for an e-mail server system for coding region localization.

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

*Biology Division.

3.70

INTEGRATED GENE RECOGNITION, MODELING AND DATABASE SEARCHING IN THE GRAIL AND GENQUEST ENVIRONMENTS

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M. Shah S. Matis
Y. Xu E. C. Uberbacher

(Abstract of paper presented at Open Problems in Computational Molecular Biology, Telluride, CO, July 11-17, 1994)

GRAIL and GenQuest provide sequence analysis environments which can be accessed either by e-mail or through an X-windows based graphical client-server user interface.

GenQuest is an integrated sequence comparison server which facilitates rapid and sensitive analysis of DNA and protein sequences by comparison to sequence and motif databases. GRAIL is a modular system which supports the recognition of gene features and gene modeling for the analysis and characterization of DNA sequences. The core of the GRAIL analysis engine continues to be based on multiple sensor-neural networks whose output is interpreted by a rule based system.

All information is presented to the user in graphic form in the X-window based client-server system XGRAIL. In addition, the user can view the positions of a number of other features including poly-A addition sites, potential promoters, CpG islands and repetitive DNA elements using this system.

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

*Biology Division.

3.71

GENE RECOGNITION, MODELING, AND HOMOLGY SEARCH IN THE GRAIL-GENQUEST SYSTEM

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(Abstract of paper presented at the DOE Contractor's Meeting, Santa Fe, NM, November 13-17, 1994)

GRAIL-genQuest is a modular expert system being constructed to analyze and characterize genomic and cDNA sequences. Recognition of gene features, gene modeling, and DNA, protein, and motif databases searches are supported by an e-mail server system and graphical client-server version. Within the last year significant improvements have been made in the sensitivity and accuracy of coding region recognition and gene modeling.

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

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3.72

AN IMPROVED SYSTEM FOR EXON RECOGNITION AND GENE MODELING IN HUMAN DNA SEQUENCES

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E. C. Uberbacher

(Abstract of paper presented at the Second International Conference on Intelligent Systems for Molecular Biology, San Francisco, CA, August 14-17, 1994)

A new version of the GRAIL system called GRAIL II, has recently been developed. GRAIL II is a hybrid AI system that supports a number of DNA sequence analysis tools including protein-coding region recognition, PolyA site and transcription promoter recognition, gene model construction, translation to protein, and DNA/protein database searching capabilities. This paper presents the core of GRAIL II, the coding exon recognition and gene model

construction algorithms. The exon recognition algorithm recognizes coding exons by combining coding feature analysis and edge signal (acceptor/donor/translation-start sites) detection. Unlike the original GRAIL system, this algorithm uses variable-length windows tailored to each potential exon candidate, making its performance almost exon length-independent. In this algorithm, the recognition process is divided into four steps. Initially a large number of possible coding exon candidates are generated. Then a rule-based prescreening algorithm eliminates the majority of the improbable candidates. As the kernel of the recognition algorithm, three neural networks are trained to evaluate the remaining candidates. The outputs of the neural networks are then divided into clusters of candidates, corresponding to presumed exons. The algorithm makes its final prediction by picking the best candidate from each cluster. The gene construction algorithm uses a dynamic programming approach to build gene models by using as input the clusters predicted by the exon recognition algorithm. Extensive testing has been done on these two algorithms. The exon recognition algorithm is a significant improvement over the original GRAIL system and the gene construction algorithm further improves the prediction results.

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

*Biology Division.

3.73

DETECTION OF PRE- AND POST-TRANSCRIPTIONAL CONTROL SEQUENCES IN DNA USING COMPUTATIONAL METHODS

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E. C. Uberbacher

(Abstract of paper presented at the Fourth Keck Symposium on Computational Biology, Pittsburgh, PA, October 24-November 5, 1993)

GRAIL (Gene Recognition Analysis Internet Link) is a computational tool designed to find and model genes in the vast amount of anonymous DNA sequence data which will be generated by the Human Genome project. GRAIL first processes

input DNA for a variety of statistical parameters then integrates the results of the primary analysis using neural networks designed to recognize key gene features. Accuracy of gene detection by GRAIL is about 90%.

Within chromosomal DNA, genes are arranged in series separated by their respective control regions. In order to increase the integrity of gene modeling by GRAIL, we have developed additional modules which score flanking regions for the presence of specific sequence elements. These regions bind multiple protein factors which participate in transcription or in processing of the primary RNA transcript. Recognition of these control sequences can set the boundaries for a gene within chromosomal DNA and can greatly facilitate automated gene modeling.

Recognition of control regions in sequence data is difficult due to the complex nature of control regions. For example, the mature 3' end of a mRNA is formed by post-transcriptional processing at a polyadenylation site. The polyA site is found at 10-30 basepairs downstream of a conserved hexamer AAUAAA. While this hexamer is found at a varying distance from the translation termination codon in the 3' ends of approximately 90% of eucaryotic genes, matches to the hexamer are scattered throughout the genome. Experimental deletion analysis has shown the requirement for other less highly conserved sequence elements found downstream of the polyA site. We have designed a module to detect polyA sites on the basis of statistical analysis of the sequence composition of regions from -6 to +59 basepairs with respect to the AAUAAA element. At least 85% of false polyA sites and 76% of true polyA sites are detected with absolute certainty using this method, while the remaining sites are scored for the likelihood of belonging to the true set of polyA sites.

Initiation of RNA transcription by RNA polymerase II is controlled by a number of sequence elements present at semi-conserved distances in the 5' end of the gene. There exists a collection of different elements which may or may not be present in a functional promoter. The TATA element is usually found upstream of the transcription start site (cap site); the CAAT box is further upstream from the TATA at an unspecified distance. In some cases a GC box or SP1 binding site is present and this sequence is thought to promote transcription in the absence of a TATA element. Some gene promoters lack all of these

elements and are thought to initiate transcription from a weakly conserved pyrimidine tract. Not all of the proposed regulatory elements are present in all genes and this property most likely reflect differences in the regulation of gene expression. In order to recognize the elaborate patterns inherent in RNA pol II promoters, a neural network is being trained with statistical information from the analysis of sequence regions flanking the elements and using distance probability information. We feel that both of these modules will allow us to recognize control regions and thus set the boundaries for genes.

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

*Biology Division.

3.74

DETECTION OF HUMAN RNA POLYMERASE II PROMOTERS USING ARTIFICIALLY INTELLIGENT METHODS

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(Abstract of paper presented at the First World Congress on Computational Medicine, Public Health and Biotechnology, Austin, TX, April 24-28, 1994)

One of the most difficult problems in the analysis of eucaryotic genes is the detection of RNA polymerase II promoter regions. RNA pol II promoters are complex in nature consisting of a collection of weakly conserved consensus sequences any of which may be absent without the loss of promoter function. The distances between most of the promoter elements are not well conserved. In previous attempts to analyze eucaryotic RNA pol II promoters, regions from all eucaryotes were used and taxonomic variation further contributed to control region ambiguities. As a result, accurate detection of eucaryotic promoters by previously devised computational methods has been disappointing.

Although the promoter vocabulary is quite rich, containing many words which may modulate transcription or dictate tissue specific function, a basic group of core promoter elements has been suggested in the literature. Approximately 62% of human promoter sequences contain a TATAA, or TATAA-like sequence element at approximately

30 bases upstream of the cap site or transcription start site. The TATAA element has been shown to bind TBF and ultimately TFIID. Other elements are the GC box which binds SP-1 and up-regulates transcription; the CAAT box; and the ATG protein initiator codon. To characterize real promoters, we searched a group of 206 experimentally mapped human promoter regions for matches to these elements and then constructed frequency matrices for each element. In addition, we constructed histograms for the distances separating the various elements

We have created a tool specific for the detection of human RNA pol II promoter regions using a unique strategy which combines statistical analysis with neural networks. In this method, the scores of the individual elements of a putative promoter and scores derived from the distance histograms are used by a neural network to score a putative promoter. Examples based on the scores generated from the various matrices and distance histograms derived from real promoter regions, combined with a similar set of false examples (which contained a TATAA or TATAA-like element) were used to train the neural network to discriminate between the two sets.

Preliminary results show that at least 86% of human TATAA containing promoters can be found using this method. Although less than 8% of the false examples were incorrectly classified as true, a further reduction of the false positive rate is desired. We are using additional training parameters, such as GC content and formulation of additional rules which depend on GRAIL's ability to find exons in anonymous DNA, to aid in promoter detection and reduction of the false positive rate.

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

*Biology Division.

3.75

DETECTION OF CONTROL REGIONS IN THE HUMAN GENOME USING INTELLIGENT SYSTEMS

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M. Shah D. Buley*
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R. J. Mural* E. C. Uberbacher

(Abstract of paper presented at Open Problems in Computational Molecular Biology, Telluride, CO, July 11-17, 1994)

GRAIL is a modular system designed to automate gene analysis, characterization, and modeling. Two versions of GRAIL, the e-mail server system and the graphical client-server system, X-GRAIL, can computationally characterize a DNA sequence and can then use the modeled gene for database queries. The heart of the GRAIL system is composed of a number of neural networks which have been trained to recognize coding regions based on statistical parameters such as word bias in coding versus non coding regions, Markov analysis and other gene features such as splice junctions. Once an optimal prediction is made for starting, middle, and terminal exons, a computational model of the gene can be constructed. The best translation of an individual exon or the gene model can then be used as substrate for database queries via the Genquest Q server. The accuracy of GRAIL, when tested on known genes is greater than 90%.

Many signal sequences are known to act *in cis* to control gene expression. Promoter and terminator regions, found at the 5' and 3' boundaries of the gene, control transcription and are thus not present in the nascent RNA transcript. Other signals such as splice junctions and polyadenylation sites are present in the transcript and function to direct post-transcriptional RNA processing. All of the afore mentioned signals are known to be constitutively controlled but there are examples of tissue specific, regulated control elements.

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

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3.76

PROTEIN STRUCTURE PREDICTION USING HYBRID AI METHODS

X Guan R. J. Mural*
E. C. Uberbacher

(Abstract of paper presented at the Tenth IEEE Conference on Artificial Intelligence for Applications, Marriott Riverwalk, San Antonio, TX, March 1-4, 1994)

This paper describes a new approach for predicting protein structures based on Artificial Intelligence methods and genetic algorithms. We combine nearest neighbor searching algorithms, neural networks, heuristic rules and genetic algorithms to form an integrated system to predict protein structures from their primary amino acid sequences. First we describe our methods and how they are integrated, and then apply our methods to several protein sequences. The results are very close to the real structures obtained by crystallography. Parallel genetic algorithms are also implemented.

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

*Biology Division.

3.77

CONSTRUCTING GENE MODELS FROM ACCURATELY-PREDICTED EXONS: AN APPLICATION OF DYNAMIC PROGRAMMING

Y. Xu R. J. Mural*
E. C. Uberbacher

[Abstract of *Computer Applications in the Biosciences* (in press)]

This paper presents a computationally efficient algorithm, the Gene Assembly Program III (GAP III), for constructing gene models from a set of accurately-predicted "exons." The input to the algorithm is a set of clusters of exon candidates, generated by a new version of the GRAIL coding region recognition system. The exon candidates of a cluster differ in their presumed edges and occasionally in their reading frames. Each exon candidate has a numerical score representing its "probability" of being an actual exon. GAP III uses a dynamic programming algorithm to construct a gene model, complete or partial, by optimiz-

ing a pre-defined objective function. The optimal gene models constructed by GAP III correspond very well with the structures of genes which have been determined experimentally and reported in the Genome Sequence Database GSDB. On a test set of 76 Human DNA sequences consisting of 534 true exons, GAP III constructed 76 gene models using 517 exons, among which 501 ($501/537 = 94\%$) are true exons and 16 ($16/517 = 3\%$) are false positive. Among the 501 true positives, 394 (79%) match the actual exons exactly, and 493 (98%) match an actual exon at least one edge. GAP III is computationally efficient. If we use E and C to represent the total number of exon candidates in all clusters and the number of clusters, respectively, the running time of GAP III is proportional to ($E \times C$).

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

*Biology Division.

3.78

RECOGNIZING EXONS IN GENOMIC SEQUENCE USING GRAIL II

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M. Shah E. Uberbacher

[Abstract of book chapter in *Genetic Engineering, Principles and Methods*, Plenum Press, Vol. 15 (1994)]

We describe an improved neural network system for recognizing protein coding regions (exons) in human genomic DNA sequences. This coding region recognition system is part of a new version of GRAIL, GRAIL II, and represents a significant improvement over the coding recognition performance of the previous GRAIL system. GRAIL II divides the process of locating exons into four steps. It first generates an exon candidate pool consisting of all possible (translation start - donor), (acceptor - donor), and (acceptor - translation stop) pairs within all open reading frames of the test sequence. The vast majority of these exon candidates are eliminated from consideration by applying a set of heuristic rules. After reducing the size of the candidate pool, GRAIL II uses three trained neural networks to evaluate the coding potential and accuracy of the edges of starting exon, internal exon and terminal exon

candidates. These networks output a set of overlapping candidates for each exon which differ by their scores and position of their edges. Multiple candidates for a given exon are grouped into a cluster based on their locations relative to candidates corresponding to other exons, and the highest scoring candidate from each cluster is used as the "best" prediction of the corresponding exon. Unlike the previous GRAIL version, GRAIL II uses variable-length windows to evaluate exon candidates and its performance is nearly independent of exon length. In addition to several strong indicators of coding potential, the system uses several other types of information including scores for splice junctions, GC composition, and the properties of the regions adjacent to an exon candidate, to aid in the discrimination process. On a large set of sequences from Genbank, GRAIL II located 93% of all exons regardless of size with a false positive rate of 12%. Among the true positives, 62% match the actual exons exactly (the exons edges are correct to the base), and 93% match at least one edge correctly. These statistics are further improved, especially the false positive rate and accuracy of the edges, through a process of gene model construction by the Gene Assembly Program (GAP III) module of GRAIL II, which uses the scored exon candidates as input and constructs optimal gene models. The gene modeling system will be described elsewhere.

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

*Biology Division.

3.79

A PRACTICAL GUIDE TO THE GRAIL E-MAIL SERVER

E. C. Uberbacher X. Guan
R. J. Mural*

[Abstract of *Automated DNA Sequencing and Analysis Techniques* (in press)]

The methods used for obtaining genome information are undergoing a revolution. One cornerstone of this revolution is an increased reliance on sequence-based computational methods to provide insight into the structure, function, and organization of the genome, and this trend will undoubtedly continue as both sequencing and infor-

matics technologies improve. The infrastructure of computational genome analysis has also changed dramatically to a distributed environment where various databases and analytical resources may be called into play to deal with a given analysis problem. In this type of distributed computing environment, it is a significant challenge for even the most skillful genome scientist to gain the expertise necessary to interact with the multitude of DNA and protein, human and model organism, mapping, sequencing, and structure databases and specialized analysis resources.

Research sponsored by U.S. DOE Office of Health and Environmental Research and Director R&D Seed Program.

*Biology Division.

3.80

INFORMATICS SUPPORT FOR MAPPING IN MOUSE-HUMAN HOMOLOGY REGIONS

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L. Hauser* R. Mural*
E. C. Uberbacher

(Abstract of paper presented at the Third Contractor-Grantee Workshop for the DOE Human Genome Program, Santa Fe, NM, February 4-7, 1993; also DOE Contractor's Meeting, Santa Fe, NM, November 13-17, 1994)

The purpose of this project is to develop databases and tools for the ORNL Mouse-Human Mapping Project, including the construction of a mapping database for the project, tools for management and archiving of cDNAs and other probes used in the laboratory, and analysis tools for mapping, inter-specific backcross, and other needs. Our initial effort has involved installing and developing a relational SYBASE database for tracking samples and probes, experimental results, analysis, etc. Recent work has focused on a corresponding ACeDB implementation containing mouse mapping data and which provides numerous graphical views of this data. The initial relational database has been constructed with SYBASE using a schema modeled from the one implemented at the LLNL center because of the available documentation for the LLNL system, and to maximize compatibility with the human chromosome 19 mapping effort (major homologies exist between human chromosome 19 and mouse chromosome 7 - the initial focus of the

ORNL work). Our ACeDB implementation has been modeled somewhat from the chromosome 21 ACeDB system at LBL (with some model modification) and is designed to contain genetic and physical mouse map data as well as homologous human chromosome data. The utility of exchanging map information with LLNL (human chromosome 19) and potentially other centers has led to the implementation of procedures for data export, and import of human mapping into the ORNL databases.

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

*Biology Division.

3.81

DYNAMIC SUBTREES: A NEW DATA STRUCTURE FOR MANIPULATING TREES

Y. Xu

(Abstract of paper presented at the 6th International Conference on Computing and Information, Peterborough, Ontario, Canada, May 26-28, 1994)

This paper presents a new data structure, called dynamic subtrees, which manipulates an undirected forest. The data structure supports three main operations *cut*, *link*, and *comp*. A *cut* operation splits a tree into two by cutting an edge of the tree; a *link* operation joins two trees by linking two arbitrarily specified vertices of the trees; a *comp* operation computes a function $f(S) = f(v_1) \odot f(v_2) \odot \dots$, for vertices v_i of S , where S is either tree of $T - e$, with T being the tree under consideration and e an arbitrarily given edge of T , $f(v) \in F$, a finite set, and $\odot$ is a closed commutative and associative binary operation over F . Assuming s_t is the time for implementing a $\odot$ operation, each of the *cut*, *link*, and *comp* operations can be implemented in $O((s_t + \log n) \log n)$ time, after a preprocessing in $O(s_t n)$ time, where n is the number of vertices of the forest under consideration.

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

3.82

A MULTIPLE DIVIDE-AND-CONQUER (MDC) ALGORITHM FOR OPTIMAL ALIGNMENTS IN LINEAR SPACE

X. Guan E. C. Uberbacher

(Abstract of ORNL/TM-12764, June 1994)

This paper describes an algorithm for optimal sequence alignments in linear space. A new multiple divide-and-conquer technique is presented that leads to a linear space alignment algorithm which improves upon an existing algorithm by Myers and Miller.

Research sponsored by Director R&D Seed Program, Office of Health and Environmental Research, U.S. DOE.

3.83

CRYSTALLIZATION OF NUCLEOSOME CORE PARTICLES CONTAINING A 146 bp DNA PALINDROME

J. M. Harp* E. Uberbacher
A. Roberson† A. Gewiess*
G. J. Bunick†

[Abstract of *The Molecular Biology* (in press)]

This laboratory is pursuing a medium to high resolution structure of the nucleosome core particle. Previously, a low resolution structure (8 Å) was published. The crystal used in the structure determination contained nucleosome core particles isolated from chicken erythrocyte nuclei. Such core particles are composed of relatively homogeneous histone protein octamers and random heterogeneous DNA sequences. Determination of the structure to significantly higher resolution requires crystallization of nucleosomes reconstituted using defined sequence DNAs. The sequence(s) must achieve precise rotational and translational phasing on the chicken histone octamer. Several sequences meeting this criterion have been developed. We have found that crystals of nucleosome core particles reconstituted using a 145 bp human alpha satellite DNA sequence diffract X-rays to 3-4 Å. We postulated that further improvement in diffraction resolution would be realized if the inherent dyad symmetry of the histone octamer were extended to the bound DNA by using a palindrome based on half of the original, human alpha

satellite sequence. This aim has been achieved by constructing an inverted repeat of one half of the native human alpha satellite fragment. Crystals of nucleosomes containing the palindrome sequence have been grown by charge-neutralization dialysis. X-ray diffraction from the crystals is anisotropic with observed reflections extending to d-spacings of 3.0-3.2 Å in the a direction, 3.5 Å in b, and 2.8 Å in c.

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

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3.84

EFFECT OF CHANGES IN THE REGION NEAR AN IMMUNOGLOBULIN SECRETORY-SPECIFIC POLYADENYLATION SITE ON THE STRENGTH OF THE SITE AND ITS REGULATION

S. Matis C. Milcarek*

(Abstract of paper presented at the Workshop on RNA 3' Ends: Formation and Function, Oxford, England, September 15-19, 1993)

An increase in the efficiency of the polyadenylation-cleavage reaction has been previously shown to accompany the developmentally regulated shift from membrane to secretory-specific forms of immunoglobulin mRNA in late stage/plasma B-cells. When stably transfected constructs where the secretory-specific polyA site alone, in the absence of the competing CH3 to M1 splice, were tested for regulated expression, we found that sequences near the relatively weak immunoglobulin γ 2B secretory polyadenylation site play an important role in this late/plasma stage regulation. In contrast, sequences near the SV40 early or the γ 2a membrane polyA sites, both of which were much more efficient polyA sites than the secretory site, were used equally by early/memory vs late/plasma B-cells (Lassman et al.). We wanted to determine which nucleotides were responsible for the regulation of the weaker,

secretory-specific site but not the stronger, SV early site, and the contribution of nucleotides in the secretory specific downstream consensus element to the relative strengths of the polyA sites. To that end, we made chimeras of the Ig secretory: SV40 early polyA sites and downstream consensus sequences, with and without di-nucleotide substitutions in the downstream elements; the sequences were carried on synthetic 31-mers and inserted into a modified pSV2gpt vector. These nearly isogenic composites were analyzed as stable transfectants in early vs late B-cell lines for their ability to direct use of the 5 foot proximal (chimeric) polyA site in stable transfectants; in each construct the default, 3 foot polyA site was the intact

SV40 early site of the pSV2gpt vector. We found that di-nucleotide alterations of the Ig secretory-specific downstream element could result in significant changes in polyA site strength. We also found that the region surrounding the site of Ig secretory-specific polyadenylation/cleavage as well as the downstream consensus element could each contribute to the B-cell stage specific use of the polyA site in the chimeras.

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

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HUMAN MACHINE INTERFACES

3.85

EXPERIMENTAL VALIDATION OF NAVIGATION WORKLOAD METRICS

J. C. Schryver J. A. Wachtel*

[Abstract of paper presented at the 38th Annual Meeting of the Human Factors and Ergonomics Society, Nashville, TN, October 24-28, 1994; Proc. Vol. 1, pp. 340-344 (1994)]

Advanced digital computer display interfaces in the control room may increase operator workload. Workstation monitors provide limited display area, and information is represented in large-scale display networks. Display navigation may generate disorienting effects, require additional resources for window management, and increase memory and data integration requirement. Six ORNL employees participated in an experiment to validate proposed metrics of navigation workload in the advanced control room. The task environment was a display network consisting of 25 windows resembling a simplified Safety Parameter Display System for Pressurized Water Reactors. A repeated measures design with 3 within-subjects factors was employed. The factors were task difficulty, navigation distance level, and a blocking factor. Participants were asked to monitor a single parameter (easy task) or two parameters (difficult task). Fourteen candidate metrics were tested. Analysis of variance of the modified task load index (MTLX) and rating subscales (confidence, dis-

orientation, effort) demonstrated substantial support for the claim that navigation of large-scale display networks can impose additional mental load. Primary and secondary task performance measures exhibited ceiling effects. Memory probes for these tasks were inadequate because they were recognition-based and coarse. Eye gaze measures were not validated, indicating a need for more refined data reduction algorithms. Strong positive correlations were found between MTLX and both navigation duration and standard deviation of pupil diameter. Further study and increased statistical power are required to validate objective navigation workload metrics.

Research sponsored by U.S. DOE and by the U.S. Nuclear Regulatory Commission, Office of Nuclear Regulatory Research.

*U.S. Nuclear Regulatory Commission, Rockville, MD.

3.86

EYE-GAZE DETERMINATION OF USER INTENT AT THE COMPUTER INTERFACE

J. H. Goldberg* J. C. Schryver

(Abstract of paper presented at the Seventh European Eye Movement Conference, University of Durham, Durham, England, August 31–September 3, 1993)

Determination of user intent at the computer interface through eye-gaze monitoring can significantly aid applications for the disabled, as well as telerobotics and process control interfaces. Whereas current eye-gaze control applications are limited to object selection and x/y gaze-point tracking, a methodology was developed here to discriminate a more abstract interface operation: zooming-in or out. This methodology first collects samples of eye-gaze location looking at controlled stimuli, at 30 Hz, just prior to a user's decision to zoom. The sample is broken into data frames, or temporal snapshots. Within a data frame, all spatial samples are connected into a minimum spanning tree, then clustered, according to user defined parameters. Each cluster is mapped to one in the prior data frame, and statistics are computed from each cluster. These characteristics include cluster size, position, and pupil size. A multiple discriminant analysis uses these statistics both within and between data frames to formulate optimal rules for assigning the observations into zoom-in, zoom-out, or no zoom conditions. The statistical procedure effectively generates heuristics for future assignments, based upon these variables. Future work will enhance the accuracy and precision of the modeling technique, and will empirically test users in controlled experiments.

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

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3.87

EYE-GAZE CONTROL OF THE COMPUTER INTERFACE: DISCRIMINATION OF ZOOM INTENT

J. H. Goldberg* J. C. Schryver

(Abstract of paper presented at the 37th Annual Meeting: Human Factors and Ergonomics Society, Seattle, WA, October 11–15, 1993)

An analysis methodology and associated experiment were developed to assess whether definable and repeatable signatures of eye-gaze characteristics are evident, preceding a decision to zoom-in, zoom-out, or not to zoom at a computer interface. This user intent discrimination procedure can have broad application in disability aids and telerobotic control. Eye-gaze was collected from 10 subjects in a controlled experiment, requiring zoom decisions. The eye-gaze data were clustered, then fed into a multiple discriminant analysis (MDA) for optimal definition of heuristics separating the zoom-in, zoom-out, and no-zoom conditions. Confusion matrix analyses showed that a number of variable combinations classified at a statistically significant level, but practical significance was more difficult to establish. Composite contour plots demonstrated the regions in parameter space consistently assigned by the MDA to unique zoom conditions. Peak classification occurred at about 1200–1600 msec. Improvements in the methodology to achieve practical real-time zoom control are considered.

Research sponsored by U.S. DOE Office of Technology Support Programs and Oak Ridge Associated Universities.

*Penn State University, University Park, PA.

3.88

EYE-GAZE CONTINGENT CONTROL OF THE COMPUTER INTERFACE: METHODOLOGY AND EXAMPLE FOR ZOOM DETECTION

J. H. Goldberg* J. C. Schryver

[Abstract of *Behavioral Research Methods, Instruments, and Computers* (in press)]

Discrimination of user intent at the computer interface solely from eyegaze can provide a powerful tool, benefiting many applications. A method-

ology of discriminating zoom-in, zoom-out, or no-zoom intent was developed here for such applications as telerobotics, disability aids, weapons systems, and process control interfaces. Using an eye tracking system, eyegaze locations on a display are collected, clustered, and then characterized. The cluster characteristics are input to a multiple linear discriminant analysis, which classifies the zoom-in, zoom-out, and no zoom conditions, from recognizable patterns. The methodologies, algorithms, and experimental data collection procedure are described, followed by example output from the computer program. Though developed specifically for real-time discrimination of zoom conditions, the methodology has a broader potential for user intent discrimination from other interface operations.

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

*Penn State University, University Park, PA.

3.89

EYE GAZE AND INTENT: APPLICATION IN 3D INTERFACE CONTROL

J. C. Schryver J. H. Goldberg*

[Abstract of paper presented at the Fifth International Conference on Human-Computer Interaction: Software and Hardware Interfaces, Orlando, FL, August 8-13, 1993; Proc. Vol. 2, pp. 573-578, G. Salvendy and M. J. Smith, Eds., Elsevier (1993)]

Computer interface control is typically accomplished with an input "device" such as keyboard, mouse, trackball, etc. An input device translates a user's input actions, such as mouse clicks and key presses, into appropriate computer commands. To control the interface, the user must first convert intent into the syntax of the input device. A more natural means of computer control is possible when the computer can directly infer user intent, without need of intervening input devices. We describe an application of eye-gaze-contingent control of an interactive three-dimensional (3D) user interface. A salient feature of the user interface is natural input, with a heightened impression of controlling the computer directly by the mind. With this interface, input of rotation and translation are intuitive, whereas other abstract

features, such as zoom, are more problematic to match with user intent. This paper describes successes with implementation to date, and ongoing efforts to develop a more sophisticated intent inferring methodology.

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

*Penn State University, University Park, PA.

3.90

THE INTEGRATED WORKSTATION SYSTEM: A COMMON, CONSISTENT LINK BETWEEN NUCLEAR PLANT PERSONNEL AND PLANT INFORMATION AND COMPUTERIZED RESOURCES

**R. T. Wood* H. E. Knee
J. A. Mullens* J. K. Munro, Jr.*
B. K. Swail* P. A. Tapp***

[Abstract of paper presented at the American Nuclear Society Topical Meeting on Nuclear Plant Instrumentation, Control, and Man-Machine Interface Technologies, Garden Plaza Hotel, Oak Ridge, TN, April 18-21, 1993; Proc. (1993)]

The increasing use of computer technology in the U.S. nuclear power industry has greatly expanded the capability to obtain, analyze, and present data about the plant to station personnel. Data concerning a power plant's design, configuration, operational and maintenance histories, and current status, and the information that can be derived from them, provide the link between the plant and plant staff. It is through this information bridge that operations, maintenance and engineering personnel understand and manage plant performance. However, it is necessary to transform the vast quantity of data available from various computer systems across communications networks into clear, concise, and coherent information. In addition, it is important to organize this information into a consolidated, structured form within an integrated environment so that various users throughout the plant have ready access at their local station to knowledge necessary for their tasks. Thus, integrated workstations are needed to provide the required information and proper software tools, in a manner that can be easily understood and used, to the proper users throughout the plant. As part of a Cooperative Research

and Development Agreement between the U.S. Department of Energy and the Electric Power Research Institute, an effort is underway at the Oak Ridge National Laboratory to address this need by developing Integrated Workstation functional requirements and implementing a limited-scale prototype demonstration. The Integrated Workstation requirements will define a flexible, expandable computer environment that permits a tailored implementation of workstation capabilities and facilitates future upgrades to add enhanced applications. In presenting the Integrated Workstation concept, the functionality to be supported by the Integrated Workstation and inherent capabilities to be provided by the workstation environment will be described. In addition, general technology areas which are to be addressed in the Integrated Workstation functional requirements will be discussed.

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

*Instrumentation and Controls Division.

3.91

HUMAN FACTORS ENGINEERING: A KEY ELEMENT OF INSTRUMENTATION AND CONTROL SYSTEM DESIGN

H. E. Knee

[Abstract of paper presented at the 39th International Instrumentation Symposium, Albuquerque, NM, May 2-6, 1993; Proc. pp. 1113-1122 (1993)]

Human factors engineering (HFE) has been in existence for a number of decades. Up until recently, however, its application to the design and operation of complex process control environments has been relatively conservative. In the nuclear industry, it took a major accident such as that at Three Mile Island - Unit 2 (TMI-2) to focus attention on the need for systematically accounting for the roles of humans in the control and maintenance of nuclear power plants (NPPs). Since TMI, the nuclear industry has made significant strides in fostering the use of HFE principals. This progress has been slowed to some degree due to the relatively anemic state of the US commercial nuclear power industry; however, new evolutionary and revolutionary nuclear design concepts are utilizing HFE principals and supporting research

for advanced HFE concepts. Furthermore, a new Department of Energy (DOE) standard on HFE design criteria is being developed. Since instrumentation and controls (I&C) provide the interface between humans and the systems to be monitored, diagnosed and controlled, much of the HFE work is key to successful I&C. This paper will discuss HFE in the nuclear industry, its recent role in nuclear I&C, and will discuss recent applications and future directions.

Research sponsored by U.S. Department of Energy.

3.92

OPERATOR ROLE DEFINITION: AN INITIAL STEP IN THE HUMAN FACTORS ENGINEERING DESIGN OF THE ADVANCED NEUTRON SOURCE (ANS)

H. E. Knee

P. F. Spelt

M. M. Houser *

W. E. Hill†

[Abstract of paper presented at the 38th Annual Meeting of the Human Factors and Ergonomics Society, Nashville, TN, October 24-28, 1994; Proc. Vol. 2, pp. 1013-1017 (1994)]

The Advanced Neutron Source (ANS) is a new basic and applied research facility sponsored by the U.S. Department of Energy that is proposed for construction. It will provide neutron beams for measurements and experiments in the fields of materials science and engineering, biology, chemistry, materials analysis, and nuclear science. The facility will provide a useful neutron beam flux that is at least five times more than is available at the world's best existing facilities. It will also provide world-class facilities for isotopes production, materials irradiation testing, materials analysis, and the production of positrons. ANS will be unique in the United States in the extent to which human factors engineering (HFE) principles will be included in its design and construction. Initial HFE accomplishments include the development of a functional analysis, an operating philosophy, and a program plan. In fiscal year 1994, HFE activities are focusing on the role of the ANS control room reactor operator (RO). An operator-centered control room model was used in conjunction with information gathered from existing ANS system design descriptions and other literature to define RO responsibilities. From this list, a survey in-

strument was developed and administered to ANS design engineers, operations management personnel at Oak Ridge National Laboratory's High Flux Isotope Reactor (HFIR), and HFIR ROs to detail the nature of the RO position. Initial results indicated that the RO should function as a high-level system supervisor with considerable monitoring, verification, and communication responsibilities. The relatively high level of control automation has resulted in a reshaping of the RO's traditional safety and investment protection roles.

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

*Engineering Division.

†Research Reactors Division.

3.93

OPERATOR-CENTERED CONTROL OF A SEMI-AUTONOMOUS INDUSTRIAL ROBOT

P. F. Spelt S. L. Jones*

(Abstract of paper presented at the 38th Annual Meeting of the Human Factors and Ergonomics Society, Nashville, TN, October 24-28, 1994)

This paper presents work done by Oak Ridge National Laboratory and Remotec, Inc., to develop a new operator-centered control system for Remotec's Andros telerobot. Andros robots are presently used by numerous electric utilities, the armed forces, and numerous law enforcement agencies to perform tasks which are hazardous for human operators. This project has automated task components and enhanced the video graphics display of the robot's position in the environment to significantly reduce operator workload. The procedure of automating a telerobot requires the addition of computer power to the robot, along with a variety of sensors and encoders to provide information about the robot's performance in and relationship to its environment. The resulting vehicle serves as a platform for research on strategies to integrate automated tasks with those performed by a human operator. The addition of these capabilities will greatly enhance the safety and efficiency of performance in hazardous environments.

Research sponsored by U.S. DOE Office of Nuclear Energy, Office of Technology.

*Remotec, Union Valley Road, Oak Ridge, TN.

3.94

TASK AUTOMATION IN A SUCCESSFUL INDUSTRIAL TELEROBOT

P. F. Spelt S. L. Jones*

[Abstract of paper presented at the AIAA/NASA Conference on Intelligent Robots in Field, Factory, Service and Space (CIRFFSS '94), Houston, TX, March 21-24, 1994; Proc. Vol. 1, pp. 88-92 (1994)]

In this paper, we discuss cooperative work by Oak Ridge National Laboratory and Remotec, Inc., to automate components of the operator's workload using Remotec's Andros telerobot, thereby providing an enhanced user interface which can be retrofit to existing fielded units as well as being incorporated into new production units. Remotec's Andros robots are presently used by numerous electric utilities to perform tasks in reactors where substantial exposure to radiation exists, as well as by the armed forces and numerous law enforcement agencies. The automation of task components, as well as the video graphics display of the robot's position in the environment, will enhance all tasks performed by these users, as well as enabling performance in terrain where the robots cannot presently perform due to lack of knowledge about, for instance, the degree of tilt of the robot. Enhanced performance of a successful industrial mobile robot leads to increased safety and efficiency of performance in hazardous environments. The addition of these capabilities will greatly enhance the utility of the robot, as well as its marketability.

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

*Remotec, Inc., Oak Ridge, TN.

3.95

**ROLE OF THE OPERATOR IN
NUCLEAR POWER PLANTS AS
DETERMINED FROM A SURVEY
OF THE NORTH AMERICAN
NUCLEAR COMMUNITY**

P. F. Spelt

[Abstract of paper presented at the American Nuclear Society Topical Meeting on Nuclear Plant Instrumentation, Control, and Man-Machine Interface Technologies, Garden Plaza Hotel, Oak Ridge, TN, April 18-21, 1993; Proc. pp. 120-127 (1993)]

Results of an empirical survey, one of the first to deal with the Role of the Operator in nuclear power plants in North America, are presented. The survey showed that the theoretical match between operators' responsibility and control (written definition of "role") is not supported by the numerical evaluations of these two concepts. Across a dimension from existing to advanced reactors, there is increasingly a shift from hands-on manipulation and readout-by-readout information integration by the operators to a role in which the operator is a passive monitor whose primary task is to give permissives to the automated control system. There is a decreasing degree of control for operators, while responsibility remains high. Decreased control coupled with high responsibility may create shift operating staff problems.

Research sponsored by the U.S. DOE Office of Technology Development.

3.96

**DRIVER PERFORMANCE DATA
ACQUISITION SYSTEM FOR
ERGONOMICS RESEARCH**

R. J. Carter M. J. Goodman*

(Abstract of paper presented at the International Ergonomics Association Congress, Toronto, Ontario, Canada, August 15-19, 1994)

A portable ergonomics data acquisition system consisting of state-of-the-art hardware is being designed. It will be employed to record driver, vehicle, and environment parameter data from a wide range of vehicles and trucks. The system will be unobtrusive to the driver and inconspicuous to the outside world. It will have three modes of data gathering and provide for extended periods of data collection. Modularity, flexibility, and cost will be key drivers in the development effort. The ergonomics data acquisition system project is being conducted in two phases - a feasibility study and a development, construction, and validation phase.

Research sponsored by the National Highway Traffic Safety Administration, Office of Crash Avoidance Research U.S. DOE.

*Office of Crash Avoidance Research, National Highway Traffic Safety Administration, Washington, DC.

Section 4

NUCLEAR ANALYSIS AND SHIELDING

4.0. INTRODUCTION

D. T. Ingersoll

The primary mission of the Nuclear Analysis and Shielding Section is to develop and apply state-of-the-art computational methods for the modeling of radiation transport and physics phenomena pertinent to a broad range of national programs. The groups within the section were reorganized twice during the reporting period in response to personnel changes and to better organize ourselves for existing and new program opportunities. Currently, the section is comprised of three groups: the Shielding and Dosimetry Group, the Reactor Physics Group, and the Applied Physics Group. Major research activities include: (1) the development of theoretical and numerical methods for modeling particle transport and physics phenomena, (2) core physics and radiation transport analyses for advanced fission reactors, (3) computational modeling of high-energy particle cascades and transport for accelerator shielding studies and physics detector analysis, and (4) nuclear vulnerability assessments and methods validation for national defense systems. The Oak Ridge Detector Center, which is also organizationally contained in the section, operates in conjunction with other laboratories and universities in the southeast region of the U.S. and coordinates basic and detector-specific research in support of national and international high-energy particle detector projects.

Research in theoretical and numerical methods centered primarily around improving the performance and features of our premier transport code, TORT. Supported by the Knolls Atomic Power Laboratory, investigations were made into improved acceleration techniques and alternative numerical methods which are more adaptable to parallel computer architectures. A new pair of codes, TORSED and TORSET were developed to provide flexible coupling between the DORT and TORT discrete ordinates codes. Progress was also made in developing the ORIGAMI visualization tool for the construction, verification, and nuclear analysis of complex geometry models. Interfaces were constructed for several different geometry data formats including formats produced by selected computer-aided-design (CAD) programs.

Over the course of the reporting period, we saw the unfortunate demise of the DOE-NE advanced reactor program, which required several adjustments and redirections of our work. Nonetheless, our staff maintained a prominent position in the national and international shielding community and expanded our prominence in the area of reactor physics. In April, 1994, section staff organized and largely ran the very successful "Advances in Reactor Physics" topical conference, which was attended by more than 200 participants representing 18 countries. Also, section staff members were assigned to represent the U.S. in an IAEA Coordinated Research Program supporting the modular high-temperature gas-cooled reactor program, and in establishing a "sister laboratory" arrangement with Thailand's Atomic Energy Office for Peace.

The central focus for our activities for fission reactor applications was the reactor physics and shielding support for the Advanced Neutron Source (ANS). Significant accomplishments in our reactor physics analyses included: (1) the optimization of fuel grading distributions resulting in a substantial gain in core performance, (2) an intense study of fuel enrichment options and the redesign of the core geometry to accommodate medium- and low-enriched fuel, and (3) significant enhancements

to the VENTURE code system. The shielding tasks for ANS were initiated during the reporting period and included large-scale global analyses of the neutron and gamma-ray fluxes in the reflector tank and adjacent regions, as well as localized analyses for identified "hot spots."

A rapidly growing effort in the area of reactor physics was initiated with the Defense Nuclear Agency (DNA) as part of their Hazard Prediction and Assessment Capability program. The goal of the program is to provide field personnel with fast-running computer simulation tools for the prediction and assessment of the hazards associated with nuclear and chemical facilities. The ORNL effort, which is being led by section staff, supports researchers in several divisions and includes: (1) the development of standard models for numerous types of nuclear facilities, (2) the generation of source term data for the facilities, (3) the characterization of potential material release and dispersion from the facilities, and (4) the development of a fast-running PC-based simulation code system for field use.

An expanded effort in the transport and shielding area was developed to support the Nuclear Regulatory Commission's Pressure Vessel Surveillance program. A major element in this expanded effort was the development and testing of a new multigroup cross section library based on ENDF/B-VI nuclear data. The library, designated BUGLE-93, is the first production-quality library to be produced from Version VI data and will be the industry standard for light-water reactor (LWR) shielding applications. Also, responsibility for a long-standing NRC program for pressure vessel dosimetry data and methods was transferred to the section. This effort includes the maintenance and upgrading of several dosimetry data bases and the development of advanced transport methods for predicting LWR pressure vessel fluences.

Our rapidly growing effort in high-energy transport and physics applications took a major blow with the sudden demise of the Superconducting Super Collider (SSC) project. Prior to the program termination, the ORNL-wide development work coordinated by the Oak Ridge Detector Center (ORDC) had grown to a yearly level of more than \$5 million. Section staff made major contributions to the designs of the Solenoidal Detector Collaboration and the Gamma-Electron-Muon detector projects and to the shielding design for the SSC experiment halls. With the loss of the SSC, research efforts focused on support for other national and international accelerator projects and basic improvements to the data and features of the CALOR and GCALOR code systems. A new major version of CALOR (CALOR93) was prepared and released for open distribution through the Radiation Shielding Information Center. In the area of fusion neutronics, a senior staff member from the section was selected to represent the U.S. on the Joint Central Team for the International Thermonuclear Experimental Reactor project and is on a long-term assignment in Garching, Germany.

A long-standing program supporting the Defense Nuclear Agency's (DNA) Radiation Environments Program was continued with emphasis on development and testing of the MASH computer code system. The first production version of the code system, which couples forward discrete ordinates methods with adjoint Monte Carlo methods, was released for restricted distribution. The code has been adopted by the NATO Panel VII Ad Hoc Group of Shielding Experts as the reference code for analysis of both NATO and non-NATO armored vehicle prompt radiation nuclear vulnerability. A workshop on MASH 1.0 was hosted by section staff and attended by approximately 30 NATO participants. Also under sponsorship of the

DNA, an investigative study was completed to resolve the outstanding discrepancies which exist in the dosimetry data resulting from the atomic weapon detonation at Hiroshima. Results from our analyses figured prominently in a requested presentation to the National Academy of Sciences.

Finally, an exploratory study of a liquid-metal engine concept resulted in a patent application being filed by MMES. The "double-duct liquid-metal magnetohydrodynamic engine with variable stroke" uses liquid metal as the effective piston mechanism to convert combustion energy to alternating current to operate electrical drive motors. The concept has the potential for producing a very lightweight engine and drive system with excellent performance and fuel efficiency.

THEORETICAL AND NUMERICAL METHODS

4.1

ADJACENT-CELL PRECONDITIONERS FOR SOLVING OPTICALLY THICK NEUTRON TRANSPORT PROBLEMS

Y. Y. Azmy

[Abstract of paper presented at the American Nuclear Society Eighth International Topical Meeting on Radiation Shielding, Arlington, TX, April 24-28, 1994; Proc. Vol. 1, pp. 193-200 (1994)]

We develop, analyze, and test a new acceleration scheme for neutron transport methods, the *Adjacent-cell Preconditioner* (AP) that is particularly suited for solving optically thick problems. Our method goes beyond Diffusion Synthetic Acceleration (DSA) methods in that its spectral radius vanishes with increasing cell thickness. In particular, for the 1D case the AP method converges immediately, i.e. in one iteration, to 10^{-4} pointwise relative criterion in problems with dominant cell size of 10 mfp or thicker. Also the AP has a simple formalism and is *cell-centered* hence, multidimensional and high order extensions are easier to develop, and more efficient to implement.

Research sponsored by U.S. Department of Energy.

4.2

CELL-CENTERED IMPOSED DIFFUSION SYNTHETIC ACCELERATION FOR WEIGHTED DIFFERENCE TRANSPORT METHODS

Y. Y. Azmy

[Abstract of *Nucl. Sci. Eng.* 115, 265 (1993)]

We compute the spectral radius for Reed's cell-centered imposed diffusion synthetic acceleration (IDSA) method applied to a fixed-weights weighted diamond-difference (WDD) scheme. We show that Reed's conclusion that IDSA is conditionally stable is strictly true only for very small magnitude spatial weights. For the zeroth-order nodal integral method, the step method (unit weights), and WDD methods with large enough weights (say larger than 0.5), a simple choice of the diffusion coefficient results in unconditionally

stable, rapidly converging iterations. Moreover, the IDSA's spectral radius vanishes in the limit of infinitely thick computational cells, thereby implying immediate convergence for sufficiently thick problems. We verify all these results via model and nonmodel test problems.

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

4.3

NEUTRON TRANSPORT METHODS ON SCALABLE SHARED MEMORY MULTIPROCESSORS

Y. Y. Azmy

[Abstract of paper presented at the American Nuclear Society Topical Meeting on Advances in Reactor Physics, Knoxville, TN, April 11-15, 1994; Proc. Vol. 1, pp. 396-405 (1994)]

We describe the parallel implementation of the Source Iterations traditionally used in solving the neutron transport equation on the highly-scalable shared memory, two-ringed Kendall Square, KSR1, with 64 cells. The program used in this work is the two-dimensional, Cartesian geometry, Arbitrarily High Order Transport (AHOT) code which has a nodal and a characteristic method option. The parallel algorithm employs an angular domain decomposition in the mesh sweep stage, and a spatial domain decomposition in the convergence test and iterate update stages, resulting in high speedup factors at parallel efficiencies in the 90% range. We construct a preliminary performance model for the parallel algorithm, and validate it against measured execution times.

Research sponsored by U.S. Department of Energy.

4.4

PERFORMANCE MODELING OF PARALLEL ALGORITHMS FOR SOLVING NEUTRON DIFFUSION PROBLEMS

Y. Y. Azmy and B. L. Kirk

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

We develop mathematical performance models for the parallel algorithm used to solve the neutron diffusion equation on message passing, and shared memory multiprocessors, represented in our study by the Intel iPSC/860, and the Sequent Balance 8000, respectively. We validate the performance models through several test problems, and use these models to estimate the performance of each of the two considered architectures in situations typical of practical applications, such as fine meshes and a large number of participating processors. We observe that while message passing computers are capable of producing speedup, the parallel efficiency deteriorates rapidly as the number of processors increases. Furthermore, the speedup fails to improve appreciably for massively parallel computers, so that only small to medium size message passing multiprocessors offer a reasonable platform for this algorithm. In contrast, the performance model for the shared memory architecture predicts very high efficiency over a wide range of number of processors reasonable for this architecture. Furthermore, the model efficiency of the Sequent remains superior to that of the hypercube if we adjust its model parameters to make its processors as fast as those of the iPSC/860. This leads us to conclude that shared memory computers are better suited for our parallel algorithm than message passing computers.

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

4.5

IMPLEMENTATION AND DISPLAY OF COMPUTER AIDED DESIGN (CAD) MODELS IN MONTE CARLO RADIATION TRANSPORT AND SHIELDING APPLICATIONS

T. J. Burns

[Abstract of paper presented at the American Nuclear Society Eighth International Topical Meeting on Radiation Shielding, Arlington, TX, April 24-28, 1994; Proc. Vol. 1, pp. 468-475 (1994)]

An Xwindow application capable of importing geometric information directly from two Computer Aided Design (CAD) based formats for use in radiation transport and shielding analyses is being developed at ORNL. The application permits the user to graphically view the geometric models imported from the two formats for verification and debugging. Previous models, specifically formatted for the radiation transport and shielding codes can also be imported. Required extensions to the existing combinatorial geometry analysis routines are discussed. Examples illustrating the various options and features which will be implemented in the application are presented. The use of the application as a visualization tool for the output of the radiation transport codes is also discussed.

Research sponsored by U.S. DOE Foreign Science Technology Center.

4.6

ORGBUG - A WINDOWS-BASED COMBINATORIAL GEOMETRY DEBUGGER

T. J. Burns

(Abstract of ORNL/TM-12020, June 1993)

ORGBUG is the second half of a two part graphical display and debugging system for combinatorial geometry. The first part of the system consists of a "view" generator, CGVIEW. ORGBUG itself is a Microsoft Windows-based application designed to run on a 386 personal computer and to display the "view" produced by CGVIEW as an aid to debugging. ORGBUG also includes specific tools to facilitate the identification of geometric features which are inconsistent or in error.

Research sponsored by Defense Nuclear Agency and U.S. DOE.

4.7

THEORETICAL BASIS OF THE LINEAR NODAL AND LINEAR CHARACTERISTIC METHODS IN THE TORT COMPUTER CODE

R. L. Childs* W. A. Rhoades

(Abstract of ORNL/TM-12246, January 1993)

Novel numerical procedures for solving the Boltzmann equation have been added to the Three Dimensional Oak Ridge Discrete Ordinates Transport Code (TORT). These procedures produce much more accuracy in the flux solutions for a given mesh size, or allow a smaller mesh to be used in order to reduce costs. The first method is a special adaptation of the linear nodal method proposed by Walters and O'Dell. The basic method has been extensively adapted in order to avoid numerical distortions that may occur in shielding problems. The second method is a characteristic procedure with linear expansion of sources and boundary flows. These methods are in widespread use in the TORT code.

Research sponsored by Defense Nuclear Agency and U.S. DOE.

*Computing Applications Division.

4.8

TIME-DEPENDENT DISCONTINUITY FACTORS FOR TRANSIENT NODAL MODELS

J. C. Gehin A. F. Henry*

[Abstract of paper presented at the Joint International Conference on Mathematical Methods and Supercomputing in Nuclear Applications, Karlsruhe, Germany, April 19-23, 1993; Proc. Vol. 1, p. 496 (1993)]

Discontinuity factors were originally introduced to make corrections for errors made in determining homogenized parameters for nodal calculations. In typical transients these discontinuity factors are assumed to be constant or are tabulated to allow for control rod motions or other material changes. An additional set of discontinuity factors is commonly used in a calculational procedure in which a lower order, but more easily solved, set of equations is forced to match higher order nodal equations. This set of discontinuity factors must

be updated periodically throughout the calculation in order to maintain accuracy of the higher order method. In this paper we investigate the time dependence of this second set of discontinuity factors. First, equations for the discontinuity factors which correct finite-difference and quadratic nodal models are developed. Calculations are then performed for a coolant inlet-temperature transient and a control rod motion transient. These calculations demonstrate that many of the discontinuity factors may be held constant at their initial values, thus avoiding the costly task of updating the discontinuity factors during the transient. In transients involving control rod motions, however, corrections in the assemblies which contain moving control rods must be performed.

Research sponsored by U.S. Department of Energy.

*Massachusetts Institute of Technology, Cambridge, MA.

4.9

CRYPTOSYSTEMS BASED ON CHAOTIC DYNAMICS

**R. A. McNees V. Protopopescu
R. T. Santoro J. S. Tolliver***

(Abstract of ORNL/TM-12440, August 1993)

An encryption scheme based on chaotic dynamics is presented. This scheme makes use of the efficient and reproducible generation of cryptographically secure pseudo random numbers from chaotic maps. The result is a system which encrypts quickly and possesses a large keyspace, even in small precision implementations. This system offers an excellent solution to several problems including the dissemination of key material, over the air rekeying, and other situations requiring the secure management of information.

Research sponsored by U.S. Department of Energy.

*Computing Applications Division.

4.10

A GENERALIZATION OF THE SCATTERING THEORY FOR LINEAR TRANSPORT EQUATIONS

V. Protopopescu

[Abstract of *C.R. Acad. Sci. Paris, Série I* 317, 1191 (1994)]

The scattering theory for transport-like equations is generalized in a framework that allows for including boundary conditions into the formalism. The existence of the wave and scattering operators is directly inferred from the properties of the evolution operators that are determined, in turn, by the physics of collisions within and at the boundaries of the scattering domain.

Research sponsored by U.S. Department of Energy.

4.11

RELATIONSHIP BETWEEN THE ALBEDO AND SCATTERING OPERATORS FOR NON-TRANSPARENT BOUNDARY CONDITIONS

V. Protopopescu

[Abstract of *C.R. Acad. Sci. Paris, Série I* 318, 83 (1994)]

The albedo and scattering operators are central objects in the theory of stationary and time-dependent transport, respectively. Their mutual relationship has recently been established by Emamirad and Arianfar for the case of transparent boundaries. In this Note, we extend the result to general boundary conditions.

Research sponsored by U.S. Department of Energy.

4.12

WAVE OPERATORS AND LOCAL DECAY FOR ABSTRACT TRANSPORT EQUATIONS

V. Protopopescu

[Abstract of *C.R. Acad. Sci. Paris, Série I* 319, 45 (1994)]

We develop an abstract approach to prove the existence of wave operators for locally decaying transport systems.

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

4.13

THE TORSED METHOD FOR CONSTRUCTION OF TORT BOUNDARY SOURCES FROM EXTERNAL DORT FLUX FILES

W. A. Rhoades

(Abstract of ORNL/TM-12359, August 1993)

The TORSED method provides a means of coupling cylindrical two-dimensional DORT fluxes or fluences to a three-dimensional TORT calculation in Cartesian geometry through construction of external boundary sources for TORT. This can be important for several reasons. The two-dimensional environment may be too large for TORT simulation. The two-dimensional environment may be truly cylindrical in nature, and thus, better treated in that geometry. It may be desired to use a single environment calculation to study numerous local perturbations.

In Section I, the TORSED code is described in detail, and the diverse demonstration problems that accompany the code distribution are discussed. In Section II, an updated discussion of the VISA code is given. VISA is required to preprocess the DORT files for use in TORSED. In Section III, the references are listed.

Research sponsored by U.S. Department of Energy.

4.14

THE TORSED AND TORSET CODES FOR COUPLING THREE-DIMENSIONAL TORT CALCULATIONS

W. A. Rhoades

[Abstract of paper presented at the American Nuclear Society Eighth International Topical Meeting on Radiation Shielding, Arlington, TX, April 24-28, 1994; Proc. Vol. 1, pp. 551-557 (1994)]

Two new codes perform "bootstrapping" of either two- or three-dimensional boundary fluxes to a TORT three-dimensional calculation. TORSED couples a DORT RZ calculation to an XYZ TORT. Two methods of directional remapping are available, each less expensive than methods previously available for this work. TORSED is compatible with the discontinuous mesh features of TORT.

The second code, TORSET, couples two XYZ TORT problems. The second problem may lie entirely inside the first, or it may touch over only a portion of its surface. TORSET can obtain most of its input data from the primary TORT problem or from an automatic mesh generator.

Research sponsored by U.S. Department of Energy.

4.15

PARABOLIC SYSTEMS WITH COMPETITIVE INTERACTIONS AND CONTROL ON INITIAL CONDITIONS

A. A. Szpiro* V. Protopopescu

[Abstract of *Applied Mathematics and Computation* 59, 215 (1993)]

We consider a two-dimensional parabolic system with general competitive interactions as a

two-player game with conflicting objectives. The controls are on the initial conditions. We demonstrate the existence of an optimal solution of the game as the saddle point for a suitably defined objective functional. The saddle point is the solution to an optimality system solved by a constructive convergence scheme.

Research sponsored by U.S. Department of Energy.

*University of California, San Diego, CA.

FISSION REACTOR APPLICATIONS

4.16

FUEL DENSITY, URANIUM ENRICHMENT, AND PERFORMANCE STUDIES FOR THE ADVANCED NEUTRON SOURCE REACTOR

E. E. Alson* J. C. Gehin
C. D. West†

(Abstract of ORNL/TM-12775, June 1994)

Using calculations performed for the Advanced Neutron Source (ANS) fuel enrichment study lead by Brookhaven National Laboratory along with additional calculations performed at Oak Ridge National Laboratory, correlations showing the effect of different enrichments and fuel densities on neutronic performance of the ANS were developed. These correlations cover the entire range from low-enriched uranium (LEU) at 20 percent to highly-enriched uranium (HEU) at 93 percent and for any fuel density range from existing technology to very advanced, undeveloped, as-yet-untested fuel. The results show that the baseline two-element core design cannot be adapted to

any practical fuel of greatly reduced enrichment without great performance penalties, but that a modification of the design, in which one additional fuel element is incorporated to provide extra volume for lower enrichment fuels, has the capability of using existing, or more advanced, fuel types to lower the uranium enrichment. The modifications adds only about 15 liters to the core volume and would have no significant impact on construction or operating costs.

Research sponsored by U.S. Department of Energy.

*Engineering Division.

†Central Management Offices.

4.17

OVERVIEW OF SHIELDING ANALYSES FOR THE MHTGR FROM 1986 TO 1991

J. A. Bucholz*

[Abstract of paper presented at the American Nuclear Society Eighth International Topical Meeting on Radiation Shielding, Arlington, TX, April 24-28, 1994; Proc. Vol. 1, pp. 316-323 (1994)]

This paper provides a historical overview of the shielding analyses performed at ORNL for the Modular High Temperature Gas-Cooled Reactor (MHTGR) between late 1985 and early 1992. While the present commercial MHTGR design has evolved considerably and is different in many respects from the 1988/89 reference design discussed in this paper, the analytical techniques used to address several key areas of concern are still in use today. This paper highlights some of those areas of concern and traces the evolution of the analytical techniques used to address them over a 6 or 7 year period.

Research sponsored by U.S. Department of Energy.

*Computing and Applications Division.

4.18

SHIELDING ANALYSIS OF THE LMR IN-VESSEL FUEL STORAGE EXPERIMENTS

J. A. Bucholz*

[Abstract of paper presented at the American Nuclear Society Eighth International Topical Meeting on Radiation Shielding, Arlington, TX, April 24-28, 1994; Proc. Vol. 2, pp. 1309-1316 (1994)]

The In-Vessel Fuel Storage (IVFS) experiments analyzed in this paper were conducted at the Oak Ridge National Laboratory's Tower Shielding Reactor (TSR) as part of the Japanese-American Shielding Program for Experimental Research (JASPER). These IVFS experiments, described in Ref. 1, were designed to study source multiplication and three-dimensional effects related to in-vessel storage of spent fuel elements in liquid metal reactor (LMR) systems. The present paper, based on Ref. 2, describes the 2- and 3-D calculations and results corresponding to a lim-

ited subset of those IVFS experiments in which the U.S. LMR program had a particular interest.

Research sponsored by U.S. Department of Energy.

*Computing and Applications Division.

4.19

APPLICATIONS OF MONTE CARLO METHODS FOR THE ANALYSIS OF MHTGR - CASE OF THE VHTRC BENCHMARK

F. C. Difilippo

(Abstract of ORNL/TM-12698, March 1994)

Monte Carlo methods, as implemented in the MCNP code, have been used to analyze the neutronics characteristics of benchmarks related to Modular High Temperature Gas-Cooled Reactors. The benchmarks are idealized versions of the Japanese (VHTRC) and Swiss (PROTEUS) facilities and an actual configurations of the PROTEUS Configuration I experiment. The purpose of the unit cell benchmarks is to compare multiplication constants, critical bucklings, migration lengths, reaction rates and spectral indices. The purpose of the full reactors benchmarks is to compare multiplication constants, reaction rates, spectral indices, neutron balances, reaction rates profiles, temperature coefficients of reactivity and effective delayed neutron fractions. All of these parameters can be calculated by MCNP, which can provide a very detailed model of the geometry of the configurations, from fuel particles to entire fuel assemblies, using at the same time a continuous energy model. These characteristics make MCNP a very useful tool to analyze these MHTGR benchmarks.

Research sponsored by U.S. DOE Office of Nuclear Energy.

4.20

APPLICATIONS OF MONTE CARLO METHODS FOR THE ANALYSIS OF MHTGR - CASE OF THE PROTEUS BENCHMARK

F. C. Difilippo

(Abstract of ORNL/TM-12711, April 1994)

Monte Carlo methods, as implemented in the MCNP code, have been used to analyze the neutronics characteristics of benchmarks related to Modular High Temperature Gas-Cooled Reactors. The benchmarks are idealized versions of the Japanese (VHTRC) and Swiss (PROTEUS) facilities and an actual configurations of the PROTEUS Configuration I experiment. The purpose of the unit cell benchmarks is to compare multiplication constants, critical bucklings, migration lengths, reaction rates, and spectral indices. The purpose of the full reactors benchmarks is to compare multiplication constants, reaction rates, spectral indices, neutron balances, reaction rates profiles, temperature coefficients of reactivity and effective delayed neutron fractions. All of these parameters can be calculated by MCNP, which can provide a very detailed model of the geometry of the configurations, from fuel particles to entire fuel assemblies, using at the same time a continuous energy model. These characteristics make MCNP a very useful tool to analyze these MHTGR benchmarks.

Research sponsored by U.S. DOE Office of Nuclear Energy.

4.21

PROBABILITY DISTRIBUTIONS FOR FIRST NEIGHBOR DISTANCES BETWEEN RESONANCES THAT BELONG TO TWO DIFFERENT FAMILIES

F. C. Difilippo

[Abstract of *Annals of Nuclear Energy* 21(4), 219 (1994)]

For a mixture of two families of resonances, we found the probability distribution for the distance, as first neighbors, between resonances that belong to different families. Integration of this distribution gives the probability of accidental overlapping of resonances of one isotope by resonance

of the other provided that the resonances of each isotope belong to a single family.

Research sponsored by U.S. Department of Energy.

4.22

SCOPING CALCULATIONS OF POWER SOURCES FOR NUCLEAR ELECTRIC PROPULSION

F. C. Difilippo

(Abstract of ORNL/TM-12703, May 1994)

This technical memorandum describes models and calculational procedures used to fully characterize the nuclear island of power sources for nuclear electric propulsion. Two computer codes were written: one for the gas cooled NERVA derivative reactor and the other for liquid metal cooled fuel pin reactors. These codes are going to be interfaced by NASA with the balance of plant in order to make scoping calculations for mission analysis.

Research sponsored by U.S. DOE and the National Aeronautical Space Administration.

4.23

SIMULATION OF PULSED NEUTRON SOURCE REACTIVITY MEASUREMENTS

**F. C. Difilippo M. Caro*
T. Williams***

(Abstract of paper presented at the Joint International Conference on Mathematical Methods and Supercomputing in Nuclear Applications, Karlsruhe, Germany, April 19-23, 1993)

A model has been developed to simulate pulsed neutron source experiments which combines a Green's function approach with the statistical samplings of the generation of neutrons by the source and the detection of them by the detector. The response pulse, measured by a multi-scaler, is thus simulated allowing confirmation of experimental procedures and analysis of data for measuring the sub criticality of nuclear reactors. The results were applied to the preparation of experiments currently underway at the PROTEUS facility.

Research sponsored by U.S. Department of Energy.

*Paul Scherrer Institute, Villigen, Switzerland.

4.24

TEMPERATURE AND VOID REACTIVITY COEFFICIENT CALCULATIONS FOR THE HIGH FLUX ISOTOPE REACTOR SAFETY ANALYSIS REPORT

W. W. Engle L. R. Williams

(Abstract of ORNL/TM-12386, July 1994)

This report provides documentation of a series of calculations performed in 1991 in order to provide input for the High Flux Isotope Reactor Safety Analysis Report. In particular, temperature and void reactivity coefficients were calculated for beginning-of-life, end-of-life, and xenon equilibrium (29 h) conditions. Much of the data used to prepare the computer models for these calculations was derived from the original HFIR nuclear design study (Ref. 1).

Research sponsored by U.S. Department of Energy.

4.25

THE DOS 1 NEUTRON DOSIMETRY EXPERIMENT AT THE HB-4-A KEY 7 SURVEILLANCE SITE ON THE HFIR PRESSURE VESSEL

K. Farrell*	F. B. Kam [†]
C. A. Baldwin*	J. V. Pace, III
W. R. Corwin*	L. Robinson [‡]
F. F. Dyer [‡]	F. M. Haggag*
F. W. Stallman [§]	B. M. Oliver [#]
L. R. Greenwood**	

(Abstract of ORNL/TM-12511, January 1994)

A comprehensive neutron dosimetry experiment was made at one of the prime surveillance sites at the High Flux Isotope Reactor (HFIR) pressure vessel to aid radiation embrittlement studies of the vessel and to benchmark neutron transport calculations. The thermal neutron flux at the key 7, position 5 site was found, from measurements of radioactivation of four cobalt wires and four silver wires, to be $2.4 \times 10^{12} \text{ n}\cdot\text{m}^{-2}\cdot\text{s}^{-1}$. The thermal flux derived from two helium accumulation monitors was $2.3 \times 10^{12} \text{ n}\cdot\text{m}^{-2}\cdot\text{s}^{-1}$. The thermal flux estimated by neutron transport calculations was $3.7 \times 10^{12} \text{ n}\cdot\text{m}^{-2}\cdot\text{s}^{-1}$. The fast

flux, $>1 \text{ MeV}$, determined from two nickel activation wires, was $1.5 \times 10^{12} \text{ n}\cdot\text{m}^{-2}\cdot\text{s}^{-1}$, in keeping with values obtained earlier from stainless steel surveillance monitors and with a computed value of $1.2 \times 10^{12} \text{ n}\cdot\text{m}^{-2}\cdot\text{s}^{-1}$. The fast fluxes given by two reaction-product-type monitors, neptunium-237 and beryllium, were $2.6 \times 10^{13} \text{ n}\cdot\text{m}^{-2}\cdot\text{s}^{-1}$ and $2.2 \times 10^{13} \text{ n}\cdot\text{m}^{-2}\cdot\text{s}^{-1}$, respectively. Follow-up experiments indicate that these latter high values of fast flux are reproducible but are false; they are due to the creation of greater levels of reaction products by photonuclear events induced by an exceptionally high ratio of gamma flux to fast neutron flux at the vessel.

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

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4.26

KCORR, A NEW MCNP OPTION-USING THE CORRELATED SAMPLING METHOD FOR STUDYING REACTIVITY EFFECTS DUE TO CHANGES OF A REACTOR ARRANGEMENT

F. X. Gallmeier

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

A new option, KCORR, for calculating the eigenvalue, k_{eff} , of fission reactor arrangements has been implemented into the Monte Carlo code MCNP. This option is based on a matrix method and has the additional feature of applying correlated sampling methods for investigating small reactivity effects which are very likely lost in the statistical uncertainties of two independent program runs with the old option KCODE. To verify the new program option, calculations of the reactivity worths of the control rod and safety rod of the FOEHN reactor and the reactivity effects of various components in the reflector pool of the FOEHN reactor were performed both with the old

option KCODE and the new option KCORR and compared against measured data. The efficiency of MCNP in calculating reactivity changes by using the option KCORR is not only improved by means of lower statistical uncertainties, but also by reduction of computing time.

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

4.27

A NEW FUEL LOADING DESIGN FOR THE ADVANCED NEUTRON SOURCE

J. C. Gehin J. P. Renier
B. A. Worley

[Abstract of paper presented at the American Nuclear Society Topical Meeting on Advances in Reactor Physics, Knoxville, TN, April 11-15, 1994; Proc. Vol. III, pp. 273-282 (1994)]

A new fuel loading design has been developed for the Advanced Neutron Source Reactor. In this reactor the combination of a small core volume and high power results in a very high power density. Using a direct optimization procedure the thermal-hydraulic margin for oxide temperature drop, centerline temperature and incipient boiling (and thus critical heat flux) were maximized to increase the limiting thermal power from 298 MW to 346 MW compared to the previous fuel grading, while maintaining the desired peak reflector thermal flux.

Research sponsored by U.S. Department of Energy.

4.28

SINBAD - A SHIELDING INTEGRAL BENCHMARK ARCHIVE AND DATABASE FOR PCs

H. T. Hunter D. T. Ingersoll
R. W. Roussin E. Sartori*
C. O. Slater

[Abstract of paper presented at the American Nuclear Society Eighth International Topical Meeting on Radiation Shielding, Arlington, TX, April 24-28, 1994; Proc. Vol. 2, pp. 795-801 (1994)]

Within the last 30 years, many shielding "benchmark" experiments, involving thermal and fast reactor spectra, as well as fusion reactor sources, have been performed world-wide. The

results provide a means to perform quality assurance and consistency checks on recently developed transport codes and cross-section libraries. An effective means for storing, locating, and retrieving these experimental and calculational benchmark results for nuclear systems is under development. A new electronic data base called SINBAD, has the flexibility and a detailed storage structure capable of handling the many types of data found in benchmarks. These data are related by classifications and subclassifications so they may be quickly and efficiently reassembled at the user's control. Output for data searching may be first pursued at the screen and then printed and/or saved to a computer file for future use in user's calculations. Future graphic display developments will allow a more comprehensive examination of the experimental geometry detail and data comparison.

Research sponsored by U.S. DOE Office of Fusion Energy.

*Nuclear Energy Agency Data Bank, France.

4.29

BUGLE-93 (ENDF/B-VI) CROSS-SECTION LIBRARY DATA TESTING USING SHIELDING BENCHMARKS

H. T. Hunter C. O. Slater
J. E. White

[Abstract of paper presented at the American Nuclear Society Eighth International Topical Meeting on Radiation Shielding, Arlington, TX, April 24-28, 1994; Proc. Vol. 2, pp. 840-847 (1994)]

Several integral shielding benchmarks were selected to perform data testing for new multigroup cross-section libraries compiled from the ENDF/B-VI data for light water reactor (LWR) shielding and dosimetry. The new multigroup libraries, BUGLE-93 and VITAMIN-B6, were studied to establish their reliability and response to the benchmark measurements by use of radiation transport codes, ANISN and DORT. Also, direct comparisons of BUGLE-93 and VITAMIN-B6 to BUGLE-80 (ENDF/B-IV) and VITAMIN-E (ENDF/B-V) were performed. Some benchmarks involved the nuclides used in LWR shielding and dosimetry applications, and some were sensitive to specific nuclear data, i.e. iron due to its dominant use in nuclear reactor systems and complex set

of cross-section resonances. Five shielding benchmarks (four experimental and one calculational) are described and results are presented.

Research sponsored by U.S. Department of Energy.

4.30

**PRODUCTION AND TESTING OF
THE VITAMIN-B6 FINE-GROUP
AND THE BUGLE-93 BROAD-
GROUP NEUTRON/PHOTON
CROSS-SECTION LIBRARIES
DERIVED FROM ENDF/B-VI
NUCLEAR DATA**

D. T. Ingersoll J. E. White
R. Q. Wright* H. T. Hunter
C. O. Slater N. M. Greene*
R. W. Roussin R. E. MacFarlane[†]

(Abstract of ORNL-6795, NUREG/CR-6214, January 1995)

A new multigroup cross section library based on ENDF/B-VI data has been produced and tested for light water reactor shielding and reactor pressure vessel dosimetry applications. The broad-group library, which is designated BUGLE-93, is intended to replace the aging BUGLE-80 and SAILOR libraries. The processing methodology is consistent with ANSI/ANS 6.1.2, since the ENDF data were first processed into a fine-group, pseudo-problem-independent format and then collapsed into the final broad-group format. The fine-group library, which is designated VITAMIN-B6, contains 120 nuclides. The BUGLE-93 47-neutron-group/20-gamma-ray-group library contains the same 120 nuclides processed as infinitely dilute and collapsed using a weighting spectrum typical of a concrete shield. Additionally, BUGLE-93 contains 105 nuclides processed with resonance self-shielding and weighted using spectra specific to BWR and PWR material compositions and reactor models. Several dosimetry response functions and kerma factors for all 120 nuclides are also included with the library. An extensive integral data testing effort was performed to qualify the new library. In general, results using the new data show significant improvements relative to earlier ENDF data.

Research sponsored by the Nuclear Regulatory Commission.

*Computing Applications Division.

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4.31

**PRODUCTION AND TESTING OF
THE VITAMIN B6 FINE-GROUP
AND THE BUGLE-93 BROAD-GROUP
NEUTRON/PHOTON CROSS-SECTION
LIBRARIES DERIVED FROM
ENDF/B-VI NUCLEAR DATA**

D. T. Ingersoll J. E. White
R. Q. Wright* H. T. Hunter
C. O. Slater N. M. Greene*
R. E. MacFarlane[†]

[Abstract of paper presented at the Eighth ASTM-EURATOM Symposium on Reactor Dosimetry, Vail, CO, August 29–September 3, 1993; Proc. pp. 660–669, H. Farrah, IV, E. P. Lippincott, J. G. Williams, and D. W. Vehar, Eds. (1994)]

A new multigroup cross-section library based on ENDF/B-VI data has been produced and tested for light water reactor shielding and reactor pressure vessel dosimetry applications. The broad-group library is designated BUGLE-93. The processing methodology is consistent with ANSI/ANS 6.1.2, since the ENDF data were first processed into a fine-group, "pseudo problem-independent" format and then collapsed into the final broad-group format. The fine-group library is designated VITAMIN-B6. An extensive integral data testing effort was also performed. In general, results using the new data show significant improvements relative to earlier ENDF data.

Research sponsored by U.S. DOE and by the U.S. Nuclear Regulatory Commission.

*Computing Applications Division.

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4.32

**ANS COLD SOURCE
NEUTRONICS ANALYSIS**

R. A. Lillie

[Abstract of paper presented at the American Nuclear Society Topical Meeting on Advances in Reactor Physics, Knoxville, TN, April 11–15, 1994; Proc. Vol. III, p. 355 (1994)]

This paper describes the calculational procedures employed in the ongoing neutronics analysis of the ANS cold source and presents in chronological order some of the more important results from the one- and two-dimensional discrete ordinates calculations performed to date in support of

the ANS cold source design. In particular, cold neutron currents from cryostat shapes which can be adequately modeled with two-dimensional geometries are compared with and without reentrant cavities. Also, results are presented from one-dimensional comparative liquid hydrogen vs liquid deuterium calculations in which the density, placement, and para-ortho mixture of liquid hydrogen is investigated. In addition, the evolution of the ANS conceptual design cold source from an initial short cylindrical cryostat with hemispherical upper and lower heads employing a natural convection liquid deuterium circulation system to the final spherical design employing a pumped system is described. Finally, performance data and heating rates are presented for some possible alternate ANS cryostat and vacuum jacket materials.

Research sponsored by U.S. Department of Energy.

4.33

**THREE-DIMENSIONAL DISCRETE
ORDINATES RADIATION
TRANSPORT CALCULATIONS OF
NEUTRON FLUXES FOR
BEGINNING-OF-CYCLE AT SEVERAL
PRESSURE VESSEL SURVEILLANCE
POSITIONS IN THE HIGH FLUX
ISOTOPE REACTOR**

**J. V. Pace, III C. O. Slater
M. S. Smith**

[Abstract of paper presented at the Eighth ASTM-EURATOM Symposium on Reactor Dosimetry, Vail, CO, August 29-September 3, 1993; Proc. pp. 140-146, H. Farrar, IV, E. P. Lippincott, J. G. Williams, and D. W. Vehar, Eds. (1994)]

The objective of this research was to determine improved thermal, epithermal, and fast fluxes and several responses at mechanical test surveillance location keys 2, 4, 5, and 7 of the pressure vessel of the Oak Ridge National Laboratory High Flux Isotope Reactor (HFIR) for the beginning of the fuel cycle. The purpose of the research was to provide essential flux data support of radiation embrittlement studies of the pressure vessel shell and beam tubes at some of the important locations.

Research sponsored by U.S. Nuclear Regulatory Commission.

4.34

**CRITICALITY SAFETY STUDIES
OF BUILDING 3019 CELL 4
AND IN-LINE STORAGE WELLS**

R. T. Primm, III

(Abstract of ORNL/TM-12374, November 1993)

New fissile material load limits for storage facilities located in Building 3019 are derived in a manner consistent with currently applicable Martin Marietta Energy Systems requirements. The limits for ^{233}U loading are 2.00, 1.80, 1.45, and 0.19 kg/ft for hydrogen-to- ^{233}U atoms ratios of 3, 5, 10, and unrestricted, respectively. Limits were also found for ^{235}U and ^{239}Pu systems. The KENO-Va Monte Carlo program and Hansen-Roach cross sections were used to derive these limits.

Research sponsored by U.S. Department of Energy.

4.35

**FISSILE MATERIAL STORAGE IN
THE OAK RIDGE RADIOCHEMICAL
DEVELOPMENT FACILITY**

R. T. Primm, III

[Abstract of paper presented at the Physics and Methods in Criticality Safety Meeting, Nashville, TN, September 19-23, 1993; Proc. pp. 234-242 (1993)]

As a part of a Department of Energy review of Oak Ridge National Laboratory facilities, nuclear safety documentation for the Radiochemical Development Facility (Building 3019) was found to be inadequate. While calculations existed which established safe limits for the storage of fissile material, these calculations were not performed with verified/validated software nor were the results reported in the manner prescribed by applicable DOE orders and ORNL procedures.

To address this deficiency, the operations conducted in Building 3019 were reviewed and conditions were compared to available critical experiment data. Applicable critical experiments were selected and multiplication factors were calculated. Subcritical limits were derived for each of three fissile materials (U-233, U-235, and Pu-239). One application of these limits was to certify the

safety of a storage array which could contain any or all of the above nuclides at varying degrees of moderation. The studies presented are believed to fulfill most of the applicable regulatory requirements.

Research sponsored by U.S. Department of Energy.

4.36

VALIDATION CALCULATIONS IN SUPPORT OF TRANSPORTATION SAFETY ANALYSES

R. T. Primm, III D. A. Tollefson*

[Abstract of paper presented at the Department of Energy Defense Programs Packaging Workshop, Hyatt Regency, Knoxville, TN, May 16-20, 1994; Proc. Conf-9405109 (1994)]

The Y-12 classified version of KENO-Va and the 27-group cross-section library from ENDF/B-IV have been validated for plutonium systems. Some biases in calculated k-effectives were observed. K-effectives averaged 1.5% high. Sufficient data are presented to derive a subcritical limit for any particular plutonium-bearing system.

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

*Health Safety Environment and Accountability Division.

4.37

ANALYSIS OF THE JASPER AXIAL SHIELD EXPERIMENT

C. O. Slater

[Abstract of paper presented at the American Nuclear Society Eighth International Topical Meeting on Radiation Shielding, Arlington, TX, April 24-28, 1994; Proc. Vol. 2, pp. 1271-1278 (1994)]

A summary of the analysis of the Axial Shield Experiment, one of several in a cooperative program between the United States Department of Energy and Japan's Power Reactor and Nuclear Fuel Development Corporation, is presented. The experimental configurations consisted of a spectrum modifier placed in front of the neutron beam from Oak Ridge National Laboratory's Tower Shielding Reactor and followed by a large concrete block containing an array of seven hexagonal-shaped axial shield assemblies. Eight different

types of axial shield assemblies were used in eleven experimental mockups. The calculated results were generally in good agreement ($\pm 20\%$) with the measured results. However, some calculated results overpredicted the measured results by more than 30%.

Research sponsored by U.S. Department of Energy.

4.38

VALIDATION OF MULTIGROUP CROSS SECTIONS FOR THE ADVANCED NEUTRON SOURCE AGAINST THE FOEHN CRITICAL EXPERIMENTAL MEASUREMENTS

L. A. Smith J. C. Gehin
B. A. Worley J. P. Renier

[Abstract of paper presented at the American Nuclear Society Topical Meeting on Advances in Reactor Physics, Knoxville, TN, April 11-15, 1994; Proc. Vol. III, pp. 444-452 (1994)]

The FOEHN critical experiments were analyzed to validate the use of multigroup cross sections in the design of the Advanced Neutron Source. Eleven critical configurations were evaluated using the KENO, DORT, and VENTURE neutronics codes. Eigenvalue and power density profiles were computed and show very good agreement with measured values.

Research sponsored by U.S. Department of Energy.

4.39

IMPLEMENTATION OF CTRLPOS, A VENTURE MODULE FOR CONTROL ROD POSITION CRITICALITY SEARCHES, CONTROL RODS WORTH CURVE CALCULATIONS, AND GENERAL CRITICALITY SEARCHES

L. A. Smith J.-P. Renier

(Abstract of ORNL/TM-12746, June 1994)

A module in the VENTURE reactor analysis code system, CTRLPOS, is developed to position control rods and perform control rod position criticality searches. The module is variably dimensioned so that calculations can be performed with any number of control rod banks each hav-

ing any number of control rods. CTRLPOS can also calculate control rod worth curves for a single control rod or a bank of control rods. Control rod depletion can be calculated to provide radiation source terms. These radiation source terms can be used to predict radiation doses to personnel and estimate the shielding and long-term storage requirements for spent control rods. All of these operations are completely automated.

The numerous features of the module are discussed in detail. The necessary input data for the CTRLPOS module is explained. Several sample problems are presented to show the flexibility of the module.

The results presented with the sample problems show that the CTRLPOS module is a powerful tool which allows a wide variety of calculations to be easily performed.

Research sponsored by U.S. DOE Applied Health Physics Practicum.

4.40

MODELING AND ANALYSIS OF CORE DEBRIS RECRITICALITY DURING HYPOTHETICAL SEVERE ACCIDENTS IN THE ADVANCED NEUTRON SOURCE REACTOR

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C. O. Slater D. L. Moses*
D. B. Simpson* V. Georgevich*

[Abstract of ORNL/TM-12382, May 1993; also paper presented at the Second ASME-JSME Nuclear Engineering Joint Conference, American Society of Mechanical Engineers, New York, March 21-24, 1993; Proc. pp. 471-479 (1993)]

This paper discusses salient aspects of severe-accident-related recriticality modeling and analysis in the Advanced Neutron Source (ANS) reactor. The development of an analytical capability using the KENO V.A-SCALE system is described including evaluation of suitable nuclear cross-section sets to account for the effects of system geometry, mixture temperature, material dispersion and other thermal-hydraulic condi-

tions. Benchmarking and validation efforts conducted with KENO V.A-SCALE and other neutron codes against critical experiment data are described. Potential deviations and biases resulting from use of the 16-group Hansen-Roach library are shown. A comprehensive test matrix of calculations to evaluate the threat of a recriticality event in the ANS is described. Strong dependencies on geometry, material constituents, and thermal-hydraulic conditions are described. The introduction of designed mitigative features is described.

Research sponsored by U.S. Department of Energy.

*Engineering Technology Division.

4.41

FAST AND THERMAL REACTOR DATA TESTING OF ENDF/B-VI

R. Q. Wright* J. E. White
D. T. Ingersoll

(Abstract of paper presented at the International Conference on Nuclear Data for Science Technology, Gatlinburg, TN, May 9-13, 1994)

The purpose of this paper is to describe the results of ENDF/B-VI data testing at the Oak Ridge National Laboratory (ORNL). Data from the VITAMIN-B6 multigroup cross-section library were used in the ENDF/B-VI benchmark calculations. VITAMIN-B6 is a coupled neutron-gamma library with 199 neutron groups (36 thermal) and 42 gamma-ray groups. The XSDRNPM module of the SCALE system was used to calculate 23 thermal reactor benchmarks and 16 fast reactor benchmarks. Calculated values of k_{eff} using the VITAMIN-B6 library are compared with corresponding results from the SCALE-4 238-group ENDF/B-V library. In addition, the VITAMIN-B6 results are also compared with results from other CSEWG data testers.

Research sponsored by the U.S. Department of Energy and the Nuclear Regulatory Commission.

*Computing Applications Division.

ACCELERATOR AND DETECTOR APPLICATIONS

4.42

RADIATION LEVELS IN THE
SSCL EXPERIMENTAL HALLS

F. S. Alsmiller R. G. Alsmiller
C. Y. Fu T. A. Gabriel
R. A. Lillie

(Abstract of paper presented at the Simulating Accelerator Radiation Environments Workshop, Santa Fe, NM, January 11-15, 1993)

Radiation levels in and around the SSCL experimental halls have been calculated using three-dimensional Monte Carlo and one-dimensional discrete ordinates transport methods. Radiation levels are presented for total beam loss, normal beam loss, and normal detector operation. These results indicate that with total beam loss the dose in the elevator shafts located at the ends of the GEM experimental hall were too high. These shafts were subsequently moved to the sides of the experimental halls. To reduce the dose to acceptable levels at the roof access areas in both the GEM and SDC experimental halls, more than 4.0 m of concrete equivalent material was found to be required. Radiation levels at the top of the GEM experimental hall access shafts and at the top of the SDC experimental hall utility and personnel shafts were calculated to be below acceptable levels. However high radiation levels were calculated at the top of the SDC experimental hall cable shaft. These high levels which were due to the absence of bends in the tunnel leading into this shaft forced a total redesign of this shaft.

Research sponsored by U.S. DOE High Energy Physics.

4.43

RADIATION LEVELS AT THE
SSCL EXPERIMENTAL HALLS
AS OBTAINED USING THE
CALOR89 SYSTEM

F. S. Alsmiller R. G. Alsmiller, Jr.
C. Y. Fu T. A. Gabriel
R. A. Lillie

[Abstract of paper presented at the International Conference on Monte Carlo Simulations in High Energy and Nuclear Physics, Florida State University, Tallahassee, FL, February 22-26, 1993; Proc. p. 180 (1993)]

Because of the increase in beam energy and intensity at the Superconducting Super Collider Laboratory (SSCL) accelerator, the biological shielding necessary for the experimental halls and access tunnels will require a much more critical review than that carried out for previous high energy physics facilities such as Fermi National Accelerator Laboratory (FNAL) or the Stanford Linear Accelerator Center (SLAC). This paper summarizes a study of the neutron and gamma-ray radiation doses that are anticipated in and around the Solenoidal Detector Collaboration (SDC) and the Gamma, Electron, and Muon (GEM) experimental halls as they were configured around March, 1992.

Research sponsored by U.S. DOE High Energy Physics.

4.44

LOW-ENERGY PARTICLE
PRODUCTION AND TRANSPORT
FOR 200 GeV/c HADRONS IN
LEAD AND COMPARISONS WITH
EXPERIMENTAL DATA

R. G. Alsmiller, Jr. F. S. Alsmiller

[Abstract of *Nucl. Instrum. Meth. Phys. Res. A* 336, 132 (1993)]

Calculated results for 200 GeV/c hadrons incident on a large lead target are presented and compared with experimental data. The calculations were carried out using the hadron transport code HETC88. Calculated results carried out with the hadron transport code FLUKA92 by Fasso et al., are also presented for comparison purposes.

The quantities that are compared are the production per unit volume of ^{18}F and ^{24}Na in aluminum, ^{32}P in sulphur, and $^{115\text{m}}\text{In}$ are due primarily to low energy (<20 MeV) neutrons and thus the comparisons here test the capabilities of HETC88 and FLUKA92 for producing and transporting these low energy neutrons. The calculated results from both HETC88 and FLUKA92 are in fair agreement with the experimental data for ^{18}F , ^{24}Na , and ^{32}P , but do not agree well with the experimental data for the production of $^{115\text{m}}\text{In}$. The two sets of calculated results are in good agreement with each other at most depths and radii and exhibit approximately the same overall agreement with the experimental data.

Research sponsored by U.S. DOE Office of High Energy and Nuclear Physics.

4.45

A MONTE CARLO STUDY OF ACCELERATOR HEAD SCATTER

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T. A. Gabriel

[Abstract of *Med. Phys.* 21(9), 1383 (1994)]

The production of off-focus x rays in the head of a 6 MV linac has been investigated using the EGS4 Monte Carlo code. The purpose of the study was to identify the sources of off-focus radiation and the relative contribution for each source. Even though a particular energy and linac were modeled, the broad conclusions are expected to be general since the effects of head scatter are similar for most conventional head designs, regardless of manufacturer energy, and model. The head components that were modeled include the exit window of the accelerating structure, target, beam stopper, flattening filter, monitor chamber, primary and secondary collimators, and air. Monoenergetic 6 MeV electrons were followed through the exit window, target, and beam stopper until all energy was expended. Primary- and higher-order x rays produced throughout the head were followed until they were either absorbed or passed through a plane at the isocenter. Sites of off-focus radiation were found to be diffusely distributed throughout the head, with the most intense sources being the primary collimator, flattening filter, and beam stopper. Data analysis shows that the collimator

effect is determined primarily by the volume of the extended head-scatter source that is exposed to the point of measurement through the collimating system. The results of this study provide a rationale for developing extended source models to calculate the collimator factor for fields defined by arbitrary collimation. An additional advantage is an improvement in the agreement between measured and calculated isodose distributions.

Research sponsored by U.S. Department of Energy.

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4.46

A SUPERCONDUCTING-COIL MULTIPURPOSE MISSION FOR AURORAL, TERRELLA, MAGNETIC PROPULSION AND SHIELDING RESEARCH

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[Abstract of *Journal of the Astronautical Sciences* (in press)]

The launching of a superconducting-coil magnet having a magnetic moment above 280,000 A·turns·m² into low-earth polar orbit would make possible the simultaneous investigation of several innovative experiments by means of a payload massing 140 kg. Launched in persistent current mode, such a coil would quantitatively test the effectiveness of charged particle radiation protection using a magnetic shield in a particle flux that was highly variable. Passage through an active auroral display could produce a number of auroral effects, including the nucleation of Alfvén waves and the creation of a pulsating aurora. Data could also be obtained via electrostatic measurement techniques on the interaction between plasma and a magnetic field moving at hypersonic velocities, and could not be duplicated by any ground-based investigation. The interaction of the payload magnetic field with the magnetic field of the earth would allow evaluation of the use of magnetic fields for not only satellite orientation, but also for orbital control (magnetic propulsion). Magnetic propul-

sion could have very wide ranging applications in satellite design, especially with the Keyhole (KH) series of satellites, whose useful lives are limited in part by the availability of maneuvering fuel.

Research sponsored by U.S. DOE High Energy Physics.

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4.47

THE CALOR93 CODE SYSTEM

T. A. Gabriel

[Abstract of paper presented at the Simulating Accelerator Radiation Environments Workshop, Santa Fe, NM, January 11-15, 1993; Proc. p. 80 (1993)]

A brief history and description of the CALOR93 code system which is used for detector (calorimeter) design and analysis, in particular and radiation transport in general, is presented.

Research sponsored by U.S. DOE High Energy Physics.

4.48

OVERVIEW OF NEW, UPGRADED, OR PROPOSED HIGH ENERGY PHYSICS FACILITIES IN THE UNITED STATES AND CANADA

T. A. Gabriel

(Abstract of paper presented at the Specialists' Meeting on Shielding Aspects of Accelerators, Targets, and Irradiation Facilities, Arlington, TX, April 28-29, 1994)

This article reviews six new, proposed, or upgraded accelerator facilities in the United States and Canada. All of the accelerators that are presented here in one form or fashion challenge the validity of the Standard Model of high energy physics; which "currently explains" all experimentally known phenomena. These facilities include the Continuous Electron Beam Accelerator Fa-

cility (CEBAF) at Newport News, Virginia, the Kaon Factory at TRIUMF in Vancouver, British Columbia, Canada, the Asymmetric B Factory at the Stanford Linear Accelerator Center (SLAC) in Palo Alto, California, the Relativistic Heavy Ion Collider (RHIC) facility at Brookhaven National Laboratory in Upton, New York, the injector upgrade project at the Fermi National Accelerator Laboratory (FNAL) in Batavia, Illinois, and the Superconducting Super Collider Laboratory (SSCL) in Waxahachie, Texas.

Research sponsored by U.S. Department of Energy.

4.49

RESPONSE TO CHARGED PIONS AND MUONS OF A CALORIMETER SIMILAR TO THAT PROPOSED FOR THE BABAR DETECTOR

T. A. Gabriel C. Y. Fu
R. A. Lillie

(Abstract of poster session presented at the CAM '94 Physics Meeting, Cancun, Mexico, September 26-30, 1994)

The BaBar detector is being proposed as the detector for the B factory at SLAC. Initially, no hadronic calorimeter with energy resolution is planned in the BaBar detector because of cost constraints. However, when the detector is upgraded, the hadronic calorimeter part of this detector will be composed of the CsI electromagnetic calorimeter and the instrumented flux return. The detector to be used in the flux return has not been totally defined but will probably be some sort of gas ionization system which can operate in the proportional mode. The analysis of the response of this calorimeter to pions and kaons in the momentum range of 0.25 to 5.0 GeV/c is being carried out using the CALOR93 and GCALOR code systems. Preliminary analysis indicates reasonably good energy resolution, on the order of 30-40% at 5 GeV/c. "Texas tower" events are also quite prevalent in the gas ionization chambers and methods are being explored to reduce their contributions to the signal without biasing the results.

Research sponsored by U.S. DOE High Energy Physics.

4.50

ENERGY DEPENDENCE OF HADRONIC ACTIVITY

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P. K. Job† N. V. Mokhov‡
G. R. Stevenson§

[Abstract of *Nucl. Instrum. Meth. A* 338, 336 (1994)]

Two features of high-energy hadronic cascades have been long known to shielding specialists: (a) in a high-energy hadronic cascade in a given material (incident $E \gtrsim 10$ GeV), the relative abundance and spectrum of each hadronic species responsible for most of the energy deposition is independent of the energy or species of the incident hadron, and (b) because π^0 production bleeds off more and more energy into the electromagnetic sector as the energy of the incident hadron increases, the absolute level of this low-energy hadronic activity ($E \lesssim 1$ GeV) rises less rapidly than the incident energy, and in fact rises very nearly as a power of the incident energy. Both features are of great importance in hadron calorimetry, where it is the "universal spectrum" which makes possible the definition of an intrinsic e/h , and the increasing fraction of the energy going into π^0 's which leads to the energy dependence of e/π . We present evidence for the "universal spectrum," and use an induction argument and simulation results to demonstrate that the low-energy activity scales as E^m , with $0.80 \lesssim m \lesssim 0.85$. The hadronic activity produced by incident pions is 15–20% less than that initiated by protons.

Research sponsored by U.S. DOE Superconducting Super Collider.

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4.51

ANALYSIS OF INTERMEDIATE ENERGY PHOTONUCLEAR REACTIONS

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S. G. Mashnik†

[Abstract of paper presented at the XII International Seminar on High Energy Physics Problems, "Relativistic Nuclear Physics and Quantum Chromodynamics," Dubna, Russia, September 12–17, 1994; Proc. E2-94-424, pp. 1–10 (1994)]

The Cascade-Exciton Model (CEM) of nuclear reactions has been extended to describe photonuclear disintegration at intermediate energies. Using CEM and the ORNL version of the Intranuclear Cascade Model for incident energies higher than the giant dipole resonance (GDR) region, and a group theory formalism based on the Interacting Boson Model in the GDR region, we have analyzed a variety of data for reactions induced by photons with energies up to ~ 1.2 GeV and target-nuclei from ^{12}C to ^{243}Am . The contributions of different photon absorption mechanisms and the relative role of different particle production mechanisms in these reactions are discussed.

Research sponsored by U.S. DOE Office of High Energy Physics.

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†Bogoliubov Laboratory of Theoretical Physics, Dubna, Russia.

4.52

NEUTRAL AND CHARGED PARTICLE BACKGROUNDS IN THE BABAR DETECTOR DUE TO BEAM LOSSES

T. A. Gabriel L. R. Williams

(Abstract of poster session presented at the CAM '94 Physics Meeting, Cancun, Mexico, September 26–30, 1994)

The BaBar detector is being proposed as the detector for the B factory at SLAC. Due to the relatively low e^+e^- collision rate as compared to hadron colliders, beam loss background, which can lead to false triggers, may represent a potential problem. Part of this problem results from the production of neutron and charged hadronic particles generated by lost beam parti-

cles of bremsstrahlung photons produced by e^+ or e^- gas interactions in the beam pipes. To estimate the magnitude of this problem production levels of protons, neutrons, and charged pions by gamma rays in the energy range of 7 MeV to 9 GeV are being calculated using up updated version of the PICA code.

Research sponsored by the U.S. DOE Department of High Energy Physics.

4.53

LASER ELECTRON ACCELERATION IN VACUUM

C. M. Haaland

[Abstract of *Optics Communications* (in press)]

This scheme involves pairs of intersecting linearly-polarized Gaussian-profile laser beams that are focused at crossover in vacuum and phased such that the effects of transverse field components cancel. The E_z components accelerate properly-phased z-axis relativistic electrons throughout a half-wave slip distance centered at crossover. The slip length is approximately 90λ for the case considered. The E_z components vanish rapidly before and after this slip region, thus providing conditions for a special case that is not included in Palmer's general acceleration theorem. Electron energy-gain gradients of several GeV/m appear to be possible.

Research sponsored by U.S. DOE Exploratory Studies Program.

4.54

NEUTRON FLUENCE CALCULATIONS FOR THE SDC DETECTOR AND THE RESULTS OF CODES COMPARISON

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T. A. Gabriel C. O. Slater
L. S. Waters† A. P. T. Palounek†
C. Zeitnitz§

[Abstract of paper presented at the American Nuclear Society Eighth International Topical Meeting on Radiation Shielding, Arlington, TX, April 24-28, 1994; Proc. Vol. 2, pp. 980-984 (1994)]

The high energy and high luminosity of the Superconducting Super Collider (SSC) cause radiation problems for the detectors. Almost all the radiation in the Solenoidal Detector Collaboration (SDC) detector comes from the 20 TeV on 20 TeV pp collisions. The design luminosity corresponds to 10^8 collisions per second. This luminosity is maintained for 10^7 seconds per year. It is important to know the radiation fields experienced by the tracking volume, calorimeter, electronics and the phototubes. For example the loss of light due to the radiation damage to the scintillators can adversely affect the physics performance of the calorimeter. In this study we use ISAJET, an event generator code, in combination with CALOR89, a particle transport code, to make an accurate prediction of neutron fluences at the various locations of the SDC detector. The low energy neutrons are important because they can produce radioactive nuclides in large quantities and substantially contribute to the radiation damage of the detector. In CALOR89 the low energy neutron fluence is accurately estimated by the MORSE code.

Research sponsored by U.S. DOE Superconducting Super Collider.

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§ University of Arizona, Tucson, AZ.

4.55

CALOR89 PREDICTIONS FOR THE HANGING FILE TEST CONFIGURATIONS

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J. Proudfoot* T. Handler†
T. A. Gabriel

[Abstract of paper presented at the International Conference on Monte Carlo Simulations in High Energy and Nuclear Physics, Florida State University, Tallahassee, FL, February 22-26, 1993; Proc. p. 180 (1993)]

We present the comparison of CALOR89 simulation with the reconfigurable stack calorimeter (Hanging Files) test beam measurements conducted at Fermilab during the period of September 1991 to January 1992. The purpose of this study is to benchmark CALOR89 code against the experimental data to enhance its reliability and predictive power. The measured e/π ratio, the electromagnetic and hadronic resolutions and the longitudinal shower profiles are compared. The results show that the CALOR89 can predict reasonably well the parameters for the scintillating plate calorimeters. We have also identified certain systematic effects in modeling the experimental configurations with CALOR89 and quantified them.

Research sponsored by U.S. DOE High Energy Physics.

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4.56

SIMULATION OF THE RECONFIGURABLE-STACK TEST CALORIMETER EXPERIMENTS WITH CALOR89

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J. Proudfoot* T. Handler†
T. A. Gabriel

[Abstract of *Nucl. Instrum. Meth. Phys. Res. A* 340, 283 (1994)]

This paper presents the simulation studies with CALOR89 for the Reconfigurable-Stack calorimeter (Hanging Files) test beam measurements conducted at Fermilab during the period of September 91 to January 92. The purpose of this study is to validate the CALOR89 code

against the experimental data and to enhance its reliability and predictive power, especially for the multi-segmented SDC calorimeters. The results of the simulation are compared with the measured e/π ratio, the electromagnetic and hadronic energy resolutions and the longitudinal shower profiles. These comparisons show that the CALOR89 can predict reasonably well the parameters for the scintillating plate calorimeters. We have also identified certain systematic effects in modeling the experimental configurations with CALOR89.

Research sponsored by the U.S. DOE Superconducting Super Collider.

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4.57

USING NEURAL NETWORKS AS AN EVENT TRIGGER IN ELEMENTARY PARTICLE PHYSICS EXPERIMENTS

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T. Handler* T. A. Gabriel
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[Abstract of paper presented at the IEEE International Conference on Neural Networks, Orlando, FL, June 28-July 2, 1994; Proc. Vol. V, pp. 3056-3060 (1994)]

Elementary particle physics experiments often have to deal with high data rates. In order to avoid having to write out all data that is occurring online processors, triggers, are used to cull out the uninteresting data. The triggers are based on some particular aspect of the physics being examined. At times these aspects are often equivalent to simple pattern recognition problems. The reliability of artificial neural networks (ANNs) in pattern recognition problems in many fields has been well demonstrated. We present here the results of a study on the feasibility of using ANNs as an online trigger for high energy physics experiments.

Research sponsored by U.S. DOE Superconducting Super Collider Lab.

* University of Tennessee, Knoxville, TN.

† Physics Division.

4.58

SHIELDING OPTIMIZATION STUDIES FOR THE DETECTOR SYSTEMS OF THE SUPERCONDUCTING SUPER COLLIDER

C. O. Slater R. A. Lillie
T. A. Gabriel

[Abstract of paper presented at the American Nuclear Society Eighth International Topical Meeting on Radiation Shielding, Arlington, TX, April 24-28, 1994; Proc. Vol. 2, pp. 972-979 (1994)]

Preliminary shielding optimization studies for the Superconducting Super Collider's Solenoidal Detector Collaboration detector system were performed at the Oak Ridge National Laboratory in 1993. The objective of the study was to reduce the neutron and gamma-ray fluxes leaving the shield to a level that resulted in insignificant effects on the functionality of the detector system. Steel and two types of concrete were considered as components of the shield, and the shield was optimized according to thickness, weight, and cost. Significant differences in the thicknesses, weights, and costs were noted for the three optimization parameters. Results from the study are presented.

Research sponsored by U.S. DOE Superconducting Super Collider Laboratory.

4.59

EXPERIMENTAL AND CALCULATED RADIONUCLIDE PRODUCTION BY PHOTONUCLEAR REACTIONS USING BREMSSTRAHLUNG PHOTONS PRODUCED BY 150 MeV ELECTRONS

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C. C. Park† T. A. Gabriel
T. A. Lewis‡ J. K. Dickens

(Abstract of paper presented at the International Conference on Nuclear Data for Science and Technology, Gatlinburg, TN, May 9-13, 1994)

We have developed an experimental apparatus to study radionuclide production by photonuclear reactions. A nearly neutron-free bremsstrahlung beam was created by incident elec-

tron interactions with a tantalum radiator. We studied photonuclear reactions in different samples, including the elements Be, Na, Si, Cl, and Ge. Decay gamma rays from radionuclides having half lives >2 min were analyzed. Using the PICA code, we calculated the yield of radionuclides for silicon. We have observed and assigned a new gamma ray transition, of $E(\gamma)=1153$ keV, to the decay of 6.6 min 29-Al.

Research sponsored by U.S. DOE Office of High Energy Physics.

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‡Instrumentation and Controls Division.

4.60

THE GEANT-CALOR INTERFACE AND BENCHMARK CALCULATIONS OF ZEUS TEST CALORIMETERS

C. Zeitnitz* T. A. Gabriel

[Abstract of Nucl. Instrum. Methods Phys. Res. A 349, 106 (1994)]

The simulation of large scale high energy physics experiments is based mainly on the GEANT package. In the current version 3.15 the simulation of hadronic interacting particles is based on GHEISHA or FLUKA. Both programs miss an accurate simulation of the interaction of low energetic neutrons ($E_{kin} < 20$ MeV) with the materials of the detector. The CALOR89 program package contains a low energetic neutron code. An interface between the CALOR program parts and the GEANT package has been developed. A comparison of simulations with ZEUS test beam measurements shows a good agreement of the energy resolution and the e/h-ratio.

Research sponsored by U.S. DOE High Energy Physics.

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DEFENSE APPLICATIONS

4.61

**MASH V1.0 ANALYSIS OF A
SIMPLIFIED BOX VEHICLE
MODEL CONTAINING OPENINGS
REPRESENTATIVE OF ARMORED
VEHICLE MODELS**

**J. D. Drischler J. O. Johnson
K. G. Kerris***

(Abstract of ORNL/TM-12755, August 1994)

Future armored vehicles and other tactical vehicles are being designed for use by the U.S. Army in both conventional and nuclear battle-field environments. Consequently, the materials to be utilized in the construction of these vehicles must provide the crew and sensitive electronic equipment protection from spall fragments from ballistic threats, and radiation from tactical nuclear weapons and dispersed radiological warfare sources. In support of this effort, the Program Executive Officer-Armored Systems Modernization (PEO-ASM) initiated the Interior Shielding Technology Development Program. The principal objective of this program is to define the spall suppression and nuclear weapon radiation shielding capabilities of selected candidate armor - radiation/spall suppression material configurations for future tactical armored vehicles.

This report summarizes the results of the Oak Ridge National Laboratory (ORNL) Monte Carlo Adjoint Shielding (MASH v1.0) code system calculations designed to investigate the effects of possible discontinuities or voids in the armor and liner of a combat vehicle. A simplified box vehicle model of approximately representative vehicle dimensions and with three different types of openings was analyzed to address the effects of armor/liner discontinuities for nine different armor/liner material configurations.

The results of this study indicate that small inconsistencies and errors in the armored vehicle geometry model will not cause a significant perturbation in the protection factor and reduction factor results if the inconsistency or error is not in a direct line of sight between the radiation source and the detector location or if it is not in an area of the armor/liner which contributes a sig-

nificant fraction of the dose to the detector location. Ill-fitting hatches or armor/liner components and missing equipment leaving "holes" in the armor/liner yield insignificant perturbations to the protection and reduction factors if the major contribution to the detector response is from scattered radiation.

Research sponsored by the U.S. Department of Energy and the Army Research Laboratory.

* Army Research Laboratory, Adelphi, MD.

4.62

**MASH V1.0 ANALYSIS OF THE ARMY
RESEARCH LABORATORY (ARL)
BOX/LINER TEST BED EXPERIMENTS
PERFORMED OCTOBER 4-8, 1993
AT THE ARMY PULSE RADIATION
FACILITY (APRF)**

**J. D. Drischler J. O. Johnson
R. T. Santoro K. G. Kerris***

(Abstract of ORNL/TM-12685, May 1994)

Future armored vehicles and other tactical vehicles are being designed for use by the U. S. Army in both conventional and nuclear battle-field environments. Consequently, the materials to be utilized in the construction of these vehicles must provide the crew and sensitive electronic equipment protection from spall fragments from ballistic threats, and radiation from tactical nuclear weapons and dispersed radiological warfare sources. In support of this effort, Tank Automotive Command (TACOM) Project Manager (PM) Survivability Systems initiated the Interior Shielding Technology Development Program. The principal objective of this program has been to define the spall suppression and nuclear weapon radiation shielding capabilities of selected candidate armor - radiation/spall suppression material configurations for future tactical armored vehicles.

This report summarizes the results of the Oak Ridge National Laboratory (ORNL) Monte Carlo Adjoint Shielding (MASH v1.0) code system calculations designed to model the series of nuclear radiation shielding experiments conducted

by Army Research Laboratory (ARL) from October 4, 1993 to October 8, 1993 at the Army Pulse Radiation Facility (APRF) in Aberdeen Proving Grounds, Maryland. In particular, the free-field environments at 400 meters were to be calculated along with measurements made using a cubical box consisting of different candidate armor/liner material configurations at the "NATO standard reference point" at 400 meters. The objective of the experimental series was to establish benchmark data for determining the validity of the computational technique using the MASH v1.0 code system. The MASH results are compared with experimental results obtained using the latest state-of-the-art integral and spectral detector systems. Results of the comparisons are to be used to validate MASH v1.0 for use in the nuclear protection analyses of other armor/liner material combinations of interest to TACOM PM Survivability Systems.

Overall, the MASH calculational results were in excellent agreement (typically within 10% with the measured reduction factor and protection factor data supplied by the APRF and ARL experimental team. Results of the comparisons validate MASH v1.0 for use in the nuclear protection analyses of other candidate armor/liner material combinations and configurations of interest to TACOM PM Survivability Systems. The analytical methodology of employing quick and inexpensive one-dimensional (ANISN) radiation transport analysis for preliminary screening of candidate armor/liner configurations, followed by three-dimensional (MASH v1.0) radiation transport analysis for detailed studies, has proven successful and is recommended for future tactical vehicle armor/liner designs. The Interior Shielding Technology Development Program has been successful in laying the foundation for the design of coupled nuclear/ballistic armor/liner configurations. From this effort, with communication between the ballistic analysts, nuclear analysts, and PM Survivability Systems, coupled nuclear/ballistic armor/liner configurations are feasible.

Research sponsored by U.S. DOE and Army Research Laboratory.

* Army Research Lab, Adelphi, MD.

4.63

NUCLEAR PERFORMANCE OF RADIATION/ARMOR SPALL LINER MATERIALS FOR ARMORED/TACTICAL VEHICLE APPLICATIONS

J. D. Drischler J. O. Johnson
R. T. Santoro K. G. Kerris*

(Abstract of ORNL/TM-12504, May 1994)

One-dimensional radiation transport calculations have been carried out to assess the neutron and gamma-ray protection characteristics of rolled homogeneous armor, aluminum, and titanium in combination with different spall liner materials and other possible radiation protecting materials that are being considered for use in advanced U.S. Army tactical vehicles. The calculations were performed using the neutron and gamma-ray spectra corresponding to the "NATO standard reference point" at 400 m from the Army Pulsed Radiation Facility. A comprehensive study was made to assess a wide range of material combinations to identify the best performance in terms of neutron protection versus total armor weight. These results suggest that armor/spall liner configurations containing aluminum achieve the best neutron protection for the lowest weight shield assemblies.

Research sponsored by U.S. DOE and Army Research Laboratory.

* Army Research Lab, Adelphi, MD.

4.64

THE MASH CODE SYSTEM, VERSION 1.0

J. O. Johnson T. J. Burns
R. T. Santoro

[Abstract of *Human Survivability* 1(2), 5 (1993)]

An armored vehicle can provide important protection against the effects of a nuclear weapon. In the case of tactical weapons, prompt radiation may be the dominant effect over a considerable area surrounding the detonation. To facilitate the calculation of radiation protection factors for armored vehicles, MASH 1.0 - the Monte Carlo Adjoint Shielding Code System, Version 1.0 was developed by the Oak Ridge National Laboratory

(ORNL) and Science Applications International Corporation (SAIC). The code system has been "benchmarked" against a series of experiments performed at the Army Pulse Radiation Facility (APRF) at Aberdeen Proving Ground, Maryland to determine its capability for reproducing measured neutron and gamma-ray integral and spectral data. As a result of these analyses and additional studies involving armored vehicles, MASH 1.0 was recommended to the U.S. Army Nuclear and Chemical Agency (USANCA) to be the reference code for future U.S. armored vehicle nuclear vulnerability calculations and is the code of choice specified in the recent update to the U.S. Army's Qualitative Research Requirements (QRR). Furthermore, the results of these analyses were used in recommendations to the NATO Panel VII Ad Hoc Group of Shielding Experts to utilize MASH 1.0 for all future armored vehicle nuclear vulnerability calculations.

Research sponsored by the U.S. DOE and Defense Nuclear Agency.

4.65

THE MASH 1.0 CODE SYSTEM: UTILIZATION OF MORSE IN THE ADJOINT MODE

J. O. Johnson R. T. Santoro

(Abstract of paper presented at the Organization for Economic Cooperation and Development, Nuclear Energy Agency, Advanced Monte Carlo Computer Programs for Radiation Transport, Centre d'Etudes, Saclay, France, April 27-29, 1993)

The Monte Carlo Adjoint Shielding Code System - MASH 1.0, principally developed at Oak Ridge National Laboratory (ORNL), represents an advanced method of calculating neutron and gamma-ray environments and radiation protection factors for complex shielding configurations by coupling a forward discrete ordinates radiation environment (i.e. air-over-ground) transport calculation with an adjoint Monte Carlo treatment of the shielding geometry. The primary application to date has been to determine the radiation shielding characteristics of armored vehicles exposed to prompt radiation from a nuclear weapon detonation. Other potential applications include analyses of the mission equipment associated with space exploration, the civilian airline industry, and other

problems associated with an external neutron and gamma-ray radiation environment. This paper will provide an overview of the MASH 1.0 code system, including the verification, validation, and application to "benchmark" experimental data. Attention will be given to the adjoint Monte Carlo calculation, the use of "in-group" biasing to control the weights of the adjoint particles, and the coupling of a new graphics package for the diagnosis of combinatorial geometry descriptions and visualization of radiation transport results.

Research sponsored by U.S. DOE and Defense Nuclear Agency.

4.66

APPLICATION OF THE MASH 1.0 CODE SYSTEM TO RADIOLOGICAL WARFARE RADIATION THREATS

J. O. Johnson R. T. Santoro
M. S. Smith

[Abstract of paper presented at the American Nuclear Society Eighth International Topical Meeting on Radiation Shielding, Arlington, TX, April 24-28, 1994; Proc. Vol. 1, pp. 531-538 (1994); also ORNL/TM-12328, October 1993]

Nuclear hardening capabilities of U.S. and foreign ground force system is a primary concern of the Department of Defense (DoD) and U.S. Army. The Monte Carlo Adjoint Shielding Code System - MASH v1.0 was developed at Oak Ridge National Laboratory (ORNL) to analyze these capabilities, i.e. the shielding effectiveness, for prompt radiation from a nuclear weapon detonation. Rapidly changing world events and the proliferation of nuclear weapons related technology have increased the kinds of nuclear threats to include intentionally dispersed radiation sources and fallout from tactical nuclear weapons used in the modern Air-Land battlefield scenario. Consequently, a DoD area of increasing interest focuses on determining the shielding effectiveness of foreign and U.S. Armored vehicles to radiological warfare and fallout radiation threats.

Research sponsored by U.S. DOE Foreign Science Technology Center.

4.67

OVERVIEW OF THE NUCLEAR DATA RELATED TO THE HIROSHIMA DOSIMETRY DISCREPANCY

J. V. Pace, III

(Abstract of paper presented at the International Conference on Nuclear Data for Science Technology, Gatlinburg, TN, May 9-13, 1994)

Nearly half a century ago the first atomic bomb was dropped on Hiroshima; several days later, a second atomic bomb was dropped on Nagasaki. Japan immediately initiated a study of all aspects of the effects of the bombings. Thus the initial effort was begun to estimate the overall risks of radiation effects in man due to nuclear detonations. By the 1950s, Japan and the United States had produced several studies that reported on the elevated risk of cancer. In 1957 the first dose estimates for survivors were designated as Tentative 1957 Doses or T57D. In 1965 a revised dosimetry system was adopted to replace T57D, and the dose estimates were designated as Tentative 1965 Doses or T65D.

The current evaluation, known as Dosimetry System 1986 or DS86, was the result of a presentation by H. H. Rossi in 1976 to the U.S. National Council on Radiation Protection and Measurements (NCRP). In the presentation, Rossi recommended that the NCRP reduce its permissible neutron dose limits by an order of magnitude. A direct result of this drastic proposal was a new dosimetry reevaluation effort. After the calculations were made and compared to the measurements, it was found that the thermal data at both cities was in disagreement.

The state-of-the-art radiation transport calculational codes require evaluated neutron and gamma-ray reaction cross-section data (which themselves were determined empirically or theoretically) to complete the cycle and calculate the measured data. This paper will review some of the more important *in situ* measured data taken over the last forty-five years, the measurement and reevaluation of some of the major cross sections required for the calculations, and the effort to agreement through calculations with some of the *in situ* measurements.

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

4.68

VULNERABILITY ASSESSMENT OF A SPACE BASED WEAPON PLATFORM ELECTRONIC SYSTEM EXPOSED TO A THERMONUCLEAR WEAPON DETONATION

C. L. Perez* J. O. Johnson

[Abstract of paper presented at the American Nuclear Society Eighth International Topical Meeting on Radiation Shielding, Arlington, TX, April 24-28, 1994; Proc. Vol. 1, pp. 611-618 (1994); also ORNL/TM-12487, May 1994]

Rapidly changing world events, the increased number of nations with inter-continental ballistic missile capability, and the proliferation of nuclear weapon technology will increase the number of nuclear threats facing the world today. Monitoring these nation's activities and providing an early warning and/or intercept system via reconnaissance and surveillance satellites and space based weapon platforms is a viable deterrent against a surprise nuclear attack. However, the deployment of satellite and weapon platform assets in space will subject the sensitive electronic equipment to a variety of natural and man-made radiation environments. These include Van Allen Belt protons and electrons; galactic and solar flare protons; and neutrons, gamma rays, and X-rays from intentionally detonated fission and fusion weapons. In this paper, the MASH v1.0 code system is used to estimate the dose to the critical electronics components of an idealized space based weapon platform from neutron and gamma-ray radiation emitted from a thermonuclear weapon detonation in space. Fluence and dose assessments were performed for the platform fully loaded, and in several stages representing limited engagement scenarios. The results indicate vulnerabilities to the Command, Control, and Communication (C³) bay instruments from radiation damage for a nuclear weapon detonation for certain source/platform orientations. The distance at which damage occurs will depend on the weapon yield (n, γ /kiloton) and size (kilotons).

Research sponsored by U.S. DOE Foreign Science Technology Center.

*University of North Carolina, Chapel Hill, NC.

4.69

AN EXPLANATION OF THE HIROSHIMA ACTIVATION DILEMMA

W. A. Rhoades J. M. Barnes*
R. T. Santoro

[Abstract of paper presented at the American Nuclear Society Eighth International Topical Meeting on Radiation Shielding, Arlington, TX, April 24-28, 1994; Proc. Vol. 1, pp. 238-244 (1994)]

A 1987 study of the radiation from the World War II nuclear weapons applied state-of-the-art data and computer techniques, providing an important advance in reliability of the results. Still, a disturbing disagreement remained between slow-neutron activation measurements and calculations for the Hiroshima event.

Newer data have confirmed the validity of the discrepancy. This work examines various potential explanations. Of those examined, only an enhancement to the weapon neutron leakage spectrum in the vicinity of the 2.3 MeV oxygen cross-section window can fit the data accurately.

Research sponsored by U.S. Department of Energy.

* Computing and Applications Division.

4.70

DNA RADIATION ENVIRONMENTS PROGRAM SPRING 1991 2-METER BOX EXPERIMENTS AND ANALYSIS

R. T. Santoro S. Y. Whitaker*

(Abstract of ORNL/TM-12161, March 1993)

This report summarizes the Spring 1991 2-m Box experiments that were performed at the Army Pulse Radiation Facility (APRF) at Aberdeen Proving Ground. These studies were sponsored by the Defense Nuclear Agency (DNA) under the Radiation Environments Program to obtain measured data for benchmarking the Adjoint Monte Carlo Code System, MASH v1.0. The

MASH code system was developed for the Department of Defense and NATO for calculating neutron and gamma-ray radiation fields and shielding protection factors for armored vehicles and military structures against nuclear weapon radiation. In the 2-m Box experiments, neutron and gamma-ray dose rates and reduction factors were measured in the free-field and as a function of position on an anthropomorphic phantom that was placed outside and inside a borated polyethylene lined steel-walled box. The data were acquired at a distance of 400-m from the APRF reactor. The measurements were performed by APRF, Armed Forces Radiobiology Research Institute (AFRRI), Etablissement Technique Central de l'Armement (ETCA), and Harry Diamond Laboratory (HDL). Calculations were carried out by the Oak Ridge National Laboratory (ORNL) and Science Applications International Corporation (SAIC).

The calculated and measured neutron and gamma-ray dose rates and reduction factors agreed on the average within the 20% demonstrate the capability of the MASH code system in reproducing measured data in nominally shielded assemblies. The agreement between the calculated and measured neutron dose rates varied with box-phantom geometry but were within the 20% calculated reduction factors ranged from good to poor depending on the box-phantom geometry with the largest disparity consistently arising for the cases when the phantom was inside the box. These disparities arise mainly from differences between the measured and calculated free-field dose rates rather than dissimilarities with the in-phantom dose rate values. The agreement among the measured gamma-ray data was, in general, within the acceptable range mandated by DNA. Large (20%) some cases when the data were compared on a team-by-team basis. The calculated gamma-ray dose rates and reduction factors were in good agreement with the data acquired by all of the experimental teams.

Research sponsored by Defense Nuclear Agency and U.S. DOE.

* Clark Atlanta University, Atlanta, GA.

THEORETICAL ENGINEERING

4.71

FOUR-PISTON DOUBLE-DUCT LIQUID METAL MHD ENGINE AND AC GENERATOR

C. M. Haaland

[Abstract of paper presented at the Annual Meeting of the Mechanical Working Group of the Interagency Advanced Power Group (IAPG), Arlington, VA, May 10-11, 1994]

Operating principles and features of the Liquid Metal (LM) engine will be presented. The advantages for automotive propulsion will be described in comparisons with current internal combustion engines, AC generators, linear alternators, Stirling engines, hybrid vehicles, and transmission systems. An R&D program will be outlined for bringing the concept of the LM engine to commercial application.

Research sponsored by U.S. Department of Energy.

Section 5

**ENGINEERING PHYSICS AND MATHEMATICS
INFORMATION CENTERS**

5.0. INTRODUCTION

R. W. Roussin

Under the management umbrella of Engineering Physics Information Centers (EPIC), we operated three activities during the reporting period, January 1, 1993 through December 31, 1994. The Radiation Shielding Information Center (RSIC), founded in FY 1963, serves the international scientific community as a technical institute and technology resource for radiation transport and safety. The second, Applied Nuclear Data Development, focuses on providing processed data, usually multigroup cross sections, for use in radiation transport computer codes. The third activity 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 had two retirements and added three new staff members. In addition, the staff was supplied with personal computers linked by a local area network. Workstations based on RISC technology were acquired and enhanced and are used not only for testing software packages but also for independent calculations. These upgrades were essential because the RSIC user community has rapidly moved to PC and workstation environments and we were able to accommodate their changing demands.

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 solving 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, transport, and safety; radiation detectors and measurements; reactor physics and criticality safety; atmospheric dispersion, environmental exposure, and waste management; 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.

RSIC has continued to participate in the work of the Cross Section Evaluation Working Group (CSEWG) to produce the U.S. Evaluated Nuclear Data File (ENDF). Both CSEWG and the Methods and Formats Subcommittee was chaired

by the RSIC director during the reporting period. Other staff members are actively involved in CSEWG and also in the American Nuclear Society (ANS) in developing radiation protection and shielding standards and standards for scientific computer programming and its documentation.

In the area of the transfer of computing technology, RSIC now makes available over 960 computer code packages and 180 data packages. RSIC entered into an agreement with the U.S. Department of Energy's Energy Science and Technology Software Center (ESTSC) to be the sole dissemination source for DOE software developed in the technical area of radiation transport and safety.

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. In addition, RSIC and the Nuclear Energy Agency Data Bank in Paris, France, exchanged staff members for two months to improve interaction between the centers.

RSIC interacts daily with, and continues to have the support of its user community, which is quite diverse and serves a broad range of government and privately sponsored programs. Because of the value of RSIC services, several new sponsored programs have been provided funding on behalf of particular segments of this user community.

Applied Nuclear Data Development (ANDD)

During this reporting period work has continued in the development of fine- and broad-group cross-section data libraries. ENDF/B-VI was released in 1990 and ANDD has processed a selected set of materials into the VITAMIN-J 175n, 42g group structure in support of Defense Nuclear Agency work on Hiroshima/Nagasaki and other studies. Data for iron isotopes was also processed for LWR pressure vessel dosimetry studies and cited by the U.S. Nuclear Regulatory Commission for its improved performance over that previously available.

Based on this early experience, the production of a major processed cross-section library for Light Water Reactor (LWR) shielding was completed. Processing of the ENDF/B-VI reference data into a 199n, 42g data set was done using the NJOY system developed at Los Alamos National Laboratory (LANL). This fine-group data has been translated into AMPX format, used in a data testing program, and was the source of a successor to the BUGLE broad group cross-section library, based on ENDF/B-IV, which has served as the standard for LWR shielding since 1980.

In order to foster the use of newly evaluated data, ANDD coordinates an international multigroup intercomparison activity which was initiated as Subgroup 7 of the Nuclear Energy Agency Nuclear Science Committee Working Party on International Evaluation Cooperation. Processed data libraries based on the VITAMIN-J group structure are being generated from evaluated data libraries from the United States, Europe, and Japan. To facilitate intercomparisons, the ANDD has sponsored and utilized a code that translates the multigroup data into the AMPX format that is commonly used at ORNL and other sites around world.

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 (SARP) 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 Martin Marietta Energy Systems, Inc. (MMES) group, (2) an Albuquerque-based group reporting to DOE Albuquerque Operations, and (3) a group from Lawrence Livermore National Laboratory (LLNL) reporting to Headquarters. Upon approval of the SARP from all committees, a transportation certificate for the package is issued by DOE.

EPIC staff members also provide supporting analysis for various Y-12 and other MMES organizations in the preparation of Transportation systems Risk Analysis (TSRA). EPIC staff members provided calculational support for predicted dose rates to Project Sapphire team members.

RADIATION TRANSPORT DEVELOPMENTS

5.1

RECENT DEVELOPMENTS AND APPLICATIONS OF THE MORSE CODE

S. N. Cramer

(Abstract of paper presented at the Seminar on Advanced Monte Carlo Computer Programs for Radiation Transport, Paris, France, April 27-29, 1993)

Several recent analyses using the multigroup MORSE Monte Carlo code are presented. In the calculation of a highly directional-dependent neutron streaming experiment it is shown that P₇ cross section representation produces results virtually identical with those from an analog code. Use has been made here of a recently released ENDF/B-VI data set. In the analysis of neutron distributions inside the water-cooled ORELA accelerator target and positron source, an analytic hydrogen scattering model is incorporated into the otherwise multigroup treatment. The radiation from a nuclear weapon is analyzed in a large concrete building in Nagasaki by coupling MORSE and the DOT discrete ordinates code. The spatial variation of the DOT-generated free-field radiation is utilized, and the building is modeled with the array feature of the MORSE geometry package. An analytic directional biasing, applicable to the discrete scattering angle procedure in MORSE, is combined with the exponential trans-

form. As in more general studies, it is shown that the combined biasing is more efficient than either biasing used separately. Other tracking improvements are included in a difficult streaming and penetration radiation analysis through a concrete structure. Proposals are given for the code generation of the required biasing parameters.

Research sponsored by U.S. DOE Office of Nuclear Energy.

5.2

A NEW COMMUNICATION SCHEME FOR THE NEUTRON DIFFUSION NODAL METHOD IN A DISTRIBUTED COMPUTING ENVIRONMENT

B. L. Kirk Y. Y. Azmy

[Abstract of paper presented at the American Nuclear Society Topical Meeting on Reactor Physics, Knoxville, TN, April 11-15, 1994; Proc. Vol. I, pp. 298-306 (1994)]

A modified scheme is developed for solving the two-dimensional nodal diffusion equations on distributed memory computers. The scheme is aimed at minimizing the volume of communication among processors while maximizing the tasks in parallel. Results show a significant improvement in parallel efficiency on the Intel iPSC/860 hypercube compared to previous algorithms.

Research sponsored by U.S. DOE Office of Science and Technology.

APPLIED NUCLEAR DATA DEVELOPMENTS

5.3

BUGLE-93 (ENDF/B-VI) CROSS-SECTION LIBRARY DATA TESTING USING SHIELDING BENCHMARKS

H. T. Hunter

(Abstract of paper presented at the Cross Section Evaluation Working Group, Oak Ridge, TN, October 25-27, 1994)

Several integral shielding benchmarks were selected to perform data testing for new multigroup cross-section libraries compiled from the ENDF/B-VI data for light water reactor (LWR) shielding and dosimetry. The new multigroup li-

braries, BUGLE-93 and VITAMIN-B6, were studied to establish their reliability and response to the benchmark measurements by use of radiation transport codes, ANISN and DORT. Also, direct comparisons of BUGLE-93 and VITAMIN-B6 to BUGLE-80 (ENDF/B-IV) and VITAMIN-E (ENDF/B-V) were performed. Some benchmarks involved the nuclides used in LWR shielding and dosimetry applications, and some were sensitive to specific nuclear data, i.e. iron due to its dominant use in nuclear reactor systems and complex set of cross-section resonances. Five shielding benchmarks (four experimental and one calculational) are described and results are presented.

Research sponsored by U.S. Department of Energy.

5.4

**NEA NSC WP INTERNATIONAL
EVALUATION COOPERATION
SUBGROUP 7/MULTIGROUP
CROSS-SECTION PROCESSING:
PROGRESS AND NEW DIRECTIONS**

R. W. Roussin E. Menapace*

(Abstract of paper presented at the International Conference on Nuclear Data for Science and Technology, Gatlinburg, TN, May 9-13, 1994)

Subgroup 7 of the NEA NSC WP-IEC stimulated interest in processing data from various international and regional evaluated cross-section libraries into the 174n, 42g VITAMIN-J multigroup energy structure for the purpose of intercomparison. Cooperation and participation came from numerous installations around the world. Most processing was done with the NJOY system, but some independent contributions were provided. At the WP-IEC meeting in June 1993, many contributions to the effort were described and the exercise proved to be useful from several aspects. It was decided to expand the role of the temporary subgroup into a long term subgroup to look at both format and processing problems. A summary of the progress of Subgroup 7 is provided and the objective and scope of the new entity, Subgroup B, is reported.

Research sponsored by U.S. DOE Office of Fusion Energy.

*Nuclear Data and Computer Codes Laboratory, Bologna, Italy.

5.5

**VITAMIN-B6: A FINE-GROUP
CROSS-SECTION LIBRARY
BASED ON ENDF/B-VI FOR
RADIATION TRANSPORTATION
APPLICATIONS**

**J. E. White R. Q. Wright*
D. T. Ingersoll R. W. Roussin
N. M. Greene* R. E. MacFarlane†**

(Abstract of paper presented at the International Conference on Nuclear Data for Science and Technology, Gatlinburg, TN, May 9-13, 1994)

A new multigroup cross-section library based on ENDF/B-VI data has been produced and tested for light water reactor shielding and reactor pressure vessel dosimetry applications. This fine-group library, which is designated VITAMIN-B6, contains 120 nuclides. Several dosimetry response functions and kerma factors for all 120 nuclides are also included with the library. Significant benchmark data testing of VITAMIN-B6 was an integral part of this development work to accelerate the qualification. Over 50 benchmarks were calculated using the VITAMIN-B6 library. In general, results using significant improvements relative to earlier ENDF data.

Research sponsored by U.S. Department of Energy.

*Computing and Applications Division.

†Los Alamos National Laboratory, Los Alamos, NM.

INFORMATION ANALYSIS CENTER ACTIVITIES

5.6

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 Simulating Accelerator Radiation Environments Workshop, Santa Fe, NM, January 11-15, 1993)

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.

5.7

CURRENT STATUS OF ENDF/B-VI

R. W. Roussin P. G. Young*
R. McKnight†

(Abstract of paper presented at the International Conference on Nuclear Data for Science and Technology, Gatlinburg, TN, May 9-13, 1994)

Version VI of the Evaluated Nuclear Data File (ENDF/B-VI) was released in 1990. For ENDF/B-VI major emphasis was placed on standard, isotopic evaluations, energy balance, improved resonance region representations, and improvement of neutronics files for important actinides. Data testing proceeds at a pace much slower than previous versions but more results are now being accumulated. Two revisions have been released to date and a third is planned after the next meeting of the Cross Section Evaluation Working Group (CSEWG), currently planned for October 1994.

Research sponsored by U.S. DOE Office of Fusion Energy.

*Los Alamos National Laboratory, Los Alamos, NM.

†Argonne National Laboratory, Argonne, IL.

APPENDICES

PERSONNEL ACTIVITY

JANUARY 1993 - DECEMBER 1994

NEW STAFF MEMBERS

A. Scientific Staff

J. Barhen, Ph.D., Nuclear Engineering/Computer Science Technion - Israel
Institute of Technology
J. M. Donato, Ph.D., Mathematics, University of California, Los Angeles,
CA (Householder Fellow)
V. V. Federov, Ph.D., Physics and Mathematics, Moscow State University,
Moscow, Russia
N. W. Grady, Ph.D., Physics, University of Virginia, Charlottesville, VA
W. C. Grimmell, Ph.D., Electrical Engineering/Mathematics, University of
Michigan, Ann Arbor, MI
X. Guan, Ph.D., Computer Science, Washington State University, Pullman,
WA
J. A. Kohl, Ph.D., Electrical/Computer Engineering, University of Iowa, Iowa
City, IA
R. W. Lee, M.S., Computer Systems, Air Force Institute of Technology, Wright
Patterson AFB, Dayton, OH
S. L. Lee, Ph.D., Computer Science, University of Illinois, Urbana, IL
L. P. MacIntyre, M.S., Chemical Engineering, University of Tennessee,
Knoxville, TN
N. M. Nachtigal, Ph.D., Applied Mathematics, Massachusetts Institute of
Technology, Cambridge, MA (Householder Fellow)
P. M. Papadopoulos, Ph.D., Electrical Engineering, University of California, San
Diego, CA
N. S. V. Rao, Ph.D., Computer Science, Louisiana State University, Baton
Rouge, LA
D. R. Tufano, Ph.D., Experimental Psychology, Princeton University, Princeton,
NJ

B. Administrative and Technical Support Staff

T. L. Barnes, Co-Op Student
K. W. Bateman, Summer Technical Support
R. G. Bilbrey, Secretary
P. S. Brantley, Technical Support
S. A. Burke, Secretary
S. W. Case, Summer Clerical
W. Chen, Summer Technical Support
D. A. Cross, Summer Technical Support
G. S. Davis, Secretary
M. D. Dewing, Summer Technical Support
B. R. Dole, Summer Technical Support
T. S. Douglas, Accounting

D. A. Gibson, Secretary
 K. A. Hall, Summer Technical Support
 R. L. Neubert, Summer Technical Support
 C. C. Parks, Summer Technical Support
 G. H. Paulino, Summer Technical Support
 J. W. Reed, Technical Support
 K. R. Sircar, Summer Technical Support
 F. A. Tulloch, Co-Op Student
 M. E. Weippert, Summer Technical Support
 C. Zhao, Summer Technical Support

DISTINGUISHED SCIENTIST

J. J. Dongarra, University of Tennessee

STAFF TRANSFERS OUT AND TERMINATIONS

A. Scientific Staff

F. S. Alsmiller (retired)
 R. G. Alsmiller (retired)
 A. L. Bangs (other employment)
 K. O. Bowman (retired)
 J. K. Dickens (retired)
 W. W. Engle (retired)
 J. A. Harvey (retired)
 T. L. Hebble (retired)
 B. L. Kirk (transferred to Central Management Organization)
 D. C. Larson (transferred to Physics Division)
 E. Leach (retired)
 W. E. Lever (retired)
 R. E. Maerker (retired)
 B. L. McGill (retired)
 T. J. Mitchell (deceased)
 F. J. Muckenthaler (retired)
 D. E. Pierce (transferred to Physics Division)
 F. G. Pin (transferred to Robotics and Process Systems Division)
 K. A. Remington (Householder term ended)
 W. A. Rhoades (retired)
 F. J. Sweeney (transferred to Energy Systems Waste Management Organization)
 L. W. Weston (retired)

B. Administrative and Technical Support Staff

J. A. Atchley (transferred to Energy Division)
 T. L. Barnes (returned to school)
 K. W. Bateman (returned to school)
 P. S. Brantley (returned to school)
 S. W. Case (other employment)
 V. M. Cauley (transferred to Chemical Technology Division)
 W. Chen (returned to school)

C. P. Coker (retired)
 D. A. Cross (returned to school)
 M. D. Dewing (returned to school)
 B. R. Dole (returned to school)
 K. A. Hall (returned to school)
 C. R. Householder (transferred to Waste Management & Remedial Action Division)
 A. L. Houston (retired)
 D. C. Human (resigned)
 L. K. Lovette (retired)
 G. A. Marvin (terminated)
 A. M. McCoy (transferred to Physics Division)
 J. L. Nave (resigned)
 R. L. Neubert (returned to school)
 C. C. Parks (returned to school)
 G. H. Paulino (returned to school)
 K. R. Sircar (returned to school)
 J. S. Trent (retired)
 F. A. Tulloch (returned to school)
 M. E. Weippert (returned to school)
 C. Zhao (returned to school)

POST-DOCTORAL ASSIGNMENTS

J. Choi, Electrical Engineering, University of Tennessee, Knoxville, TN
 F. X. Gallmeier, Physics, Technical University of Munich, Munich, Germany
 X. Guan, Computer Science/Human Genome,
 S. Matis, Computational Biology, University of Pittsburgh, Pittsburgh, PA
 K. Rahmani, Robotics/Mechanical Engineering, Purdue University, Carmel, IN
 H. J. Schmiedmayer, Physics, Technische Universitat, Wien, Austria
 S. S. Shekhar, Mechanical Engineering, Stanford University, Stanford, CA
 B. Straughan, Applied Mathematics, Heriot-Watt University, England
 R. Wunstorff, Physics, University of Tennessee, Knoxville, TN
 Y. Xu, Computer Science, University of Colorado, Boulder, CO
 H. Zhou, Computer Science, University of Zurich, Zurich, Switzerland

GUESTS AND SHORT-TERM APPOINTMENTS

A. University/Industry Research Collaborators

R. G. Alsmiller, Jr., High Energy Physics (retired)
 M. A. Abidi, Electrical/Computer Engineering, University of Tennessee, Knoxville, TN
 X. Bai, Engineering, Shenyang Institute of Automation, Chinese Academy of Sciences
 F. S. Barickman, Engineering/Robotics, Midwest Technical, Oak Ridge, TN
 D. Bash, Mathematics, U.S. Army Nuclear and Chemical Agency
 B. L. Bishop, Statistics, Ore Company, Oak Ridge, TN (retiree)
 J. Borenstein, Robotics, Univ. of Michigan, Ann Arbor, MI
 J. E. Brehm, Computer Science, University of Hannover, Institut fuer Rechnerstrukturen und Betriebssystem, Hannover, Germany
 R. W. Brockett, EPM Advisory Committee, Electrical Engineering/Computer Science, Harvard University, Cambridge, MA
 R. F. Carlton, Physics, Middle Tennessee State University, Murfreesboro, TN

- C.-X. Chen, Electrical Engineering, University of Tennessee, Knoxville, TN
 P. V. Cherkukuri, Nuclear Engineering, University of Florida, Gainesville, FL
 S. C. Chiang, Robotics, University of Florida, Gainesville, FL
 J. C. Courtney, Nuclear Engineering, Louisiana State University, Baton Rouge, LA
 W. L. Dunn, Nuclear Engineering, Quantum Research Services, Durham, NC
 C. L. Dyer, Statistics, Self-Employed Consultant, Knoxville, TN
 G. Einstein, Robotics, Tennessee State University, Nashville, TN
 M. S. Elsasser, Robotics, Fachhochschule fur Technik und Wirtschaft, Germany
 W. Fabritz, Physics, Atominsitute, Vienna, Austria
 L. Feng, Mechanical Engineering, University of Michigan, Ann Arbor, MI
 R. J. Fraga, Mathematics/Computer Science, Rippon College, Rippon, WI
 J. S. Faulkner, Physics, Self-Employed Consultant, Boca Raton, FL
 P. A. Forsyth, Mathematics, Herndon, VA
 F. W. Garber, Physics, Intraspac, Inc., Oak Ridge, TN
 J. A. George, Computer Science, University of Waterloo, Waterloo, Canada
 M. Goldstein, Nuclear Engineering, Nuclear Research Center, Israel
 R. C. Gonzalez, Robotics, Self-Employed Consultant, Knoxville, TN
 A. T. Goshaw, Physics, Duke University, Durham, NC
 F. Guess, Statistics, University of Tennessee, Knoxville, TN
 R. Gwin, Physics, Self-Employed Consultant, Oak Ridge, TN (retiree)
 B. L. Gyorffy, Physics, Self-Employed Consultant, Bristol, England
 C. P. J. Halloy, Computer Science, University of Tennessee, Knoxville, TN
 D. R. Hart, Mathematics, Knox College, Galesburg, IL
 J. A. Harvey, Physics, Oak Ridge, TN (retiree)
 L. J. Hauser, Computational Biology, University of Tennessee, Knoxville, TN
 N. W. Hill, Physics, Self-Employed Consultant, Knoxville, TN (retiree),
 M. E. Kittrell, Business Administration, ORAU, Oak Ridge, TN
 L. E. Klobe, Business, Midwest Technical, Inc., Oak Ridge, TN
 D. S. Koltick, High Energy Physics, Purdue University, Lafayette, IN
 J. E. Lumpp, Electrical Engineering/Computer Science, University of Kentucky,
 Lexington, KY
 Roger L. Macklin, Physics, Oak Ridge, TN
 F. C. Maienschein, Physics, Oak Ridge, TN (retiree)
 L. T. Mashburn, History, University of Tennessee, Knoxville, TN
 S. G. Mashnik, Nuclear Research, Joint Institute for Nuclear Research, Russia
 B. F. Maskewitz, Psychology, Powell, TN (retiree)
 A. Mau, Nuclear Engineering, Research Center Juelich Ltd/, Juelich, Germany
 R. A. McNees, Physics/Mathematics, University of North Carolina, Raleigh, NC
 M. C. Moxon, Physics, AEA Technology, Harwell, England
 A. Nanthakumar, Statistics, University of Kentucky, Lexington, KY
 Y. I. Noy, Human Factors, Transport Canada, Ottawa, Ontario, Canada
 J. M. Ortega, Mathematics, University of Virginia, Charlottesville, VA
 L. S. Ostrouchov, Computer Science, University of Tennessee, Knoxville, TN
 R. W. Peelle, Physics, Consultant-Self-Employed (retiree)
 S. Petrov, Mathematics, University of Tennessee, Knoxville, TN
 R. Pozo, Computer Science, University of Tennessee, Knoxville, TN
 S. Ramachandramurthi, Mathematics, University of Tennessee, Knoxville, TN
 J. J. Reidy, Physics, University of Mississippi, Oxford, MS
 J. P. Riehs, Physics, Institute fur Kernphysik, Wien, Austria
 R. H. Rockwell, Cognitive Systems, Columbus, OH
 E. Sartori, Nuclear Physics, Organization for Economic Cooperation and Development,
 Nuclear Energy Agency, France
 M. B. Shah, Computer Science, University of Tennessee, Knoxville, TN

R. A. Schrack, Physics, National Institute of Standards and Technology, Washington, D.C.
 K. N. Sigmon, Mathematics, University of Florida, Gainesville, FL
 M. H. Smith, Statistics, Oak Ridge Associated Universities, Oak Ridge, TN
 C. A. Sparrow, Nuclear Engineering, Mississippi State University, Starkeville, MS
 L. S. Tonsunoglu, Robotics Control, University of Texas, Austin, TX
 M. Trivedi, Electrical Engineering, University of Tennessee, Knoxville, TN
 D. K. Trubey, Computer Science, Self-Employed Consultant, Citrus Springs, FL (retiree)
 V. R. Uppurluri, Mathematics, Oak Ridge, TN (retiree)
 F. J. Walter, Physics, Intraspec, Inc., Oak Ridge, TN
 O. A. Wasson, Physics, National Institute of Standards and Technology, Washington, D.C.
 Y. Watanabe, Robotics, University of Tsukuba, Japan
 D. K. Wehe, Robotics, University of Michigan, Ann Arbor, MI
 R. R. Winters, Nuclear Physics, Denison University, Granville, OH
 B. Xiaobo, Engineering, Shenyang Institute of Automation, Shenyang, China
 M. S. Zien-Sabattou, Electrical Engineering, Tennessee State University, Nashville, TN

B. Faculty Research Participation Program

J. B. Conway, Mathematics, University of Tennessee, Knoxville, TN
 J. C. Courtney, Nuclear Engineering, Louisiana State University, Baton Rouge, LA
 A. S. Cover, Mathematics, Clemson University, Clemson, SC
 G. J. Davis, Mathematics, Georgia State University, Atlanta, GA
 N. Deo, Electrical Engineering, University of Central Florida, Orlando, FL
 P. A. Forsyth, University of Waterloo, Waterloo, Canada
 J. A. George, Computer Science, University of Waterloo, Waterloo, Ontario
 G. W. Howell, Mathematics, Florida Institute of Technology, Melbourne, FL
 J. H. Goldberg, Psychology, Pennsylvania State University, College Park, PA
 S. Li, Robotics, Nanjing Aeronautical Institute, Nanjing, China
 J. W. H. Liu, Computer Science, York University, Oakville, Ontario, Canada
 N. Manickam, Mathematics, DePauw University, Greencastle, IN
 D. R. Marpaka, Electrical Engineering, Tennessee State University, Nashville, TN
 A. Nanthakumar, Statistics, University of Tennessee, Martin, Chattanooga, TN
 H. N. Narang, Applied Mathematics, Tuskegee University, Tuskegee, AL
 U. I. Pisingan, Education Administration, Kadena High School, Okinawa, Japan
 J. A. Reneke, Mathematics, Clemson, Clemson, SC
 C. D. Rosaly, Mathematics, Van Buren Jr. High School, Tampa, FL
 S. R. Seidel, Michigan Technological University, Houghton, MI

C. Graduate Students Research Participation Program

M. B. Abdulghafour, Computer Vision, University of Tennessee, Knoxville, TN
 A. H. Barfield, Mathematics, North Carolina Central University, Durham, NC
 B. Bundrage, Electrical Engineering, Tennessee State University, Nashville, TN
 S. Chaudhry, Nuclear Engineering, University of Florida, Gainesville, FL
 M. W. Craven, Computer Science, University of Wisconsin, Madison, WI
 A. K. Dalmia, Robotics, University of Tennessee, Knoxville, TN
 M. D. Dewing, Physics, University of Illinois, Urbana, IL
 O. H. Doerum, Robotics Vision, Norwegian Institute of Technology, Norway
 J. B. Duffie, Electrical Engineering, Clemson University, Clemson, SC
 L. Feng, University of Michigan, Ann Arbor, MI

D. K. Ghosh, Structural Engineering, Vanderbilt University, Nashville, TN
 J. M. Graham, Mathematics, North Carolina State University, Raleigh, NC
 A. Hammerle, Physics, Technical University of Vienna, Vienna, Austria
 A. Hampapur, Computer Science, University of Michigan, Ann Arbor, MI
 D. Ioannou, Engineering, University of Florida, Gainesville, FL
 C. T. Jenson, Computer Science, Aalborg University, Aalborg, Denmark
 W. T. Johnson, Mathematics, University of Tennessee, Knoxville, TN
 G. V. Jones, Computer Science, University of Tennessee, Knoxville, TN
 T. Katsaounis, Mathematics, University of Tennessee, Knoxville, TN
 Y. Kim, Computer Science, University of Tennessee, Knoxville, TN
 G. M. Kofler, Physics, Atominstute, Vienna, Austria
 Y. Koren, Robotics, University of Michigan, Ann Arbor, MI
 P. F. Locascio, Electrical Engineering, University of Westminster, England
 C. C. Large, Physics, University of Tennessee, Knoxville, TN
 J. T. Louallen, Mathematics, University of Tennessee, Knoxville, TN
 J. D. Martens, Electrical Engineering, Case Western Reserve, Euclid, OH
 A. P. Merlo, Computer Engineering, Universita of Pavia, Italy
 S. A. Mikkelsen, Engineering, Aalborg University, Aalborg, Denmark
 B. R. Moore, Nuclear Engineering, North Carolina State University, Raleigh, NC
 K. A. Morgansen, Mechanical Engineering, Boston University, Boston, MA
 S. A. Moulton, Computer Science, University of Tennessee, Knoxville, TN
 R. L. Neubert, Marketing, University of Tennessee, Knoxville, TN
 Q. H. Nguyen, Mechanical Engineering, University of Texas, Austin, TX
 J. A. Nichols, Mathematics, University of Tennessee, Knoxville, TN
 E. J. Nisewonder, Mathematics/Physics, Elon College, Elon College, NC
 J. H. Noerrellykke, Engineering, University of Aalborg, Aalborg, Denmark
 B. S. Park, Mechanical Engineering, Korea Atomic Energy Research Institute, Daejeon, Korea
 G. Rajeev, Computer Science, University of Tennessee, Knoxville, TN
 J. C. Reeb, Mathematics, University of Tennessee, Knoxville, TN
 L. A. Smith, Nuclear Engineering, University of Florida, Tallahassee, FL
 T. Steinell, Robotics, Fachhochschule Wiesbaden, Wiesbaden, Germany
 A. S. Stoffel, Mathematics, Siena College, Loudonville, NY
 R. N. Stewart, Mathematics/Statistics, University of Tennessee, Knoxville, TN
 S. S. Takkella, Michigan Technological University, Houghton, MI
 A. Yarkhan, Computer Science, University of Tennessee, Knoxville, TN

D. Undergraduate Student Research Participation Program

M. Abdelrazek, Physics, University of Tennessee, Knoxville, TN
 E. G. Balas, Computer Science, Saint Joseph's College, Collegeville, IN
 F. S. Barickman, Engineering/Robotics, Gannon University, Erie, PA
 R. F. Barrett, Mathematics, University of Tennessee, Knoxville, TN
 D. Blau, Mathematics, Oak Ridge High School, Oak Ridge, TN
 D. A. Boozer, Mechanical Engineering, University of Alaska, Fairbanks, Alaska
 M. K. Campin, Applied Mathematics, Western Washington University, Bellingham, WA
 D. D. Carlson, Electrical Engineering/Computer Science, University of Nevada, Reno, NV
 M. P. Coddington, Mathematics, Oak Ridge High School, Oak Ridge, TN
 M. W. Craven, Computer Science, University of Wisconsin, Madison, WI
 M. L. Dennard, Computer Science, Morris Brown College, Atlanta, GA
 R. A. Haire, Mathematics, Oak Ridge High School, Oak Ridge, TN
 M. B. Hall, Applied Mathematics, Oregon State University, Corvallis, OR

- T. S. Hamilton, Physics, University of Tennessee, Knoxville, TN
 E. J. Harris, Electrical Engineering, Prairie View A&M University, Prairie View, TX
 T. A. Hodge-Diaz, Industrial Engineering, University of Puerto Rico, Mayaguez, PR
 A. W. Hoover, Computer Science, University of South Florida, Tampa, FL
 S. A. Ingracia, Electrical Engineering, University of Missouri-Rolla, Rolla, MO
 Y. Iwanaga, Engineering Physics, Cornell University, Ithaca, NY
 S. R. Johnson, Mathematics, Alabama A&M,
 C. K. Karlof, Mathematics, University of Tennessee, Knoxville, TN
 S. Kopecky, Physics, Institut fur Kernphysik, Vienna, Austria
 M. Krenn, Physics, Technical University, Vienna, Austria
 Q. Luo, Mathematics/Computer Science, University of The South, Sewanee, TN
 L. C. Lupo, Electrical Engineering, Moorpark College, Moorpark, CA
 S. B. Martin, Mathematics, University of New Hampshire, Durham, NH
 R. A. Mir, Computer Science, Morris Brown College, Atlanta, GA
 J. A. Nichols, Mathematics, University of Tennessee, Knoxville, TN
 N. Olman, Mathematics, Oak Ridge High School, Oak Ridge, TN
 A. M. Ortiz-Cotto, Industrial Engineering, University of Puerto Rico, Mayaguez, PR
 R. C. Penland, Nuclear Engineering, North Carolina State University, Raleigh, NC
 C. L. Perez, Mathematics, University of North Carolina, Chapel Hill, NC
 J. C. Reeb, Mathematics, Illinois State University, Normal, IL
 J. V. Reynolds, Mathematics, Wesleyan College, Macon, GA
 A. H. Skees, Mathematics/Physics, Centenary College, Shreveport, LA
 F. W. Starr, Physics, University of Tennessee, Knoxville, TN
 S. Toemoe, Computer Science, Fachhochschule Wiesbaden, Wiesbaden, Germany
 S. T. Wallace, Molecular Genetics, University of Wien, Vienna, Austria
 S. Y. Whitaker, Mathematics, Clark-Atlanta College, Atlanta, GA
 C. T. White, Mathematics, University of Tennessee, Knoxville, TN
 J. Wu, Computer Science/Mathematics, Denison University, Granville, OH
 A. Xia, Mathematics/Wabash College, Crawfordsville, IN
 M. Yeh, Cognitive Science/Applied Mathematics, Rice University, Houston, TX
 C. Zhao, Mathematics, Denison University, Granville, OH
 V. A. Zarkian, Mathematics/Computer Science, University of Tennessee,
 Knoxville, TN
 J. Zhu, Mathematics, Knox College, Galesburg, IL

SCIENTIFIC AND PROFESSIONAL ACTIVITIES

January 1993 — December 1994

V. Alexiades

Professor

- Mathematics Department, University of Tennessee, Knoxville, TN.

Coordinator

- Metric Coordinator for EPM.

Award

- UTK-ORNL Science Alliance Research Incentive Award, 1986–1991, 1994.

Reviewer

- *Mathematics Reviews*

Referee

- *SIAM Journal of Mathematical Analysis*
- *Nonlinear Analysis*
- *International Journal of Heat and Mass Transfer*
- *ASME Journal of Heat Transfer*
- NSF and DOE Proposals

Invited lecture

- “In-Situ-Vitrification: Some Modeling Issues,” DOE/OSC Applied Mathematics Workshop, Albuquerque, NM, February 3–5, 1993.

Invited papers

- “A Weak Formulation for Phase Change Problems with Bulk Movement Due to Unequal Densities,” (with J. B. Drake) Vol. 281, pp. 82–87 in *Free Boundary Problems Involving Solids*, Eds., J. M. Chadam and H. Rasmussen, Pitman Research Notes, Longman, New York, 1993.
- “Heat Transfer Analysis of a Field-Scale Melting Experiment,” (with A. D. Solomon and G. K. Jacobs) *International Communications in Heat and Mass Transfer* 20(6), 793 (1993).
- “Constraints on Mass Balance of Soil Moisture During In Situ Vitrification,” (with G. K. Jacobs and N. W. Dunbar) *Environmental Geology* 23, 83 (1994).

- "Solidification Modeling of In Situ Vitrification Melts," (with G. K. Jacobs) pp. 11-16 in Proc. of Dynamic Systems and Applications, Vol. 1, Eds., G. S. Ladde and M. Sambandham, Dynamic Publishers, July 1994.

F. S. Alsmiller

Invited papers

- "Radiation Levels in the SSCL Experiment Halls," (with R. G. Alsmiller, Jr., C. Y. Fu, T. A. Gabriel, and R. A. Lillie) Workshop on Simulating Accelerator Radiation Environments, Santa Fe, NM, January 11-15, 1993.
- "Radiation Levels at the SSCL Experimental Halls as Obtained Using the CALOR89 System," (with R. G. Alsmiller, Jr., C. Y. Fu, T. A. Gabriel, and R. A. Lillie) International Conference on Monte Carlo Simulations in High Energy and Nuclear Physics Florida State University, Tallahassee, FL, February 22-26, 1993.
- "Radiation Levels in the SSC Experimental Facilities," (with R. G. Alsmiller, Jr., C. Y. Fu, T. A. Gabriel, R. A. Lillie, and C. O. Slater) 1993 Winter Meeting of the American Nuclear Society, San Francisco, CA, November 14-19, 1993; *Trans. Am. Nucl. Soc.* 69, 433-437 (1993).

Y. Y. Azmy

Member

- Executive Committee Mathematics and Computation Division of the American Nuclear Society.
- Technical Program Committee, ANS M&C Topical Meeting, Portland, OR, 1995.
- Technical Program Committee, ANS Reactor Physics Meeting, Knoxville, 1994.
- Assistant to the General Chairman of the Reactor Physics Meeting, Knoxville, TN, 1994.

Referee

- *National Academy of Science*
- *Nuclear Science and Engineering*
- *Journal Computational Physics*
- *Transport Theory and Statistical Physics*
- *International Science Foundation*

Invited talk

- "Multiprocessing for Neutron Transport and Diffusion Methods," Faculty at the University of California, Santa Barbara, CA, March 8-10, 1993.

Invited papers

- "Neutron Transport Methods on Scalable Shared Memory Multiprocessors," pp. 396-405 in Proc. of 1994 ANS Reactor Physics Meeting, Knoxville, TN, April 11-15, 1994.
- "Adjacent-Cell Preconditioners for Solving Optically Thick Neutron Transport Problems," Eighth International Conference on Radiation Shielding, Arlington, TX, April 24-27, 1994.
- "Arbitrarily High Order Nodal and Characteristic Methods," *Trans. Am. Nucl. Soc.* **71**, 228 (1994).

A. L. Bangs**Invited paper**

- "Research and Applications of Cooperating Mobile Robots," 1993 IEEE International Conference on Robotics and Automation, Workshop on Needs for Research in Cooperating Robots, Atlanta, GA, May 2-7, 1993.

C. O. Beasley**Member**

- American Physical Society.
- Facility Management Steering Committee (ORNL).
- Solid Low-Level Waste Characterization Task Team (ORNL).

Chairman

- Subcommittee on Training.

Invited talk

- "Information Technology at ORNL," International Atomic Energy Agency, Vienna, Austria, October 20, 1994.

Referee

- *Nuclear Fusion*
- *Physics of Fluids*
- *Plasma Physics*

Safety officer

- Engineering Physics and Mathematics Division.

Radiation control officer

- Engineering Physics and Mathematics Division.

Quality assurance coordinator

- Engineering Physics and Mathematics Division.

Training coordinator

- Engineering Physics and Mathematics Division.

Environmental protection officer

- Engineering Physics and Mathematics Division.

Facility manager

- Engineering Physics and Mathematics Division.

HAZCOM coordinator

- Engineering Physics and Mathematics Division.

J. J. Beauchamp**Member**

- EPMD Representative to ORNL Values Committee.

Invited talk

- "Statistics: An Aid to Better Understanding," Oral Presentation, Restoring Our Waters Workshop, Oak Ridge, TN, July 13, 1993.

K. O. Bowman**Member**

- The President's Committee on Employment of People with Disabilities.
- Committee on Statistics and Disability, American Statistical Association.
- Advisory Board, *Journal of Statistical Computation and Simulations*.
- International Editorial Board, Communications in Statistics.
- International Organizing Committee, Indo-U.S.-Japan Conference.
- Advisory Board, Quality through Engineering Design, Indo-U.S. Japan Conference.
- Grant Application Review Committee, The Foundation for Science and Disability.

Contributing editor

- *Current Index to Statistics*

President

- The Foundation for Science and Disability.

Grant

- Indo-U.S.-Japan Conference, National Science Foundation

Reviewer

- *Science, American Association for the Advancement of Science*
- Research Proposal, National Science Foundation

Referee

- *The Annals of the Institute of Statistical Mathematics*
- *Communications in Statistics*

Invited lecture

- "Employment Opportunities in Science for Persons with Disabilities," National Symposium on Americans with Disabilities from Diverse Cultural Communities, 1994 Annual National Conference, Atlanta, GA, May 17, 1994.

Invited papers

- "Contribution to the Discussion on the Paper by R. C. H. Cheng and L. Taylor on Non-Regular Maximum Likelihood Problems, on 19 January 1994," (with L. R. Shenton) *Journal of Royal Statistical Society* (in press).
- "NSF Office for Disabled Scientists and Engineers Opens," *Amstat News*, p. 19 (February 1993).
- "EEOC Publication Explains Your Rights Under the Americans with Disabilities Act," *Amstat News*, p. 10 (March 1993).
- "AAAS Explores Problems for Scientists and Engineers," *Amstat News*, p. 12 (April 1993).
- "Your Rights Under ADA—Continued" *Amstat News*, p. 10 (May 1993).
- "FSD Works to Increase Options for Students with Disabilities," *Amstat News*, p. 16 (June 1993).
- "ADA Passes Its First Anniversary," *Amstat News*, pp. 26–27 (August–September 1993).
- "ADA Can Only Work for Those Who Identify Themselves," *Amstat News*, pp. 34–35 (October 1993).
- "Note from the Committee on Statistics and Disability," *Amstat News* (November 1993).

T. J. Burns**Invited presentation**

- "Radiation Environments Program," (with J. O. Johnson) handouts for the Radiation Sciences Simulation and Modeling Conference, Williamsburg, VA, November 29–December 1, 1994.

R. J. Carter**Member**

- Human Factors and Ergonomics Society Surface Transportation Special Interest Group Abstract Review Committee.
- Human Factors and Ergonomics Society Safety Technical Group Abstract Review Committee.
- Human Factors and Ergonomics Society Publications Committee.
- DOE Human Factors Standards Steering Committee.
- Intelligent Vehicle Highway Society of America Safety and Human Factors Committee.
- ANS Human Factors Topical Meeting Technical Program Committee.
- Human Factors and Ergonomics Society Best Technical Group Newsletter Award Committee.

Liaison

- Human Factors and Ergonomics Society, ANS Human Factors Topical Meeting.

Chair

- Human Factors and Ergonomics Society Best Bulletin Article Award Committee.
- Human Factors and Ergonomics Society Annual Meeting Local Organizing Committee.

Editor

- *Human Factors and Ergonomics Society Bulletin*

E. F. D'Azevedo**Member**

- Society for Industrial and Applied Mathematics.

J. K. Dickens**General chairman**

- International Conference on Nuclear Data for Science and Technology, Gatlinburg, TN, May 9-13, 1994.

Member

- American Nuclear Society Standards Committee ANS-19.
- American Nuclear Society Standards Working Group 5.1, Decay Heat Standard.
- American Nuclear Society Standards Working Group 19.8, Fission Product Yields.

- American Nuclear Society Standards Working Group 19.9, Delayed Neutrons Standard.
- International Atomic Energy Agency Nuclear Data Section Coordinated Research Program on, "Measurement, Calculation, and Evaluation of Photon Production Data."

Referee

- *Nuclear Science and Engineering*
- U.S. Department of Energy

Invited papers

- "Physics of Neutron Production at the Oak Ridge Electron Linear Accelerator," *Trans. Am. Nucl. Soc.* **69**, 424-425 (1993).
- "Experimental and Calculated Radionuclide Production by Photonuclear Reactions Using Bremsstrahlung Photons Produced by 150 MeV Electrons," (with R. Wunstorf, W. M. Bugg, C. C. Park, T. A. Gabriel, and T. A. Lewis) International Conference on Nuclear Data for Science and Technology, Gatlinburg, TN, May 9-13, 1994.
- "In-Beam Gamma-Ray Spectrometric Measurements of Multi-Body Breakup Reactions for E_n Between Threshold and 40 MeV," Specialists' Meeting on Measurement, Calculation and Evaluation of Photon Production Data, Bologna, Italy, November 8-11, 1994.
- "Precision Measurement of the ^{56}Fe Cross Section for the $R_\gamma=846$ -keV Transition and for E_n Between Threshold and 4 MeV," IAEA First Research Coordination Meeting on Measurement, Calculation and Evaluation of Photon Production Data, Bologna, Italy, November 14-17, 1994.

F. C. Difilippo

Member

- National and Mathematics Division Program Committees of the American Nuclear Society.

Fellow

- American Nuclear Society

Listed

- International Directory of Nuclear Criticality Safety Personnel.

Special assignment

- DOE Technical Representative Gas Cooled Reactor Program at Paul Scherrer Institute, Villigen, Switzerland:
Analysis and Quality Assurance of Experiments Performed at the PROTEUS Facility, July 7-31, 1993.
Fifth Coordination Research Program Meeting on Validation of Safety Related Physics Calculations for Low-Enriched Gas-Cooled Reactors, May 16-20, 1994.

Academic

- Adjunct Professor, Department of Nuclear Engineering, University of Tennessee, Knoxville, TN.

Referee

- *Nuclear Science and Engineering*

Invited lectures

- "Nuclear Power Sources for Space Propulsion," University of Tennessee, March 17, 1993.
- "Scoping Calculations of Power Sources for NEP," NASA-Lewis Research Center, Cleveland, OH, April 20, 1993.
- "Experiments Analysis with Monte Carlo Methods: Benchmarking MCNP," 5th Research Coordination Meeting on Validation of Safety Related Physics Calculations for Low Enriched Gas Cooled Reactors, Villigen, Switzerland, May 16-18, 1994.

J. B. Drake

Member

- CHAMMP Executive Committee.
- ESnet Steering Committee.

J. R. Einstein

Invited talks

- "Integrated Gene Recognition, Modeling, and Data Base Searching in the GRAIL and GenQuest Environments," (with R. J. Mural, D. M. Buley, X. Guan, S. Matis, M. Shah, Y. Xu, and E. C. Uberbacher) Open Problems in Computational Molecular Biology, Telluride, CO, July 11-17, 1994.
- "Detection of Control Regions in the Human Genome Using Intelligent Systems," (with S. Matis, Y. Xu, M. Shah, D. M. Buley, X. Guan, R. J. Mural, and E. C. Uberbacher) Open Problems in Computational Molecular Biology, Telluride, CO, July 11-17, 1994.
- "An Improved System for Exon Recognition and Gene Modeling in Human DNA Sequences," (with Y. Xu, R. J. Mural, M. Shah, and E. C. Uberbacher) The Second International Conference on Intelligent Systems for Molecular Biology, Stanford, CA, August 14-17, 1994.
- "Integrated Gene Recognition, Modeling and Database Searching in the GRAIL and genQuest Environments," (with R. J. Mural, X. Guan, M. Shah, S. Matis, Y. Xu, and E. C. Uberbacher) International Conference on the Human Genome Project, Washington, DC, October 2-5, 1994.
- "Gene Recognition, Modeling, and Homology Search in the GRAIL-genQuest System," (with M. Shah, S. Matis, Y. Xu,

X. Guan, D. M. Buley, S. Petrov, L. Hauser, R. J. Mural, and Uberbacher) DOE Contractor's Meeting, Santa Fe, NM, November 13-17, 1994.

Invited papers

- "An Improved System for Exon Recognition and Gene Modeling in Human DNA Sequences," (with Y. Xu, R. J. Mural, M. Shah, and E. C. Uberbacher) pp. 373-384 in Proc. of The Second International Conference on Intelligent Systems for Molecular Biology, Stanford University, San Francisco, CA, August 14-17, 1994.
- "Integrated Gene Recognition, Modeling and Database Comparison in the GRAIL and GenQuest Environments," (with R. J. Mural, D. M. Buley, X. Guan, S. Matis, M. Shah, Y. Xu, and E. C. Uberbacher) *Computers in Chemistry* (in press).
- "Detection of Control Regions in Human DNA Sequence Using Intelligent Systems," (with S. Matis, Y. Xu, M. Shah, D. Buley, R. J. Mural, and E. C. Uberbacher) *Computers & Chemistry* (in press).

W. W. Engle, Jr.

Fellow

- American Nuclear Society

Executive committee member

- Radiation Protection and Shielding Division, American Nuclear Society

Honors and awards committee member

- Radiation Protection and Shielding Division, American Nuclear Society

D. M. Flanagan

Award

- MMES Significant Event Award: Development of Y-12 Repair History Data Collection and Reporting System Prototype.

E. L. Frome

Member

- 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.

Statistical Consultant

- Radiation Research Society.

Referee

- *The American Journal of Epidemiology*
- *The American Statistician*
- *Radiation Research*

Invited talk

- “Statistical Methods for the Blood Lymphocyte Proliferation Test,” (with M. H. Smith, L. G. Littlefield, R. L. Neubert, and S. P. Colyer) Conference on Beryllium Disease Research, Triangle Park, NC, November 8–10, 1994.

C. Y. Fu**Invited talk**

- “Comparison of Calculated $^{58}\text{Ni}(n, \alpha)$ Cross-Sections and α -Particle Emission Spectra Using Two Level-Density Formalisms Normalized at Two Energies,” Second IAEA RCM Meeting on Improvement of Measurements, Calculations and Evaluations of Neutron-Induced Helium Production Cross Sections, Beijing, China, November 1–4, 1994.

Invited papers

- “Radiation Levels at the SSCL Experimental Halls as Obtained Using the CALOR89 System,” (with F. S. Alsmiller, R. G. Alsmiller, Jr., T. A. Gabriel, and R. A. Lillie) International Conference on Monte Carlo Simulations in High Energy and Nuclear Physics Florida State University, Tallahassee, FL, February 22–26, 1993.
- “TNG Calculations and Evaluations of Photon Production Data for Some ENDF/B-VI Materials,” OECD NEANSC Specialists’ Meeting on Measurement, Calculation and Evaluation of Photon Production Data, Bologna, Italy, November 8–11, 1994.

T. A. Gabriel**Director**

- Oak Ridge Detector Center

Member

- Southeastern Association for High Energy Physics (SAHEP) Executive Committee.
- SAHEP Steering Committee.

- BaBar Detector Collaboration Institutional Board.
- Membership Committee – BaBar Detector Collaboration.
- Institutional Board International Accelerator Radiological Protection E-Mail (IARPE).
- Nuclear Energy Agency, Nuclear Science Committee (NEANSC)
 - Neutron Cross Section from 20 to 100 MeV.

Conference session organizer

- Transport Code Session for the Accelerator Radiation Environmental Workshop, Santa Fe, NM, January 11–15, 1993.
- Detector Session for the MC-93 Conference, Tallahassee, FL, February 22–26, 1993.
- Detector Session for the Fifth Annual Industrial Symposium on the Superconducting Super Collider, San Francisco, CA, May 6–8, 1993.
- Physics User Facilities Session for the Southeastern Section of the American Physics Society, Columbia, SC, November, 1993.

Conference organizing committee

- Accelerator Radiation Environment Workshop, Santa Fe, NM, January 11–15, 1993.
- International Conference on Monte Carlo Simulations in High Energy and Nuclear Physics, Tallahassee, FL, February 22–26, 1993.

Invited talks

- “CALOR89: Benchmarking and Applications,” (with P. K. Job and T. Handler) Workshop on Simulating Accelerator Radiation Environments, Santa Fe, NM, January 11–15, 1993.
- “Introduction to CALOR,” Workshop on Simulating Accelerator Radiation Environments, Santa Fe, NM, January 11–15, 1993.
- “Overview of the Codes and Cross Sections Libraries for Shielding the Muon Chambers from Neutrons and Gammas,” Solenoidal Detector Collaboration Muon Workshop, Superconducting Super Collider Laboratory, Dallas, TX, January 18–29, 1993.
- “Background and Trigger Studies for the BaBar Detector,” BaBar Detector Collaboration Meeting, Stanford Linear Accelerator Center, Stanford, CA, July 7–12, 1994.

Invited papers

- “The CALOR93 Code System,” Simulating Accelerator Radiation Environments Workshop, Santa Fe, NM, January 11–15, 1993.
- “Radiation Levels in the SSCL Experiment Halls,” (with F. S. Alsmiller, R. G. Alsmiller, Jr., C. Y. Fu, and R. A. Lillie) Workshop on Simulating Accelerator Radiation Environments, Santa Fe, NM, January 11–15, 1993.

- "CALOR89: Predictions for the Hanging File Test Configurations," (with P. K. Job, L. Price, J. Proudfoot, and T. Handler) International Conference on Monte Carlo Simulations in High Energy and Nuclear Physics, Florida State University, Tallahassee, FL, February 22–26, 1993.
- "Radiation Levels at the SSCL Experimental Halls as Obtained Using the CALOR89 System," (with F. S. Alsmiller, R. G. Alsmiller, Jr., C. Y. Fu, and R. A. Lillie) International Conference on Monte Carlo Simulations in High Energy and Nuclear Physics Florida State University, Tallahassee, FL, February 22–26, 1993.
- "Radiation Levels in the SSC Experimental Facilities," (with F. S. Alsmiller, R. G. Alsmiller, Jr., C. Y. Fu, R. A. Lillie, and C. O. Slater) 1993 Winter Meeting of the American Nuclear Society, San Francisco, CA, November 14–19, 1993; *Trans. Am. Nucl. Soc.* **69**, 433–437 (1993).
- "Overview of New, Upgraded, or Proposed High Energy Physics Facilities in the United States and Canada," Specialists' Meeting on Shielding Aspects of Accelerators Targets and Irradiation Facilities, Arlington, TX, April 28–29, 1994.
- "Experimental and Calculated Radionuclide Production by Photonuclear Reactions Using Bremsstrahlung Photons Produced by 150 MeV Electrons," (with R. Wunstorf, W. M. Bugg, C. C. Park, T. A. Lewis, and J. K. Dickens) International Conference on Nuclear Data for Science and Technology, Gatlinburg, TN, May 9–13, 1994.
- "Analysis of Intermediate Energy Photonuclear Reactions," (with G. Maino and S. G. Mashnik) XII International Seminar on High Energy Physics Problems, Relativistic Nuclear Physics and Quantum Chromodynamics, Dubna, Russia, September 12–17, 1994.
- "A Monte Carlo Study of Accelerated Head Scatter," (with E. L. Chaney and T. J. Culip) *Medical Physics* **21**(9), 1383 (1994).

G. A. Geist

Member

- SIAM Society

General chairman

- PVM Users Group Meeting 1994

Invited talks

- "PVM Tutorial," Convex Corporation, Dallas, TX, January 27, 1993.
- "The Evolution of the PVM Concurrent Computing System," Compcon Conference, San Francisco, CA, February 25, 1993.
- "PVM 3.0 Features and How to Extend the Interface," Hewlett-Packard Corporation, San Francisco, CA, February 26, 1993.

- "Using PVM 3.0 to Run Grand Challenge Applications on a Heterogeneous Network of Parallel Computers," (with R. Manchek and W. Jiang) 6th SIAM Conference on Parallel Processing for Scientific Computing, Norfolk, VA, March 22-24, 1993.
- "Software Tools for Computational Grand Challenges," Conference on High Speed Computing, Salishan Lodge, OR, March 31, 1993.
- "PVM 3 Beyond Network Computing," University of Kentucky, Lexington, KY, April 28, 1993.
- "The Development of the SCF-KKR-CPA Electronic Structure Method Within a Heterogeneous Distributed Computing Environment," (with W. A. Shelton and G. M. Stocks) SIAM 1993 Annual Meeting, Philadelphia, PA, July 8, 1993.
- "The Development of the SCR-KKR-CPA Electronic Structure Method Within a Heterogeneous Distributed Computing Environment," (with W. A. Shelton and G. M. Stocks) 1993 SIAM Annual Meeting, Philadelphia, PA, July 15, 1993.
- "MPI: A Standard Message Passing Interface for Distributed Memory Concurrent Computers," (with D. W. Walker) ICASE/LARC Short Course on Parallel Computation, Hampton, VA, July 27, 1993.
- "PVM 3 Beyond Network Computing," 2nd International ACPC Conference on Parallel Software, Vienna, Austria, October 4-6, 1993.
- "PVM Tutorial," Supercomputing '93, Portland, OR, November 15, 1993.
- "PVM What's New, What's Coming," Cluster Workshop '93, Florida State University, Tallahassee, FL, December 8, 1993.
- "PVM Tutorial," Maui High Performance Computing Center, Maui, HI, February 16, 1994.
- "PVM 3.3: New Features, New Directions," Thinking Machines Corporation, Cambridge, MA, April 5, 1994.
- "Cluster Computing: The Wave of the Future?" Workshop on Parallel Scientific Computing, Lyngby, Denmark, June 19-23, 1994.

Invited papers

- "PVM 3 Beyond Network Computing," Second International Conference of the Austrian Center for Parallel Computation, Gmunden, Austria, October 4-6, 1993.
- "Distributed Computing's Future," Supercomputing '93, Portland, OR, November 18, 1993; Proc. IEEE Computer Society Press, Los Alamitos, CA, p. 762 (1993).
- "MPI Workshop," Supercomputing '93, Portland, OR, November 19, 1993; Proc. IEEE Computer Society Press, Los Alamitos, CA, pp. 878-883 (1993).

- "PVM A Platform for Portable Distributed Computing," High Performance Computing Conference '94, National University of Singapore, Singapore, September 29–30, 1994.
- "Visualization and Debugging in a Heterogeneous Environment," (with A. Beguelin, J. J. Dongarra, and V. Sunderam) *Computer* (in press).

Awards

- 1994 R&D 100 Award
- SC '93 Heterogeneous Challenge Award

C. W. Glover

Member

- Program Committee for 1994 IEEE International Conference on Neural Networks.
- Program Committee for 1994 SPIE Conference on Neural Networks.

Invited talks

- "Hybrid Pattern Recognition System Capable of Self-Modification," Second International Conference on Information and Knowledge Management, Washington, DC, November 1993.
- "Neural Networks for Fault Diagnoses and Predictive Maintenance," DOE Symposium on Predictive Maintenance, Atlanta, GA, May 1994.

Invited Paper

- "Hybrid Pattern Recognition System Capable of Self-Modification," Knowledge Discovery in Scientific Data Bases, Second International Conferences on Information and Knowledge Management, Washington, DC, 1994.

L. J. Gray

Member

- Scientific Organizing Committee for the IABEM-95 International Conference, Hawaii, July 30–August 3, 1995.

Committee

- ORNL Awards Night Publication Committee.
- Science Alliance Faculty Awards Committee.

Editorial board

- Engineering Analysis with Boundary Elements.
- Boundary Elements: Abstracts and Newsletters.

Referee

- *International Journal for Numerical Methods in Engineering*
- *SIAM J. Applied Mathematics*
- *Engineering Analysis with Boundary Elements*

Invited talks

- "Crack Propagation Modeling," Institute for Mathematics and Its Applications, Minneapolis, MN, October 15, 1993.
- "Boundary Integral Methods for Crack Propagation Modeling," University of Minnesota, Department of Civil and Mineral Engineering, Minneapolis, MN, April 6–8, 1994.

Invited papers

- "Hypersingular Integrals at a Corner," (with L. L. Manne) BEM (Boundary Element Methods) 15 Conference, Worcester, MA, August 10–12, 1993.
- "Morphological Stability of Thin Films," (with M. F. Chisholm and T. Kaplan) pp. 181–190 in Computational Mechanics Publications, BETECH-93 (Boundary Element Technology) Vilamoura, Portugal, November 9–11, 1993.
- "Crack Propagation Modeling," (with D. O. Potyondy, E. D. Lutz, P. A. Wawrzynek, L. F. Martha, and A. R. Ingraffea) *Mathematical Models and Methods in Applied Sciences* 4, 179 (1994).
- "Local Error Estimation for Boundary Element Calculations," (with V. Zarikian and G. Paulino) pp. 253–260 in Boundary Element Technology IX, Eds., C. A. Brebbia and A. J. Kassab, Computational Mechanics Publications (1994).

X. Guan

Awards

- Oak Ridge National Laboratory R&D Accomplishment Award, 1994.
- Oak Ridge National Laboratory World Class Team Work Award, 1993.

Invited talks

- "Integrated Gene Recognition, Modeling, and Data Base Searching in the GRAIL and GenQuest Environments," (with R. J. Mural, D. M. Buley, J. R. Einstein, S. Matis, M. Shah, Y. Xu, and E. C. Uberbacher) Open Problems in Computational Molecular Biology, Telluride, CO, July 11–17, 1994.
- "Detection of Control Regions in the Human Genome Using Intelligent Systems," (with S. Matis, Y. Xu, M. Shah, D. M. Buley, J. R. Einstein, R. J. Mural, and E. C. Uberbacher) Open Problems in Computational Molecular Biology, Telluride, CO, July 11–17, 1994.

- "Integrated Gene Recognition, Modeling and Database Searching in the GRAIL and genQuest Environments," (with R. J. Mural, J. R. Einstein, M. Shah, S. Matis, Y. Xu, and E. C. Uberbacher) International Conference on the Human Genome Project, Washington, DC, October 2-5, 1994.
- "Gene Recognition, Modeling, and Homology Search in the GRAIL-genQuest System," (with M. Shah, J. R. Einstein, S. Matis, Y. Xu, D. M. Buley, S. Petrov, L. Hauser, R. J. Mural, and E. C. Uberbacher) DOE Contractor's Meeting, Santa Fe, NM, November 13-17, 1994.

Invited papers

- "A Practical Guide to the GRAIL E-Mail Server," (with E. C. Uberbacher and R. J. Mural) Automated DNA Sequencing and Analysis Techniques.
- "Integrated Gene Recognition, Modeling and Database Comparison in the GRAIL and GenQuest Environments," (with R. J. Mural, D. M. Buley, J. R. Einstein, S. Matis, M. Shah, Y. Xu, and E. C. Uberbacher) *Computers in Chemistry* (in press).
- "Detection of Control Regions in Human DNA Sequence Using Intelligent Systems," (with S. Matis, Y. Xu, M. Shah, D. Buley, J. R. Einstein, R. J. Mural, and E. C. Uberbacher) *Computers & Chemistry* (in press).

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*

Invited paper

- "Four-Piston Double-Duct Liquid Metal MHD Engine and AC Generator," Annual Meeting of the Mechanical Working Group of the Interagency Advanced Power Group (IAPG), Arlington, VA, May 10-11, 1994.

Patent

- Application filed with U.S. Patent Office, "Double-Duct Liquid Metal Magneto-Hydrodynamic Engine," May 12, 1994.

D. T. Ingersoll**Member**

- Advisory Committee for International Conference on Nuclear Data for Science and Technology.
- Program Committee for 8th International Conference on Radiation Shielding.

Chairman

- Shielding Data Testing Subcommittee, Cross-Section Evaluation Working Group (CSEWG).

Reviewer

- *Nuclear Technology Journal*.

Invited talks

- "Design and Neutronics Issues for the Advanced Neutron Source," North Carolina State University, Raleigh, NC, December 8, 1994.
- "Design and Neutronics Issues for the Advanced Neutron Source," Nuclear Engineering Seminar, Georgia Institute of Technology, Atlanta, GA, November 4, 1994.

J. O. Johnson**Member**

- American Nuclear Society Radiation Protection and Shielding Division Technical Program Committee.

Invited talks

- "The MASH 1.0 Code System: Utilization of MORSE in the Adjoint Mode," (with R. T. Santoro) Organization for Economic Cooperation and Development (OECD) Nuclear Energy Agency (NEA), Seminar on Advanced Monte Carlo Computer Programs for Radiation Transport, Centre d'Etudes, Saclay, France, April 27-29, 1993.
- "Sample Problem Definition," MASH (Monte Carlo Adjoint Shielding) Workshop Pollard Auditorium, Oak Ridge, TN, November 16-18, 1993.
- "DORT A Two-Dimensional Discrete Ordinates Transport Code Input Instructions," MASH (Monte Carlo Adjoint Shielding) Seminar/Workshop, Pollard Auditorium, Oak Ridge, TN, November 16-18, 1993.
- "VISTA Variable Input Source Transformation and Assembly Code User Input Instructions," MASH (Monte Carlo Adjoint Shielding) Seminar/Workshop, Pollard Auditorium, Oak Ridge, TN, November 16-18, 1993.
- "Overview of the MASH Code System v1.0," MASH (Monte Carlo Adjoint Shielding) Seminar/Workshop, Pollard Auditorium, Oak Ridge, TN, November 16-18, 1993.

- "Application of the Adjoint Monte Carlo Shielding Code System - MASH - in Nuclear Operations," (with R. T. Santoro and M. S. Smith) 61st Military Operations Research Society Symposium, Wright Patterson Air Force Base Dayton, OH, June 22-24, 1993.

Invited presentations

- "Radiation Environments Program," (with T. J. Burns) handouts for the Radiation Sciences Simulation and Modeling Conference, Williamsburg, VA, November 29-December 1, 1994.
- "MASH the Nuclear Vulnerability Assessment Code of the U.S. Army," Radiation Sciences Simulation and Modeling Conference, Williamsburg, VA, November 29-December 1, 1994.

Invited paper

- "The MASH Code System, Version 1.0," (with T. J. Burns and R. T. Santoro) *Human Survivability* 1(2), 5-10 (1993).

B. L. Kirk

Member

- American Nuclear Society (ANS-10 Standards Committee).
- American Nuclear Society, Professional Women in ANS.
- American Nuclear Society, Math and Computation Division Technical Program Committee for 1995 International Topical.
- American Nuclear Society/Radiation Protection and Shielding Division Technical Program Committee for 1994 International Topical.

Secretary

- American Nuclear Society, Radiation Protection and Shielding Division.

Board Member

- American Nuclear Society, Oak Ridge/Knoxville Chapter.

Member

- Organization for Economic Cooperation and Development (OECD)/Nuclear Energy Agency (NEA) Working Party on Advanced Computing: Task Force on Adapting Computer Codes in Nuclear Applications to Parallel Architectures
- Society for Industrial and Applied Mathematics

J. A. Kohl

Member

- IEEE
- IEEE Computer Society

- Association for Computing Machinery (ACM)
- ACM SIGCHI
- Eta Kappa Nu National Electrical Engineering Honorary (HKN)
- Tau Beta Pi National Engineering Honorary (TBPI)
- MENSA International

Official reviewer

- *IEEE Computer*

Invited lectures

- "XPVM: A Graphical Console and Monitor for PVM," (with G. A. Geist) PVM Users Group Meeting, Garden Plaza Hotel, Oak Ridge, TN, May 19-20, 1994.
- "Equate Relationships in the IMPROV Program Visualization Environment," (with T. L. Casavant) Workshop on Environments and Tools for Parallel Scientific Computing, Blackberry Farm, TN, May 25-27, 1994.
- "The IMPROV Custom Animation Environment for Parallel Program Visualization," (with T. L. Casavant) PTOOLS Parallel Tools Consortium, First General Meeting, NASA Ames Research Center, Moffett Field, CA, June 8-10, 1994.

Award

- SC '93 - Heterogeneous Computer Challenge, "Most Elegant Interface."

H. E. Knee

Member

- Executive Committee: Human Factors Division of the American Nuclear Society, 1991-1994.
- American Nuclear Society, 1984 to present.
- Smoky Mountain Chapter of the Human Factors and Ergonomics Society (founding member).
- Corporate member, ITS-America, 1993 to present.
- Energy Facilities Contractors Group (EFCOG)/Safety Analysis Working Group, 1992 to present.

Technical chairman

- ANS Topical Meeting on Nuclear Plant Instrumentation, Control and Man-Machine Interface Technologies, Oak Ridge, TN, April 18-21, 1993.

Public relations chair

- 38th Annual Meeting of the Human Factors and Ergonomics Society; People & Technology in Harmony, to be held in Nashville, TN, October 24-28, 1994.

Proposal reviewer

- Department of Energy.
- Federal Highway Administration.

Invited talks

- "Capabilities and Resources of the Oak Ridge National Laboratory for Establishment of a NRC Human Factors Regulatory Research Facility," NRC Technical Training Center, Chattanooga, TN, June 24, 1993.
- "Development of an In-Vehicle Signing Specification," The Federal Highway Administration, Overview of the Development of an In-Vehicle Signing Specification, Washington, DC, June 21, 1994.

Invited paper

- "Human Factors Engineering: A Key Element of Instrumentation and Control System Design," pp. 1113-1122 in Instrument Society of America, 39th International Instrumentation Symposium, Albuquerque, New Mexico, May 2-6, 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*

Invited talk

- "Fusion Data Measurement Capabilities at the Oak Ridge Electron Linear Accelerator (ORELA)," 1993 Symposium on Nuclear Data, Tokai Research Establishment, Japanese Atomic Energy Research Institute, Tokai, Japan, November 18–19, 1993.

Invited papers

- "Status of Nuclear Data for Iter Applications," (with E. T. Cheng, F. M. Mann, and G. Saji) International Conference on Nuclear Data for Science and Technology, Gatlinburg, TN, May 9–13, 1994.
- "In-Beam Gamma-Ray Spectrometric Measurements of Multi-Body Breakup Reactions for E_n Between Threshold and 40 MeV," Specialists' Meeting on Measurement, Calculation and Evaluation of Photon Production Data, Bologna, Italy, November 8–11, 1994.

E. Leach**Award**

- DOE Award of Excellence.

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*

Invited talks

- "A Brief Description of Discrete Ordinates," Workshop on Simulating Accelerator Radiation Environments, Santa Fe, NM, January 11–15, 1993.
- "Theory of Discrete Ordinates," MASH (Monte Carlo Adjoint Shielding) Workshop, Pollard Auditorium, Oak Ridge, TN, November 16–18, 1993.

Invited papers

- "Radiation Levels in the SSCL Experiment Halls," (with F. S. Alsmiller, R. G. Alsmiller, Jr., C. Y. Fu, and T. A. Gabriel) Workshop on Simulating Accelerator Radiation Environments, Santa Fe, NM, January 11–15, 1993.

- "Radiation Levels at the SSCL Experimental Halls as Obtained Using the CALOR89 System," (with F. S. Alsmiller, R. G. Alsmiller, Jr., C. Y. Fu, and T. A. Gabriel) International Conference on Monte Carlo Simulations in High Energy and Nuclear Physics Florida State University, Tallahassee, FL, February 22–26, 1993.
- "Radiation Levels in the SSC Experimental Facilities," (with F. S. Alsmiller, R. G. Alsmiller, Jr., C. Y. Fu, T. A. Gabriel, and C. O. Slater) 1993 Winter Meeting of the American Nuclear Society, San Francisco, CA, November 14–19, 1993; *Trans. Am. Nucl. Soc.* **69**, 433–437 (1993).
- "ANS Cold Source Neutronics Analysis," ANS 1994 Topical Meeting on Advances in Reactor Physics: Reactor Physics Faces the 21st Century, Knoxville, TN, April 11–15, 1994; *Proc. Vol. III*, p. 355 (1994).

R. C. Mann

Member

- Advisory Committee, Demand Activated Manufacturing Architecture Project, AMTEX.

Program committee

- ANS Fifth Topical Meeting on Robotics and Remote Systems, Monterey, CA, February 5–10, 1995.

Reviewer

- *IEEE Computer*
- DOE SBIR Program
- *IEEE Trans. Neural Networks*

Invited paper

- "Supporting Robotics Technology Requirements Through Research in Intelligent Machines," Robotics Industry Forum and Annual Meeting, Orlando, FL, November 2–4, 1994.

S. Matis

Invited talks

- "Detection of Pre- and Post-Transcriptional Control Sequences in DNA Using Computational Methods," (with R. J. Mural and E. C. Uberbacher) The Fourth Keck Symposium on Computational Biology, Pittsburgh, PA, October 24–November 5, 1993.
- "Integrated Gene Recognition, Modeling and Database Comparison in the GRAIL and GenQuest Environments," (with R. J. Mural, D. M. Buley, J. R. Einstein, X. Guan, M. Shah, Y. Xu, and E. C. Uberbacher) Open Problems in Computational Molecular Biology, Telluride, CO, July 11–17, 1994.

- "Detection of Control Regions in the Human Genome Using Intelligent Systems," (with Y. Xu, M. Shah, D. M. Buley, X. Guan, J. R. Einstein, R. J. Mural, and E. C. Uberbacher) Open Problems in Computational Molecular Biology, Telluride, CO, July 11–17, 1994.
- "Integrated Gene Recognition, Modeling and Database Searching in the GRAIL and genQuest Environments," (with R. J. Mural, J. R. Einstein, X. Guan, M. Shah, Y. Xu, and E. C. Uberbacher) International Conference on the Human Genome Project, Washington, DC, October 2–5, 1994.
- "Gene Recognition, Modeling, and Homology Search in the GRAIL-genQuest System," (with M. Shah, J. R. Einstein, Y. Xu, X. Guan, D. M. Buley, S. Petrov, L. Hauser, R. J. Mural, and E. C. Uberbacher) DOE Contractor's Meeting, Santa Fe, NM, November 13–17, 1994.

Invited papers

- "Integrated Gene Recognition, Modeling and Database Comparison in the GRAIL and GenQuest Environments," (with R. J. Mural, D. M. Buley, J. R. Einstein, X. Guan, M. Shah, Y. Xu, and E. C. Uberbacher) *Computers in Chemistry* (in press).
- "Detection of Control Regions in Human DNA Sequence Using Intelligent Systems," (with Y. Xu, M. Shah, D. Buley, X. Guan, J. R. Einstein, R. J. Mural, and E. E. Uberbacher) *Computers & Chemistry* (in press).
- "Detection of Human RNA Polymerase II Promoters Using Artificially Intelligent Methods," (with M. B. Shah, R. J. Mural, and E. C. Uberbacher) *CompMed94*, (Proceedings of the First World Congress on Computational Medicine, Public Health and Biotechnology), M. Witten, Ed. (in press).

M. D. Morris

Associate editor

- *Technometrics*

Editorial consultant statistician

- *Radiation Research*

Invited lectures

- "Design and Analysis for an Inverse Problem of Advective-Dispersive Fluid Flow," (with A. D. Solomon) University of Tennessee Statistics Department, Knoxville, TN, October 28, 1993.
- "A Stepwise Technique for Computer Experimentation: Experimental Design, Input Screening, and Predictive Modeling," ASA Meeting, Toronto, August 17, 1994.
- "A Case Study of Statistics Used in Environmental Remediation: Remediation of the X-231B Site," Spatial Sampling for the Environment, Chapel Hill, September 22, 1994.

- "Some Recent Developments in the Design and Analysis of Computer Experiments, and an Input Screening Example," National Institute of Standards and Technology, November 16, 1994.

Fellow

- American Statistical Association

N. M. Nachtigal

Award

- SIAM Activity Group on Linear Algebra Prize for most outstanding paper in applicable linear algebra published in 1991–1993.

Invited presentations

- "First Principles Simulations of Material Properties," (with W. A. Shelton and G. M. Stocks) Southeastern-Atlantic Section of SIAM Regional Meeting, Wake Forest University, Winston-Salem, NC, March 25–26, 1994.
- "A Look-Ahead Variant of TFQMR," (with R. W. Freund) Colorado Conference on Iterative Methods, Breckenridge, CO, April 5–9, 1994.
- "First Principles Simulations of Material Properties," (with W. A. Shelton and G. M. Stocks) Numerical Linear Algebra with Applications, Mathematical Research Institute at Oberwolfach, F.R. of Germany, April 9–16, 1994.
- "A Look-Ahead Variant of TFQMR," Eidgenossische Technische Hochschule, Zurich, Switzerland, April 19, 1994.
- "QMRPACK and Applications," (with R. W. Freund) Fifth SIAM Conference on Applied Linear Algebra, Snowbird, UT, June 15–18, 1994.
- "A New Krylov Subspace Method for Symmetric Indefinite Linear Systems," (with R. W. Freund) 14th IMACS World Congress, Atlanta, GA, July 11–15, 1994.
- "QMRPACK and Applications," (with R. W. Freund) 14th IMACS World Congress, Atlanta, GA, July 11–15, 1994.
- "QMR Methods in Computational Fluid Dynamics," International Workshop on Solution Techniques for Large-Scale CFD Problems, Montreal, Canada, September 26–28, 1994.

E. Ng

Member

- IMACS Technical Committee on Computational Linear Algebra.
- IMACS Technical Committee on Parallel and Super-Computing.
- Ph.D. Thesis Committee in the Computer Science Department at the University of Tennessee, Knoxville.

Invited lectures

- "Parallel Sparse Matrix Computations," Intevap Company, Mathematical and Statistics Department, Caracas, Venezuela, January 25, 1993.
- "Sparse Matrix Research at ORNL," (with B. W. Peyton) DOE/OSC (Office of Scientific Computing) Applied Mathematics Workshop, Albuquerque, NM, February 3–5, 1993.
- "Parallel Sparse Cholesky Factorization Algorithms for Shared-Memory Multiprocessor Systems," (with B. W. Peyton, E. Rothberg, and A. Gupta) Sixth SIAM Conference on Parallel Processing for Scientific Computing, Norfolk, VA, March 22–24, 1993.
- "An Efficient Algorithm to Compute Row and Column Counts for Sparse Cholesky Factorization," (with J. Gilbert and B. W. Peyton) IBM Thomas J. Watson Research Center, Yorktown Heights, NY, July 28–31, 1993.
- "Sparse Cholesky Factorization Algorithms," (with B. W. Peyton) Laboratoire National d'Hydraulique, Electricite de France, Paris, France, September 27, 1993.
- "Algorithms for the Direct Solution of Sparse Nonsymmetric Linear Systems," Laboratoire National d'Hydraulique, Electricite de France, Paris, France, September 28, 1993.
- "A Comparison of Some Direct Methods for Solving Sparse Nonsymmetric Linear Systems," International Workshop on Sparse Matrix Computations, St. Giron, France, July 11–15, 1994.
- "Direct Solution of Sparse Linear Systems: Algorithms, Codes, and Performance," University of Wisconsin, Madison, WI, October 31, 1994.

Invited papers

- "Separators and Structure Prediction for Nonsymmetric Matrix Factorizations," (with J. R. Gilbert) Pure and Applied Linear Algebra: The New Generation, The 3rd Conference of the International Linear Algebra Society, University of West Florida and the Pensacola Hilton Hotel, Pensacola, FL, March 17–20, 1993.
- "On the Solution of Stokes Pressure System Using Supernodal Cholesky Factorization," (with B. W. Peyton and B. Nitrosso) SIAM 18th Annual Southeastern-Atlantic Section Meeting, Winston-Salem, NC, March 25–26, 1994.
- "Separators and Structure Prediction in Sparse Orthogonal Factorization," with (J. R. Gilbert and B. W. Peyton) *Linear Algebra and Its Applications* (in press).
- "A Comparison of Some Direct Methods for Solving Sparse Nonsymmetric Linear Systems," SIAM Conference on Applied Linear Algebra, Minisymposium on Sparse Direct Methods, Snowbird, UT, June 15–18, 1994.

- "On the Solution of Stokes Pressure System Using Supernodal Cholesky Factorization," (with B. W. Peyton and B. Nitrosso) Computer Science Colloquium, Sandia National Laboratory, Albuquerque, NM, June 20, 1994.
- "Recent Developments in Parallel Method of Lines Solutions of Partial Differential Equations," (with W. F. Lawkins and S. Thompson) 14th IMACS World Congress on Computation and Applied Math, Georgia Institute of Technology, Atlanta, GA, July 11-15, 1994.
- "Linear Systems," (with B. W. Peyton) to appear in CRC Handbook of Discrete and Combinatorial Mathematics.

G. Ostrouchov

Associate editor

- *Journal of Statistical Computation and Simulation*
- *Technometrics*

Adjunct faculty

- Oak Ridge Science Semester

J. V. Pace, III

Member

- Working Group on the Reassessment of A-Bomb Dosimetry of the U.S. DOE.
- 1996 RPSD Topical Meeting Technical Program Committee.
- DOE Technical Review Group (TRG) for the Reactor Spent Fuels Cask Systems Development Program (CSDP).

Invited paper

- "Overview of the Nuclear Data Related to the Hiroshima Dosimetry Discrepancy," International Conference on Nuclear Data for Science and Technology, Gatlinburg, TN, May 9-13, 1994.

L. E. Parker

Invited paper

- "ALLIANCE: An Architecture for Fault Tolerant, Cooperative Control of Heterogeneous Mobile Robots," 1994 IEEE/RSJ/GI International Conference on Intelligent Robots and Systems (IROS '94), Munich, Germany, September 12-16, 1994.

Thesis

- "Heterogeneous Multi-Robot Cooperation," Massachusetts Institute of Technology Ph.D. Dissertation, January 1994.

Awards

- Elected full member of Sigma Xi, MIT Chapter.
- Elected Institute Fellow of the KISS Institute for Practical Robotics.

Referee

- *IEEE Control Systems*
- *Journal of Machine Learning*
- *IEEE Expert*
- *DOE SBIR Program*
- *IEEE Transactions on Robotics and Automation*

S. Petrov

Invited talks

- "Gene Recognition, Modeling, and Homology Search in the GRAIL-genQuest System," (with M. Shah, J. R. Einstein, S. Matis, Y. Xu, X. Guan, D. M. Buley, L. Hauser, R. J. Mural, and E. C. Uberbacher) DOE Contractor's Meeting, Santa Fe, NM, November 13-17, 1994.
- "Informatics Support for Mapping in Mouse-Human Homology Regions," (with M. Shah, L. Hauser, R. J. Mural, and E. C. Uberbacher) DOE Contractor's Meeting, Santa Fe, NM, November 13-17, 1994.

B. W. Peyton

Invited talks

- "Sparse Matrix Research at ORNL," (with E. Ng) DOE/OSC (Office of Scientific Computing) Applied Mathematics Workshop, Albuquerque, NM, February 3-5, 1993.
- "Partitioning a Chordal Graph into Transitive Subgraphs for Parallel Sparse Triangular Solution," (with A. Pothén and X. Yuan) Pure and Applied Linear Algebra Conference: The New Generation, Pensacola, FL, March 17-20, 1993.
- "Parallel Sparse Cholesky Factorization Algorithms for Shared-Memory Multiprocessor Systems," (with E. Rothberg, A. Gupta, and E. Ng) Sixth SIAM Conference on Parallel Processing for Scientific Computing, Norfolk, VA, March 22-24, 1993.
- "An Efficient Algorithm to Compute Row and Column Counts for Sparse Cholesky Factorization," (with E. G. Ng and J. Gilbert) IBM Thomas J. Watson Research Center, Yorktown Heights, NY, July 28-31, 1993.

Invited papers

- "Partitioning a Chordal Graph into Transitive Subgraphs for Parallel Sparse Triangular Solution," (with A. Pothén and X. Yuan) *Linear Algebra and Its Applications* (in press).

- “On the Solution of Stokes Pressure System Using Supernodal Cholesky Factorization,” (with E. G. Ng and B. Nitrosso) SIAM 18th Annual Southeastern-Atlantic Section Meeting, Winston-Salem, NC, March 25–26, 1994.
- “On the Solution of Stokes Pressure System Using Supernodal Cholesky Factorization,” (with E. G. Ng and B. Nitrosso) Computer Science Colloquium, Sandia National Laboratory, Albuquerque, NM, June 20, 1994.
- “Chordal-Graph Algorithms for Sparse Cholesky Factorization,” Seventh SIAM Conference on Discrete Mathematics, Albuquerque, NM, June 22–25, 1994.

R. T. Primm, III

Chairman

- Technical Program Chairman, 1994 Reactor Physics Topical Meeting.
- Vice Chairman, Local Section, American Nuclear Society, January 1993 to June 1993.
- Chairman, Local Section, American Nuclear Society, July 1993 to June 1994.
- Past Chairman, Local Section, American Nuclear Society, July 1994 to June 1995.

Referee

- *Nuclear Science and Technology*

Invited talk

- “Validation Calculations in Support of Transportation Analyses,” (with D. A. Tollefson) 1994 U.S. Department of Energy Defense Programs Packaging Workshop, Knoxville, TN, May 19, 1994.

V. A. Protopopescu

Member

- Editorial Board of the *CRC Mathematical Modelling Series*.
- Editorial Board of the Journal *Mathematical Models and Methods in Applied Sciences*.
- Editorial Board of the Journal *Transport Theory and Statistical Physics*.

Adjunct professor

- Mathematics Department, University of Tennessee, Knoxville, TN.

Reviewer

- *Mathematical Reviews*

Referee

- *Journal of Statistical Physics*
- *Transport Theory and Statistical Physics*
- *Mathematical Models and Methods in Applied Sciences*
- *Journal of Physics*
- *Numerical Methods in Partial Differential Equations*

Invited talks

- "Linear Chaos: A Mathematical Artifact?" Boston University, Boston, MA, February 15, 1993.
- "Chaos and Fractals: Potential Relevance for Medical Applications," Emory Medical School, Atlanta, GA, March 22, 1994.
- "Optimal Control for Cooperative-Competitive Systems," 879th Meeting of the American Mathematical Society, Knoxville, TN, March 26-27, 1993.
- "Chaos in Linear Systems: A Mathematical Artifact?" Virginia Polytechnic Institute, Blacksburg, VA, April 1, 1994.
- "Wave and Scattering Operators for General Transport Equations," 14th Annual Southeastern-Atlantic Regional Conference on Differential Equations, University of Tennessee, Knoxville, TN, October 21-22, 1994.

N. S. V. Rao**Member**

- Program Committee, Dedicated Conference on Supercomputer Applications in the Transportation Industries, Aachen, Germany, October 31 - November 4, 1994.

Academic

- Adjunct Assistant Professor, Department of Computer Science, University of Tennessee, Knoxville, TN.

Invited talk

- "Fusion-Rule Estimation in Multiple Sensor Systems Using Learning," Dagstuhl, Germany, October 24-28, 1994.

Invited papers

- "Hybrid Pattern Recognition System Capable of Self-Modification," (with C. W. Glover and E. M. Oblov) 2nd International Conference on Information and Knowledge Management, Washington, DC, May 1-5, 1993.
- "Fusion Rule Estimation in Multiple Sensor Systems with Unknown Noise Distributions," Indo-U.S. Workshop on Distributed and Parallel Signal and Image Integration, Pune, India, December 16-18, 1993.

- "On Fast Planning of Sub-Optimal Paths Amidst Polygonal Obstacles in Plane," *Theoretical Computer Science* (in press).

D. B. Reister

Patent

- Patent application filed by D. B. Reister and M. A. Unseren, "Method for Controlling a Vehicle with Two or Four Independently Steered Wheels," amended August 1994.

K. A. Remington

Travel Award

- Computing Research Association to attend the Grace Hopper Conference on Women in Computing in June 1994.

W. A. Rhoades

Invited paper

- "An Explanation of the Hiroshima Activation Dilemma," (with J. M. Barnes and R. T. Santoro) Vol. 1, pp. 238-244 in Proc. of American Nuclear Society, Eighth International Conference on Radiation Shielding, Arlington, TX, April 24-28, 1994.

R. W. Roussin

Member

- 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.
- Executive Committee, CSEWG.
- Methods and Experiments Subcommittee, Department of Energy, DNFSB Recommendation 93-2 Response Team.

International liaison

- 8th International Conference on Radiation Shielding, Arlington, TX.

Chairman

- Cross Section Evaluation Working Group (CSEWG).
- Methods and Formats Committee, CSEWG.
- Photon Interaction Evaluation Subcommittee, CSEWG.
- Subgroup B, Cross Section Processing, NEANSC Working Party on International Evaluation Cooperation.

Executive committee

- American Nuclear Society (ANS) Radiation Protection and Shielding Division (RPSD).

Referee

- *Nuclear Science and Engineering*
- *Nuclear Technology/Fusion*
- *Trans. of Symposia on Space Nuclear Power Systems*

Award

- American Nuclear Society Fellow

T. H. Rowan**Collaborating scientist**

- Computer Science Department at the University of Tennessee.

Member

- HPCC Software Exchange Technical Working Group.
- SLATEC Common Mathematical Library Committee (ORNL site representative).
- Society for Industrial and Applied Mathematics.
- Association for Computing Machinery.

Reviewer

- Department of Energy - Advanced Software Development.
- ACM Transactions on Mathematical Software.

R. T. Santoro**Special assignment**

- ITER Joint Work Site, Max-Planck-Institute fur Plasmaphysik, Garching, Germany, October 1993-October 1998.

Referee

- *Fusion Technology*
- *Nuclear Science and Engineering*
- *Nuclear Technology/Fusion*

Invited talks

- "The MASH 1.0 Code System: Utilization of MORSE in the Adjoint Mode," (with J. O. Johnson) Organization for Economic Cooperation and Development (OECD) Nuclear Energy Agency (NEA), Seminar on Advanced Monte Carlo Computer Programs for Radiation Transport, Centre d'Etudes, Saclay, France, April 27-29, 1993.

- "Application of the Adjoint Monte Carlo Shielding Code System – MASH – in Nuclear Operations," (with J. O. Johnson and M. S. Smith) 61st Military Operations Research Society Symposium, Wright Patterson Air Force Base Dayton, OH, June 22–24, 1993.
- "Shielding Analysis for the ITER Divertor and Vacuum Pumping Ducts," (with M. Sawan and Y. Gohar) Third International Symposium on Fusion Technology, UCLA Conference Center, Los Angeles, CA, June 27–July 1, 1994.
- "ITER Shielding Analysis," (with Y. Gohar, G. Shatalov, and R. R. Parker) Third International Symposium on Fusion Technology, UCLA Conference Center, Los Angeles, CA, June 27–July 1, 1994.
- "ITER Nuclear Engineering: Blanket and Shield Design, and R&D Program," (with Y. Gohar, A. Antipenkov, A. Cardella, G. Kalinin, K. Mohri, R. Raffrey, R. Parker, and P. H. Rebut) Fifteenth International Conference on Plasma Physics and Controlled Nuclear Fusion, Seville, Spain, September 26–October 1, 1994.
- "ITER Vacuum Vessel, Blanket and Shield," (with R. R. Parker, A. Antipenkov, A. Cardella, T. Iizuka, W. Gauster, Y. Gohar, K. Ioki, G. Johnson, G. Kalinin, K. Mohri, R. Raffray, P.-H. Rebut, K. Shimizu, and D. Williamson) Fifteenth International Conference on Plasma Physics and Controlled Nuclear Fusion, Seville, Spain, September 26–October 1, 1994.

Invited papers

- "The MASH Code System, Version 1.0," (with J. O. Johnson and T. J. Burns) *Human Survivability* 1(2), 5–10 (1993).
- "An Explanation of the Hiroshima Activation Dilemma," (with W. A. Rhoades and J. M. Barnes) Vol. 1, pp. 238–244 in Proc. of American Nuclear Society, Eighth International Conference on Radiation Shielding, Arlington, TX, April 24–28, 1994.

B. D. Semeraro

Invited paper

- "QMR Methods for Solution of the Euler Equations," (with N. Nachtigal) International Workshop on Solution Techniques for Large-Scale CFD Problems, September 1994.

M. Shah

Invited talks

- "Integrated Gene Recognition, Modeling and Database Comparison in the GRAIL and GenQuest Environments," (with R. J. Mural, D. M. Buley, J. R. Einstein, X. Guan, S. Matis, Y. Xu, and E. C. Uberbacher) Open Problems in Computational Molecular Biology, Telluride, CO, July 11–17, 1994.
- "Detection of Control Regions in the Human Genome Using Intelligent Systems," (with S. Matis, Y. Xu, D. M. Buley, X. Guan,

- J. R. Einstein, R. J. Mural, and E. C. Uberbacher) Open Problems in Computational Molecular Biology, Telluride, CO, July 11-17, 1994.
- "An Improved System for Exon Recognition and Gene Modeling in Human DNA Sequences," (with Y. Xu, J. R. Einstein, R. J. Mural, and E. C. Uberbacher) The Second International Conference on Intelligent Systems for Molecular Biology, Stanford University, San Francisco, CA, August 14-17, 1994.
 - "Integrated Gene Recognition, Modeling and Database Searching in the GRAIL and genQuest Environments," (with R. J. Mural, J. R. Einstein, X. Guan, S. Matis, Y. Xu, and E. C. Uberbacher) International Conference on the Human Genome Project, Washington, DC, October 2-5, 1994.
 - "Gene Recognition, Modeling, and Homology Search in the GRAIL-genQuest System," (with J. R. Einstein, S. Matis, Y. Xu, X. Guan, D. M. Buley, S. Petrov, L. Hauser, R. J. Mural, and E. C. Uberbacher) DOE Contractor's Meeting, Santa Fe, NM, November 13-17, 1994.
 - "Informatics Support for Mapping in Mouse-Human Homology Regions," (with S. Petrov, L. Hauser, R. J. Mural, and E. C. Uberbacher) DOE Contractor's Meeting, Santa Fe, NM, November 13-17, 1994.

Invited papers

- "Recognizing Exons in Genomic Sequence Using GRAIL II," (with Y. Xu, R. J. Mural, and E. C. Uberbacher) *Genetic Engineering, Principles and Methods* 16, 241 (1994).
- "An Improved System for Exon Recognition and Gene Modeling in Human DNA Sequences," (with Y. Xu, J. R. Einstein, R. J. Mural, and M. Shah) pp. 373-384 in Proc. of The Second International Conference on Intelligent Systems for Molecular Biology, Stanford University, San Francisco, CA, August 14-17, 1994.
- "Integrated Gene Recognition, Modeling and Database Comparison in the GRAIL and GenQuest Environments," (with R. J. Mural, D. M. Buley, J. R. Einstein, X. Guan, S. Matis, Y. Xu, and E. C. Uberbacher) *Computers in Chemistry* (in press).
- "Detection of Control Regions in Human DNA Sequence Using Intelligent Systems," (with S. Matis, Y. Xu, D. Buley, X. Guan, J. R. Einstein, R. J. Mural, and E. C. Uberbacher) *Computers & Chemistry* (in press).
- "Detection of Human RNA Polymerase II Promoters Using Artificially Intelligent Methods," (with S. Matis, R. J. Mural, and E. C. Uberbacher) *CompMed94*, (Proceedings of the First World Congress on Computational Medicine, Public Health and Biotechnology), M. Witten, Ed. (in press).

P. F. Spelt

Invited papers

- "Robotics and Artificial Intelligence for Hazardous Environments," XVII Congreso de Investigación Científica Universidad, Interamericana de Puerto Rico, San Juan, Puerto Rico, February 11-12, 1993.
- "Task Automation in a Successful Industrial Telerobot," AIAA/NASA (American Institute of Aeronautics and Astronauts/National Aerospace and Space Administration) Conference on Intelligent Robots in Field, Factory, Service and Space (CIRFFSS '94), Houston, TX, March 21-24, 1994.
- "A Wall-Crawling Robot for Reactor Vessel Inspection in Advanced Reactors," (with C. Crane, L. Feng, M. Abidi, and S. Tosunoglu) AIR '94, Application of Artificial Intelligence and Robotics to Nuclear Plants, Tokai-mura, Naka-gun, Ibaraki, Japan, May 29-June 2, 1994.
- "Design of the Reactor Vessel Inspection Robot for the Advanced Liquid Metal Reactor," (with C. Crane, L. Feng, M. Abidi, and S. Tosunoglu) ISRAM '94 (International Symposium on Robotics and Manufacturing), Wailea, Maui, August 15-17, 1994.
- "Operator Role Definition: An Initial Step in the Human Factors Engineering Design of the Advanced Neutron Source (ANS)," (with H. E. Knee, M. M. Houser, and W. E. Hill) Human Factors and Ergonomics Society Annual Meeting, Nashville, TN, October 23-28, 1994.

R. R. Spencer

Chairman

- EPMD Safety Committee.

E. C. Uberbacher

Conference program committees

- The First International Symposium on Pattern-Matching in Molecular Biology, Seattle, June 11-13, 1994.
- The Second International Conference on Intelligent Systems for Molecular Biology, Stanford University, San Francisco, CA, August 14-17, 1994.

Invited talks

- "Detection of Pre- and Post-Transcriptional Control Sequences in DNA Using Computational Methods," (with S. Matis and R. J. Mural) The Fourth Keck Symposium on Computational Biology, Pittsburgh, PA, October 24-November 5, 1993.
- "Neural Network Systems for Exon and Intron Recognition," The Human Genome Project - Commercial Implications, San Francisco, February 28-March 2, 1994.

- "Annotation of Genomic DNA Sequence Using the GRAIL Neural Network System," Modulation of Signal Transduction and Gene Expression, Bethesda, MD, April 25-27, 1994.
- "Integrated Gene Recognition, Modeling and Database Comparison in the GRAIL and GenQuest Environments," (with R. J. Mural, D. M. Buley, J. R. Einstein, X. Guan, S. Matis, M. Shah, and Y. Xu) Open Problems in Computational Molecular Biology, Telluride, CO, July 11-17, 1994.
- "Detection of Control Regions in the Human Genome Using Intelligent Systems," (with S. Matis, Y. Xu, M. Shah, D. M. Buley, X. Guan, J. R. Einstein, and R. J. Mural) Open Problems in Computational Molecular Biology, Telluride, CO, July 11-17, 1994.
- "An Improved System for Exon Recognition and Gene Modeling in Human DNA Sequences," (with Y. Xu, J. R. Einstein, R. J. Mural, and M. Shah) The Second International Conference on Intelligent Systems for Molecular Biology, Stanford University, San Francisco, CA, August 14-17, 1994.
- "Integrated Gene Recognition, Modeling and Database Searching in the GRAIL and genQuest Environments," (with R. J. Mural, J. R. Einstein, X. Guan, M. Shah, S. Matis, and Y. Xu) International Conference on the Human Genome Project, Washington, DC, October 2-5, 1994.
- "Gene Recognition, Modeling, and Homology Search in the GRAIL-genQuest System," (with M. Shah, J. R. Einstein, S. Matis, Y. Xu, X. Guan, D. M. Buley, S. Petrov, L. Hauser, and R. J. Mural) DOE Contractor's Meeting, Santa Fe, NM, November 13-17, 1994.
- "Informatics Support for Mapping in Mouse-Human Homology Regions," (with S. Petrov, M. Shah, L. Hauser, and R. J. Mural) DOE Contractor's Meeting, Santa Fe, NM, November 13-17, 1994.

Invited papers

- "Recognizing Exons in Genomic Sequence Using GRAIL II," (with Y. Xu, R. J. Mural, and M. Shah) *Genetic Engineering, Principles and Methods* 16, 241 (1994).
- "An Improved System for Exon Recognition and Gene Modeling in Human DNA Sequences," (with Y. Xu, J. R. Einstein, R. J. Mural, and M. Shah) pp. 373-384 in Proc. of The Second International Conference on Intelligent Systems for Molecular Biology, Stanford University, San Francisco, CA, August 14-17, 1994.
- "ORNL Announces genQuest and X-GRAIL," *Human Genome News* 5(5), 8 (1994).
- "Integrated Gene Recognition, Modeling and Database Comparison in the GRAIL and GenQuest Environments," (with R. J. Mural, D. M. Buley, J. R. Einstein, X. Guan, S. Matis, M. Shah, and Y. Xu) *Computers in Chemistry* (in press).
- "Detection of Control Regions in Human DNA Sequence Using Intelligent Systems," (with S. Matis, Y. Xu, M. Shah, D. Buley,

X. Guan, J. R. Einstein, and R. J. Mural) *Computers & Chemistry* (in press).

- "Detection of Human RNA Polymerase II Promoters Using Artificially Intelligent Methods," (with S. Matis, M. B. Shah, and R. J. Mural) *CompMed94*, (Proceedings of the First World Congress on Computational Medicine, Public Health and Biotechnology), M. Witten, Ed. (in press).

Patent

- "Resolving Sequencing by Hybridization Reconstruction Branchpoints Using Intentionally Generated DNA Polymorphism," (pending).

M. A. Unseren

Chair

- Special Invited Session on Multiple Manipulators at the Fifth International Symposium on Robotics and Manufacturing (ISRAM '94), Maui, HI, August 15, 1994.

Invited papers

- "Experimental Investigations of Sensor-Based Surface Following Tasks by a Mobile Manipulator," (with D. B. Reister, J. E. Baker, and F. G. Pin) International Symposium on Experimental Robotics, Kyoto, Japan, October 27-29, 1993.
- "A New Technique for Dynamic Load Distribution When Two Manipulators Mutually Lift a Rigid Object - Part 1: The Proposed Technique," Proc. Vol. 2, pp. 359-365 in Proc. of Intelligent Automation and Soft Computing, Trends in Research, Development, and Applications, Maui, HI, August 14-17, 1994.
- "A New Technique for Dynamic Load Distribution When Two Manipulators Mutually Lift a Rigid Object - Part 2: Derivation of Entire System Model and Control Architecture," Proc. Vol. 2, pp. 367-372 in Proc. of Intelligent Automation and Soft Computing, Trends in Research, Development, and Applications, Maui, HI, August 14-17, 1994.

Patent

- Patent application filed by D. B. Reister and M. A. Unseren, "Method for Controlling a Vehicle with Two or Four Independently Steered Wheels," amended August 1994.

D. W. Walker

Member

- ORNL CRADA Review Committee.
- Editorial Board of *Concurrency: Practice and Experience*

Chairman

- 1994 Scalable High Performance Computing Conference Program Committee.
- Parkbench Compact Applications Subcommittee.

Guest Editor

- Special Issue on Message Passing of Parallel Computing.

Board member

- ACM Signum

Invited talks

- "MPI: A Standard Message Passing Interface for Distributed Memory Concurrent Computers," (with G. A. Geist) ICASE/LARC Short Course on Parallel Computation, Hampton, VA, July 26-30, 1993.
- "Message Passing Interface: The New Parallel Programming Standard?" SHARE81 Summer 1993 Meeting, Washington, DC, August 18, 1993.
- "MPI: A Standard Message Passing Interface for Distributed Memory Environments," Intel Supercomputer User's Group Meeting, St. Louis, MO, October 4, 1993.
- "Issues in the Design of Scalable Software Libraries for Distributed Memory Concurrent Computers," (with J. Choi and J. J. Dongarra) Workshop on Environments and Tools for Parallel Scientific Computing, Walland, TN, May 26-27, 1994.
- "The Design of a Parallel, Dense Linear Algebra Software Library: Reduction to Hessenberg, Tridiagonal, and Bidiagonal Form," (with J. Choi and J. J. Dongarra) Workshop on Environments and Tools for Parallel Scientific Computing, Walland, TN, May 26-27, 1994.
- "Using the Advanced Features of MPI," Department of Computer Science, Rice University, Houston, TX, August 1, 1994.

Invited papers

- "CRPC Research into Linear Algebra Software for High Performance Computers," (with J. Choi, J. J. Dongarra, R. Pozo, and D. Sorensen) *International Journal of Supercomputer Applications* 8(2), 99 (1994).
- "The Design of a Parallel, Dense Linear Algebra Software Library: Reduction to Hessenberg, Tridiagonal, and Bidiagonal Form," (with J. Choi and J. J. Dongarra) pp. 1180-1182 in Proc. of the Fourteenth IMACS World Congress on Computation and Applied Mathematics, Atlanta, GA, July 11-15, 1994.
- "Parallel Matrix Transpose Algorithms on Distributed Memory Concurrent Computers," (with J. Choi and J. J. Dongarra) pp. 245-252 in Proc. of the 1992 Scalable Parallel Libraries

Conference, IEEE Computer Society Press, Starkville, MS, October 6-8, 1993.

- "The Design of a Standard Message Passing Interface for Distributed Memory Concurrent Computers," *Parallel Computing* 20(4), 657 (1994).
- "Scalability Issues Affecting the Design of a Dense Linear Algebra Library," (with J. J. Dongarra and R. A. van de Geijn) *Journal of Parallel and Distributed Computing* 22(3), 523 (1994).
- "Paradigms and Strategies for Scientific Computing on Distributed Memory Concurrent Computers," (with I. T. Foster) pp. 252-257 in Proc. of the High Performance Computing 1994, Society for Computer Simulation, San Diego, CA, April 10-15, 1994.
- "The Design of Scalable Software Libraries for Distributed Memory Concurrent Computers," (with J. Choi and J. J. Dongarra) pp. 792-799 in Proc. of the Eighth International Parallel Processing Symposium, IEEE Computer Society Press, Cancun, Mexico, April 26-29, 1994.
- "An Object Oriented Design for High Performance Linear Algebra on Distributed Memory Architectures," (with J. J. Dongarra and R. Pozo) Proc. of the Object Oriented Numerics Conference, 1993.
- "LAPACK for Distributed Memory Architectures: the Next Generation," (with J. Demmel, J. J. Dongarra, and R. A. van de Geijn) pp. 323-329 in Proc. of the Sixth SIAM Conference on Parallel Processing for Scientific Computing, SIAM Press, Norfolk, VA, March 22-24, 1993.
- "LAPACK++: A Design Overview of Object-Oriented Extensions for High Performance Linear Algebra," (with J. J. Dongarra and R. Pozo) pp. 162-171 in Proc. of Supercomputing '93, IEEE Computer Society Press, Portland, OR, November 15-19, 1993.
- "PB-BLAS: A Set of Parallel Block Basic Linear Algebra Subprograms," (with J. Choi and J. J. Dongarra) pp. 534-541 in Proc. of the 1994 Scalable High Performance Computing Conference, IEEE Computer Society Press, Knoxville, TN, May 23-25, 1994.

R. C. Ward

Member

- College of Engineering Advisory Council, North Carolina State University, 1991-93.
- Advisory Committee, Second International Conference on Computational Physics, Beijing, China, 1993.
- Program Committee, Supercomputing '93, Portland, OR, November 15-19, 1993.
- General Purpose Equipment Committee, ORNL, FY 1994.
- Tutorials Committee, Supercomputing '94, Washington, DC, November 14-18, 1994.

- Technical Achievement Committee, Martin Marietta Awards, 1994.
- Tutorials Committee, Supercomputing '95, San Diego, CA, December 4–8, 1995.

Fellow

- American Association for Advancement of Science.

J. E. White

Member

- American Nuclear Society 6.2 and 19.1 Standards Committees.

Reviewer

- *Nuclear Technology Journal*

L. R. Williams

Invited talks

- “FIDO Input Instructions,” MASH (Monte Carlo Adjoint Shielding) Seminar/Workshop, Pollard Auditorium, Oak Ridge, TN, November 16–18, 1993.
- “GIP Input Instructions,” MASH (Monte Carlo Adjoint Shielding) Seminar/Workshop, Pollard Auditorium, Oak Ridge, TN, November 16–18, 1993.

T. Wright

Research Fellow

- U.S. Bureau of the Census (sponsored by American Statistical Association, National Science Foundation, and the U.S. Bureau of the Census).

Member

- Sampling and Estimation Design Committee for 1995 Census Test, U.S. Bureau of the Census.
- Steering Committee, Tennessee Mathematics Coalition.
- Steering Committee, Tennessee Systemic Initiative, Tennessee Board of Education.

Invited discussant

- 1993 Research Conference on Undercounted Ethnic Populations, U.S. Bureau of the Census.
- 1994 Technical Session, “Fundamental Change: The 1995 Census Design Test,” Joint Statistical Meetings, Toronto, August, 1994.

Editorial board

- *The American Journal of Mathematical and Management Sciences.*

Board of directors and treasurer

- Tennessee Mathematics and Computer Sciences Foundation, Inc.

Associate professor

- (Mathematics) Knoxville College, Knoxville, TN.
- (Statistics/Mathematics) University of Tennessee, Knoxville, TN.

Reviewer

- *Mathematical Reviews*

Referee

- *Journal of the American Statistical Association*
- *The American Statistician*
- *Survey Methodology* (2)
- *Metrika*

B. A. Worley**Member**

- Executive Committee of Reactor Physics Division of the American Nuclear Society.

Invited paper

- "Validation of Multigroup Cross Sections for the Advanced Neutron Source Against the FOEHN Critical Experimental Measurements," (with L. A. Smith, J. C. Gehin, and J. P. Renier) pp. 444-452, Vol. III in Proc. of the American Nuclear Society 1994 Topical Meeting on Advances in Reactor Physics, Knoxville, TN, April 11-15, 1994.

U.S. Representative

- IAEA Coordinated Research Program on Validation of Safety Related Physics Calculations for Gas Cool Reactors.

Y. Xu**Invited talks**

- "Integrated Gene Recognition, Modeling, and Data Base Searching in the GRail and GenQuest Environments," (with R. J. Mural, D. M. Buley, J. R. Einstein, X. Guan, M. Shah, S. Matis, and E. C. Uberbacher) Open Problems in Computational Molecular Biology, Telluride, CO, July 11-17, 1994.
- "Detection of Control Regions in the Human Genome Using Intelligent Systems," (with S. Matis, M. Shah, D. Buley, X. Guan,

- J. R. Einstein, R. J. Mural, and E. C. Uberbacher) Open Problems in Computational Molecular Biology, Telluride, CO, July 11–17, 1994.
- “An Improved System for Exon Recognition and Gene Modeling in Human DNA Sequences,” (with J. R. Einstein, R. J. Mural, M. Shah, and E. C. Uberbacher) The Second International Conference on Intelligent Systems for Molecular Biology, Stanford, CA, August 14–17, 1994.
 - “Gene Recognition, Modeling, and Homology Search in the GRAIL-genQuest System,” (with M. Shah, J. R. Einstein, S. Matis, X. Guan, D. Buley, S. Petrov, L. Hauser, R. J. Mural, and E. C. Uberbacher) DOE Contractor’s Meeting, Santa Fe, NM, November 13–17, 1994.
 - “Dynamic Subtrees: A New Data Structure for Manipulating Trees,” The 6th International Conference on Computing and Information, Peterborough, Ontario, Canada, May 25–28, 1994.
 - “Integrated Gene Recognition, Modeling and Database Searching in the GRAIL and genQuest Environments,” (with R. J. Mural, J. R. Einstein, X. Guan, M. Shah, S. Matis, and E. C. Uberbacher) International Conference on the Human Genome Project, Washington, DC, October 2–5, 1994.
 - “Gene Recognition, Modeling, and Homology Search in the GRAIL-genQuest System,” (with M. Shah, J. R. Einstein, S. Matis, X. Guan, D. M. Buley, S. Petrov, L. Hauser, R. J. Mural, and E. C. Uberbacher) DOE Contractor’s Meeting, Santa Fe, NM, November 13–17, 1994.

Invited papers

- “An Improved System for Exon Recognition and Gene Modeling in Human DNA Sequences,” (with J. R. Einstein, R. J. Mural, M. Shah, and E. C. Uberbacher) pp. 376–384 in Proc. of the Second International Conference on Intelligent Systems for Molecular Biology, AAAI Press (1994).
- “Recognizing Exons in Genomic Sequence Using GRAIL II,” (with R. J. Mural, M. Shah, and E. C. Uberbacher) *Genetic Engineering, Principles and Methods* 16, 241 (1994).
- “Detection of Control Regions in Human DNA Sequence Using Intelligent Systems,” (with S. Matis, M. Shah, D. Buley, X. Guan, J. R. Einstein, R. J. Mural, and E. C. Uberbacher) *Computers and Chemistry* (in press).
- “An Improved System for Exon Recognition and Gene Modeling in Human DNA Sequences,” (with J. R. Einstein, R. J. Mural, M. Shah, and E. C. Uberbacher) pp. 373–384 in Proc. of The Second International Conference on Intelligent Systems for Molecular Biology, Stanford University, San Francisco, CA, August 14–17, 1994.
- “Integrated Gene Recognition, Modeling and Database Comparison in the GRAIL and GenQuest Environments,” (with R. J. Mural, D. M. Buley, J. R. Einstein, X. Guan, S. Matis, M. Shah, and E. C. Uberbacher) *Computers in Chemistry* (in press).

CONFERENCES

1993**"Training Course for SCALE Users," July 19-23, 1993, Oak Ridge, TN**

Organizers: R. W. Roussin, C. V. Parks, S. O. Bowman, and L. M. Petrie

Attendees: 64

Sponsors: U.S. Department of Energy

"MASH Workshop," November 16-18, 1993, Oak Ridge, TN

Organizers: J. O. Johnson and S. P. Shriner

Attendees: 45

Sponsors: Defense Nuclear Agency

1994**"American Nuclear Society Topical Meeting on Advances in Reactor Physics," April 11-15, 1994, Knoxville, TN**

Organizers: R. T. Primm and B. A. Worley

Attendees: 250

Sponsors: American Nuclear Society (ANS), Oak Ridge/Knoxville Section, ANS Reactor Physics Division, and ANS Mathematics and Computation Division

"NEANSC Accelerator Specialists Meeting, April 28-29, 1994, Arlington, TX

Organizers: R. W. Roussin, E. Sartori, and S. Tanaka

Attendees: 25

Sponsors: Organization for Economic Cooperation and Development, Nuclear Energy Agency

"Nuclear Energy Agency Nuclear Science Committee Working Party on International Evaluation Cooperation, May 4-6, 1994, Oak Ridge, TN

Organizers: R. W. Roussin, D. C. Larson, and C. Nordborg

Attendees: 30

Sponsors: ORNL, Radiation Shielding Information Center, Organization for Economic Cooperation and Development, Nuclear Energy Agency

"1994 Scalable High Performance Computing Conference," May 22-25, 1994, Knoxville, TN

Organizers: J. J. Dongarra and D. W. Walker

Attendees: 320

Sponsors: IEEE Computer Society, EPMD, UT Computer Science Department

"Cross Section Evaluation Working Group, October 25-27, 1994, Oak Ridge, TN

Organizers: R. W. Roussin and M. Bhat

Attendees: 50

Sponsors: ORNL, Radiation Shielding Information Center

SEMINARS AT ORNL

Y. Y. Azmy was the seminar coordinator during the period covered by this report. The following seminars were held during January 1993 through December 1994.

- C. A. Alund, ITM – Swedish Institute of Applied Mathematics, "PVM 3.2 Versions of the NAS Parallel Benchmarks Kernels," October 28, 1993
- R. C. Arkin, Associate Professor, College of Computing, Georgia Institute of Technology, "Cooperation and Communication in Multi-Agent Reactive Robotic Systems," August 4, 1993
- S. B. Baden, University of Wisconsin, "Digital Alchemy: From Atoms to Abstractions," November 3, 1994
- C. F. Baillie, Physics Department, University of Colorado at Boulder, "Porting a Well-Posed Topographical Meteorological Model to the KSR Parallel Supercomputer," May 21, 1993
- J. E. Baker, Engineering Physics and Mathematics Division, "Image Accuracy and Representational Enhancement Through Low-Level, Multi-Sensor Integration Techniques," February 10, 1993
- A. L. Bangs, Engineering Physics and Mathematics Division, "Cooperating Robots: Where They've Been, Where We're Going," January 8, 1993
- J. Barhen, Jet Propulsion Laboratory and California Institute of Technology, Pasadena, CA, "New Directions in Neurocomputing," March 11, 1994
- J. J. Beauchamp, Engineering Physics and Mathematics Division, "Statistics: An Aid to Better Understanding," July 13, 1993
- E. Biham, The Technion, Haifa, Israel, "Differential Cryptanalysis: Survey and Latest Results," August 18, 1993
- J. Brehm, University of Hannover, Germany, "Multiprocessor Benchmarking Using Parameterized Workloads," April 27, 1993
- J. E. Brehm, University of Hannover, Germany, "Benchmarking Massively Parallel Systems Using Parameterized Workloads," October 27, 1994
- H. I. Christensen, Aalborg University, Denmark, "Recent Accomplishments in Robotic Manipulation and Navigation," December 8, 1994
- E. D'Azevedo and C. Romine, Engineering Physics and Mathematics Division, "Shared Memory Library Simplifies Programming for PVM Paragon," November 9, 1994
- T. DeSchepper, Talarian, Atlanta, "RT Works: Network Communications and Graphical Displays for Real-Time Computing," May 10, 1993

- F. C. Difilippo, Engineering Physics and Mathematics Division, "Nuclear Power Sources for Space Propulsion," March 17, 1993
- T. Dunigan, Engineering Physics and Mathematics Division, "UNIX Workstation Users Group Meeting," February 4, 1994
- M. Engelhardt, Idaho National Engineering Laboratory, Idaho Falls, ID, "Analysis of a Power-Law Process with Missing Data," March 3, 1993
- B. Enk, Applied Parallel Research, Bethesda, MD, "FORGE 90 Parallelization Tools Applied Parallel Research," April 21, 1993
- V. V. Fedorov, Carlson School of Management, University of Minnesota, "Experimental Design for Local Regression," March 21, 1994
- P. A. Forsyth, University of Waterloo, "Three Dimensional Modeling Studies of Air Sparging and Steam Injection for Remediation of DNAPL Contaminated Sites," October 22, 1993
- J. I. Frankel, The University of Tennessee, Knoxville, "Cumulative Variable Formulation for Transient Radiative Transport," January 27, 1994
- R. W. Freund, AT&T Bell Laboratories, Murray Hill, NJ, "Efficient Linear Circuit Analysis by Pade Approximation via the Landzos Process," May 18, 1994
- G. A. Geist, Engineering Physics and Mathematics Division, "Network Computing with PVM," April 16, 1993
- G. A. Geist, Engineering Physics and Mathematics Division, "Network Computing with PVM," July 30, 1993
- G. A. Geist, Engineering Physics and Mathematics Division, and G. W. Howell, Department of Applied Mathematics, Florida Institute of Technology, Melbourne, FL, "Computing Eigenvalues of 'Skinny' Hessenberg Matrices," August 17, 1994
- J. H. Goldberg, Associate Professor, Penn State University, University Park, PA, "Understanding User Intent at the Computer Interface: Discrimination of Zoom Condition Solely from Eye Gaze," April 22, 1993
- G. H. Golub, Computer Science Department, Stanford University, Stanford, CA, "Orthogonal Polynomials and Least Squares," October 22, 1993
- W. C. Grimmell, Director, Engineering Innovation, Warner Lambert Company, Morris Plains, NJ, "Vision Systems Inspection of a Pharmaceutical Product," September 16, 1993
- D. Hitlin, Professor of Physics, California Institute of Technology, Pasadena, CA, "Measuring CP-Violating Asymmetries at PEP-11 at SLAC," January 26, 1994

- C. J. Jacobus, Cybernet Systems Corporation, Ann Arbor, MI, "A 3-D Mapping and Inspection System for Inside-Tank Robotics Applications," March 1, 1993
- D. E. Keyes, Department of Mechanical Engineering, Yale University, New Haven, CT, "Domain Decomposition: A Bridge Between Nature and Parallel Computers," March 18, 1993
- C. Laugier, Director of the Robotics Group at LIFIA/INRIA Rhône-Alpes, Grenoble Cedex, France, "Autonomous Robots in Non-Manufacturing Applications," May 6, 1993
- R. D. Lawrence, IBM Research Division, Yorktown Heights, NY, "Scalable Parallel Processing," March 19, 1993
- M. B. Leahy, Jr., San Antonio Air Logistics Center, Kelly Air Force Base, TX, "Unified Telerobotic Architecture Project Program Overview," February 24, 1994
- T. C. Leuth, University of Karlsruhe, Karlsruhe, Germany, "Institute for Real-Time Computer Systems, and Robotics," December 2, 1993
- A. Liegmann, Integrated Systems Laboratory, Zurich, Switzerland, "Supernodal Techniques in Semiconductor Device Simulation," February 23, 1993
- P. C. Liewer, California, Institute of Technology, Pasadena, CA, "Particle-in-Cell Algorithms for 3D PIC Codes on MIMD Parallel Computers," July 8, 1993
- A. M. Linkov, Institute of Problems of Mechanical Engineering, Russian Academy of Science, "Real and Complex Hypersingular Integrals and Integral Equations in Computational Mechanics," May 6, 1994
- Y. Lirov, Salomon Brothers, Rutherford, NJ, "Embedded Artificial Intelligence for Distributed Systems Management," August 26, 1993
- B. P. Miller, Computer Science Department, University of Wisconsin, Madison, WI, "Paradyn Parallel Performance Tool Project," October 29, 1993
- I. Muchnik, University of Boston, Boston, MA, "Quasi-Convex Clustering Models," May 13, 1993
- T. Newman, Research Assistant, Department of Computer Science, Michigan State University, East Lansing, MI, "Experiments in 3D CAD-Based Inspection Using Range Images," August 10, 1993
- D. W. Nigg, Manager of Reactor and Radiation Physics, Idaho National Engineering Laboratory, "Boron Neutron Capture Therapy," April 13, 1994
- C. A. Papadopoulos, University of California, Santa Barbara, CA, "Domain Decomposition and Splitting Techniques for Free Boundary Problems," January 22, 1993

- P. M. Papadopoulos, University of California, Santa Barbara, CA, "Large-Scale and Ill-Conditioned Matrix Equations in Control," January 21, 1993
- L. E. Parker, Engineering Physics and Mathematics Division, "Heterogeneous Multi-Robot Cooperation," March 16, 1994
- L. Petzold, Department of Computer Science, University of Minnesota, Minneapolis, MN, September 15, 1994
- F. G. Pin, Engineering Physics and Mathematics Division, "Approximate Reasoning on VLSI Chips for Autonomous Robots," March 1, 1993
- D. Prawel, Spatial Technology, Boulder, CO, "Using the ACIS 3D Tool Kit to Develop Software for Visualization, Simulation, and User Interfaces," May 26, 1994 and June 15, 1994
- H. K. Qammar, University of Akron, Akron, OH, "Chaotic Time Series Prediction: Neural Networks vs Fuzzy Logic," January 5, 1993
- D. I. Radin, Department of Psychology, University of Edinburgh, "Human Factors Issues in Personalized Information Retrieval Systems," October 6, 1993
- K. Rahmani, Engineering Physics and Mathematics Division, "Directions Toward Global Path Planning for Combined Mobility and Manipulation," January 13, 1993
- M. L. Realff, Assistant Professor, School of Textile & Fiber Engineering, Georgia Institute of Technology, Atlanta, GA, "From Fiber to Yarn to Fabric: A Micromechanical Approach to Fabric Modeling," January 7, 1993
- L. A. Reibling, Smiths Industries Aerospace & Defense Systems, Inc., Grand Rapids, MI, "A Massively Parallel Architecture for Path Planning," August 19, 1993
- D. B. Reister and M. A. Unseren, Engineering Physics and Mathematics Division, "Position and Constraint Force Control of a Vehicle with Two or More Steerable Drive Wheels," May 28, 1993
- T. Riddenberry, Sun Microsystems, Knoxville, "Global Workstation Conferencing Demonstration," August 31, 1993
- F. Saied, Department of Computer Science, University of Illinois, Champaign-Urbana, "Parallel Solvers for Underwater Acoustics," April 18, 1994
- H. M. Sardar, Clemson University, Clemson, SC, "Attenuation of Structural Vibrations in Motion Controlled Mechanical Systems," October 20, 1993
- S. Seidel, Michigan Institute of Technology, "Broadcasting on Linear Arrays and Meshes," March 16, 1993
- I. K. Sethi, Vision and Neural Networks Laboratory, Department of Computer Science, Wayne State University, Detroit, MI, "Decision Trees and Feedforward Neural Networks," May 21, 1993

- T. Shinbrot, Northwestern University, Evanston, IL, "Will Control of Chaos Ever Lead to Control of Turbulence?" September 23, 1994
- C. Shoemaker, Cornell University, Ithaca, NY, "Large Scale Nonlinear Optimal Control Algorithms with Applications to Groundwater Remediation," November 12, 1993
- S. Simunovic, Metals and Ceramics Division, "Porting DYNA3D to the Kendall Square Research Computer," April 29, 1994
- A. L. Solomonoff, Institute for Math and Its Applications, University of Minnesota, "Fast Algorithms for Micromagnetic Calculations," February 21, 1994
- T. Steinel, Polytechnic Institute of Wiesbaden, Germany, "Collision Detection for Two Manipulators," March 22, 1993
- S. Stothoff, University of Vermont, Burlington, VT, "Semi-Analytic Solution of Conservation Equations," February 5, 1993
- X.-H. Sun, ICASE, NASA Langley Research Center, "Parallel Matrix Algorithms for High Resolution Discretizations," October 21, 1993
- A. Tsao, Supercomputing Research Center, Bowie, MD, "Performance of a Parallel Eigensolver Based on the Invariant Subspace Decomposition Algorithm for Dense Symmetric Matrices," August 26, 1993
- R. Van De Geijn, University of Texas, Austin, TX, "Efficient Communication on Mesh Architectures," February 11, 1993
- H. A. Van Der Vorst, Department of Mathematics, Utrecht University, "Further Improvements in Nonsymmetric Hybrid CG Methods," December 10, 1993
- R. C. Ward, C. O. Beasley, R. C. Mann, D. T. Ingersoll, D. C. Larson, and R. W. Roussin, Engineering Physics and Mathematics Division, "Research and Capabilities of the Engineering Physics and Mathematics Division," May 20, 1993
- T. Y. C. Woo, Department of Computer Sciences, University of Texas at Austin, "Authentication and Authorization in Distributed Systems," April 14, 1994
- J. Xiao, University of North Carolina, Charlotte, NC, "Contact-Based Replanning of Robot Motion in the Presence of Uncertainties," March 9, 1994
- K. Yelick, Department of Computer Science, University of California, Berkeley, "Programming Irregular Applications on Distributed Memory Multiprocessors," February 24, 1993
- H. Zhang, Department of Mathematical Sciences, Clemson University, Clemson, SC, "On the Waveform Relaxation Method," October 21, 1993
- Z. Zhang, Center for Telecommunications Research, Columbia University, "Integrated Voice/Data TDMA Schemes in BISDN/ATM Networks," March 14, 1994

PUBLICATIONS

ADAMS, S. M.,* K. D. HAM,* AND J. J. BEAUCHAMP

"Application of Canonical Variate Analysis in the Evaluation and Presentation of Multivariate Biological Response Data," *Environmental Toxicology and Chemistry* **13**(10), 1673 (1994). (1.105)[†]

ALEXIADES, V., G. K. JACOBS,* AND N. W. DUNBAR*

"Constraints on Mass Balance of Soil Moisture During in Situ Vitrification," *Environmental Geology* **23**, 83 (1994). (1.47)

ALSMILLER, R. G., JR., AND F. S. ALSMILLER

"Low-Energy Particle Production and Transport for 200 GeV/c Hadrons in Lead and Comparisons with Experimental Data," *Nucl. Instrum. Meth. Phys. Res. A* **336**, 132 (1993). (4.44)

ALSMILLER, R. G., JR., AND R. A. LILLIE

"Design Calculations for the ANS Cold Neutron Source II: Heating Rates," *Nucl. Instrum. Methods Phys. Res. A* **321**, 265 (1992). (1992)

ALSON, E. E.,* J. C. GEHIN, AND C. D. WEST*

"Fuel Density, Uranium Enrichment, and Performance Studies for the Advanced Neutron Source Reactor," ORNL/TM-12775 (June 1994). (4.16)

AZMY, Y. Y.

"General Order Nodal Transport Methods and Application to Parallel Computing," *Transport Theory and Statistical Physics* **22**(2&3), 359 (1993). (1992)

"Cell-Centered Imposed Diffusion Synthetic Acceleration for Weighted Difference Transport Methods," *Nucl. Sci. Eng.* **115**, 265 (1993). (4.2)

BAKER, J. E.

"Terrain Following and Mapping of Arbitrary Surfaces Using High Precision Proximity Data," *Optical Engineering* **32**(5), 1117 (1993). (3.12)

"Image Accuracy and Representational Enhancement Through Low-Level Multi-Sensor Integration Techniques," ORNL/TM-12218 (May 1993). (3.38)

* Not a member of Engineering Physics and Mathematics Division.

[†] In most cases, the number shown in parentheses following the publication corresponds to the number of an abstract included in this report. In some cases the number is a year, which means the abstract was published in an earlier progress report published that year. If neither an abstract number nor a year appears, then an abstract was not available for this report.

BALAKRISHNA, C.* L. J. GRAY, AND J. H. KANE*

"Efficient Analytical Integrations of Symmetric Galerkin Boundary Integrals Over Curved Elements; Thermal Conduction Formulation," *Comput. Methods Appl. Mech. Eng.* 111, 335 (1994). (1.48)

BANGS, A. L.

"An Evaluation of Integration of the Trace Assertion Method with the Box Structure Method for Coding in C++," ORNL/TM-12439 (August 1993). (3.66)

BLAIR, J. R. S.,* AND B. W. PEYTON

"On Finding Minimum-Diameter Clique Trees," *Nordic Journal of Computing* 1, 173 (1994). (1.31)

BOWMAN, K. O.

"Committee on Statistics and Disabilities Reaches Out to Members," *Amstat News*, p. 8 (December 1992).

"NSF Office for Disabled Scientists and Engineers Opens," *Amstat News*, p. 19 (February 1993).

"EEOC Publication Explains Your Rights Under the Americans with Disabilities Act," *Amstat News*, p. 10 (March 1993).

"AAAS Explores Access Problems for Scientists and Engineers," *Amstat News*, p. 12 (April 1993).

"Your Rights Under ADA—Continued," *Amstat News*, p. 10 (May 1993).

"FSD Works to Increase Options for Students with Disabilities," *Amstat News*, p. 16 (June 1993).

"ADA Passes Its First Anniversary," *Amstat News*, pp. 26–27 (August–September 1993).

"ADA Can Only Work for Those Who Identify Themselves," *Amstat News*, pp. 34–35 (October 1993).

"Note from the Committee on Statistics and Disability," *Amstat News* (November 1993).

BOWMAN, K. O., AND M. A. KASTENBAUM*

"Overdispersion of Aggregated Genetic Data," *Mutation Research* 272, 133 (1992). (1992)

BOWMAN, K. O., M. K. MILLER,* AND L. R. SHENTON*

"The Use of Moment Estimators to Determine the Parameters of Concentration Fluctuations in Random Area Atom Probe Analyses," *Applied Surface Science* 367, 424 (1993). (1992)

BOWMAN, K. O., AND L. R. SHENTON*

"Additional Bowman-Shenton Approximate Percentage Points for Pearson Distributions Based on Pearson Type VI," *Commun. Statist.-Simula.* **23(3)**, 583 (1994). (1.122)

BROWNE, S. V.,* J. J. DONGARRA, S. C. GREEN,* K. MOORE,* T. H. ROWAN, AND R. C. WADE*

"Netlib Services and Resources," ORNL/TM-12680 (April 1994). (1.2)

BURNS, T. J.

"ORGBUG - A Windows-Based Combinatorial Geometry Debugger," ORNL/TM-12020 (June 1993). (4.6)

BUTLER, P. L.,* AND J. P. JONES

"A Modular Control Architecture for Real-Time Synchronous and Asynchronous Systems," in *Experimental Environments in Computer Vision and Image Processing*, H. I. Christensen and J. L. Corwley, Eds., Vol. 18, pp. 157-182, World Scientific Press, Singapore (1994). (3.58)

CHANEY, E. L.,* T. J. CULIP,* AND T. A. GABRIEL

"A Monte Carlo Study of Accelerated Head Scatter," *Medical Physics* **21(9)**, 1383 (1994). (4.45)

CHEN, W.*

"Implementation and Parallelization of Fast Matrix Multiplication for a Fast Legendre Transform," ORNL/TM-12285 (September 1993). (1.67)

CHILDS, R. L.,* AND W. A. RHOADES

"Theoretical Basis of the Linear Nodal and Linear Characteristic Methods in the TORT Computer Code," ORNL/TM-12246 (January 1993). (4.7)

CHOI, J., J. J. DONGARRA, R. POZO,* D. C. SORENSEN,* AND D. W. WALKER

"CRPC Research into Linear Algebra Software for High Performance Computers," *International Journal of Supercomputer Applications* **8(2)**, 99 (1994). (1.24)

CHOI, J., J. J. DONGARRA, AND D. W. WALKER

"PUMMA: Parallel Universal Matrix Multiplication Algorithms on Distributed Memory Concurrent Computers," ORNL/TM-12252 (August 1993). (1.26)

"Parallel Matrix Transpose Algorithms on Distributed Memory Concurrent Computers," ORNL/TM-12309 (October 1993). (1.27)

CRAMER, S. N., AND C. O. SLATER

"Investigation of Radiation Effects in Hiroshima and Nagasaki Using a General Monte Carlo-Discrete Ordinates Coupling Scheme," *Nucl. Sci. Eng.* 114(1), 1 (1993). (1992)

D'AZEVEDO, E. F.

"Are Bilinear Quadrilaterals Better Than Linear Triangles?" ORNL/TM-12388 (August 1993). (1.49)

D'AZEVEDO, E. F., AND C. H. ROMINE

"DONIO: Distributed Object Network I/O Library," ORNL/TM-12743 (September 1994). (1.3)

"DOLIB: Distributed Object Library," ORNL/TM-12744 (October 1994). (1.4)

DICKENS, J. K., AND M. A. MILLER*

"Measurements and Calculations of Radionuclides Created by $^{181}\text{Ta}(\gamma, xn_{yp})$ Reactions for Bremsstrahlung Photons Produced by 150-MeV Electrons," *Nucl. Sci. Eng.* 114, 149 (1993). (1992)

DIFILIPPO, F. C.

"Probability Distributions for First Neighbor Distances Between Resonances that Belong to Two Different Families," *Annals of Nuclear Energy* 21(4), 219 (1994). (4.21)

"Applications of Monte Carlo Methods for the Analysis of MHTGR - Case of the VHTRC Benchmark," ORNL/TM-12698 (March 1994). (4.19)

"Applications of Monte Carlo Methods for the Analysis of MHTGR - Case of the PROTEUS Benchmark," ORNL/TM-12711 (April 1994). (4.20)

"Scoping Calculations of Power Sources for Nuclear Electric Propulsion," ORNL/TM-12703 (May 1994). (4.22)

DONATO, J. M.

"The Fourier Analysis Technique and Epsilon-Pseudo-Eigenvalues," ORNL/TM-12347 (July 1993). (1.69)

"A Comparison of Iterative Methods for a Model Coupled System of Elliptic Equations," ORNL/TM-12447 (August 1993). (1.70)

DONGARRA, J. J., R. HEMPEL,* A. J. G. HEY,* AND D. W. WALKER

"A Proposal for a User-Level, Message Passing Interface in a Distributed Memory Environment," ORNL/TM-12231 (February 1993). (1.5)

DONGARRA, J. J., T. H. ROWAN, AND R. C. WADE*

"Software Distribution Using Xnetlib," ORNL/TM-12318 (June 1993). (1.6)

DONGARRA, J. J., R. A. VAN DE GEIJN, AND D. W. WALKER

"Scalability Issues Affecting the Design of a Dense Linear Algebra Library," *Journal of Parallel and Distributed Computing* 22(3), 523 (1994). (1.29)

DONGARRA, J. J., AND D. W. WALKER

"The Design of Linear Algebra Libraries for High Performance Computers," ORNL/TM-12404 (August 1993). (1.30)

DRISCHLER, J. D., J. O. JOHNSON, AND K. G. KERRIS*

"MASH V1.0 Analysis of a Simplified Box Vehicle Model Containing Openings Representative of Armored Vehicle Models," ORNL/TM-12755 (August 1994). (4.61)

DRISCHLER, J. D., J. O. JOHNSON, R. T. SANTORO, AND K. G. KERRIS*

"MASH V1.0 Analysis of the Army Research Laboratory (ARL) Box/Liner Test Bed Experiments Performed October 4-8, 1993 at the Army Pulse Radiation Facility (APRF)," ORNL/TM-12685 (May 1994). (4.62)

"Nuclear Performance of Radiation/Armor/SPALL Liner Materials for Armored/Tactical Vehicle Applications," ORNL/TM-12504 (May 1994). (4.63)

DUNIGAN, T. H.

"Multi-Ring Performance of the Kendall Square Multiprocessor," ORNL/TM-12331 (March 1994). (1.8)

"Early Experiences and Performance of the Intel Paragon," ORNL/TM-12194 (August 1994). (1.7)

ENGLE, W. W., JR., AND L. R. WILLIAMS

"Temperature and Void Reactivity Coefficient Calculations for the High Flux Isotope Reactor Safety Analysis Report," ORNL/TM-12386 (July 1994). (4.24)

FARRELL, K.,* F. B. KAM,* C. A. BALDWIN,* J. V. PACE, III, W. R. CORWIN,* L. ROBINSON,* F. F. DYER,* F. M. HAGGAG,* F. W. STALLMAN,* B. M. OLIVER,* AND L. R. GREENWOOD*

"The DOS 1 Neutron Dosimetry Experiment at the HB-4-A Key 7 Surveillance Site on the HFIR Pressure Vessel," ORNL/TM-12511 (January 1994). (4.25)

FOSTER, I. T.,* AND P. H. WORLEY

"Parallel Algorithms for the Spectral Transform Method," ORNL/TM-12507 (April 1994). (1.85)

FREUND, R. W.,* AND N. M. NACHTIGAL

"QMRPACK and Applications," ORNL/TM-12753 (October 1994). (1.75)

"A New Krylov-Subspace Method for Symmetric Indefinite Linear Systems," ORNL/TM-12754 (October 1994). (1.73)

FREUND, R. W.,* N. M. NACHTIGAL, AND J. C. REEB*

"QMRPACK User's Guide," ORNL/TM-12807 (October 1994). (1.76)

FROME, E. L., M. H. SMITH,* L. G. LITTLEFIELD,* R. L. NEUBERT, AND S. P. COLYER*

"Statistical Methods for the Analysis of a Screening Test for Chronic Beryllium Disease," ORNL-6818 (October 1994). (1.106)

GABRIEL, T. A., D. E. GROOM,* P. K. JOB,* N. V. MOKHOV, AND G. R. STEVENSON

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Knoxville, TN, March 17, 1993*

DIFILIPPO, F. C., "Nuclear Power Sources for Space Propulsion."

*Pure and Applied Linear Algebra: The New Generation, The 3rd Conference of the
International Linear Algebra Society, University of West Florida and the Pensacola
Hilton Hotel, Pensacola, FL, March 17-20, 1993*

GILBERT, J. R.,* AND E. G. NG, "Separators and Structure Prediction for
Nonsymmetric Matrix Factorizations." (1.33)

PEYTON, B. W., A. POTHEN,* AND X. YUAN,* "Partitioning a Chordal
Graph into Transitive Subgraphs for Parallel Sparse Triangular Solution,"
(oral presentation only).

*The Second International Conference on Nuclear Engineering (ICONE-2), San
Francisco, CA, March 21-24, 1993*

KWANT, W.,* N. L. RAMSOUR,* AND F. J. SWEENEY, "Robotics
Application for In-Service Inspection of the ALMR." (3.60)

*The Second ASME-JSME Nuclear Engineering Joint Conference, American Society
of Mechanical Engineers, New York, March 21-24, 1993; Proc. (1993)*

TALEYARKHAN, R. P.,* S. H. KIM,* C. O. SLATER, D. L. MOSES,*
D. B. SIMPSON,* AND V. GEORGEVICH,* "Modeling and Analysis of Core
Debris Recriticality During Hypothetical Severe Accidents in the Advanced
Neutron Source Reactor," pp. 471-479. (4.40)

American Physical Society 1993 Annual Meeting, Seattle, WA, March 22, 1993

SEIFU, D.,* F. J. PINSKI,* W. A. SHELTON, G. M. STOCKS,* AND D.
D. JOHNSON,* "Total Energy of Ordered and Disordered $\text{Cu}_e\text{Au}_{1-e}$ Alloys."
(1.93)

*Sixth SIAM Conference on Parallel Processing for Scientific Computing, Norfolk,
VA, March 22-24, 1993; Proc. (1993)*

BENNETT, K. R., "Fast Direct Solvers for Three-Dimensional Poisson and
Helmholtz Problems on Distributed Memory Machines," (oral presentation
only).

D'AZEVEDO, E. F., V. EIJKHOUT,* AND C. H. ROMINE, "A Matrix Framework for Conjugate Gradient Methods and Some Variants of CG with Less Synchronization Overhead," Vol. II, pp. 644-646. (1.50)

FOSTER, I. T.,* AND P. H. WORLEY, "Parallelizing the Spectral Transform Method: A Comparison of Alternative Parallel Implementations," pp. 100-107. (1.84)

GEIST, G. A., R. MANCHEK,* AND W. JIANG,* "Using PVM 3.0 to Run Grand Challenge Applications on a Heterogeneous Network of Parallel Computers," (oral presentation only).

LEETE, C. A., B. W. PEYTON, AND R. F. SINCOVEC, "Toward a Parallel Recursive Spectral Bisection Mapping Tool." (1.44)

PEYTON, B. W., E. ROTHBERG,* A. GUPTA,* AND E. NG, "Parallel Sparse Cholesky Factorization Algorithms for Shared-Memory Multiprocessor Systems," (oral presentation only).

7th National Conference on Undergraduate Research, University of Utah, Salt Lake City, UT, March 25-27, 1993; Proc. (1993)

SZPIRO, A. A.,* AND V. PROTOPOPESCU, "Two-Sided Game for a Reaction-Diffusion System with Competitive Interactions and Controls on Initial Conditions," pp. 817-821.

Oral Presentation, American Mathematical Society, Southeastern Section, Knoxville, TN, March 26-27, 1993

PROTOPOPESCU, V., "Optimal Control for Competitive Parabolic Systems."

Second IEEE International Conference on Fuzzy Systems, San Francisco, CA, March 28-April 1, 1993; Proc. (1993)

PIN, F. G., AND Y. WATANABE,* "Driving a Car Using Reflexive Fuzzy Behaviors," pp. 1425-1430. (3.20)

Oral Presentation, Conference on High Speed Computing, Salishan Lodge, OR, March 31, 1993

GEIST, G. A., "Software Tools for Computational Grand Challenges."

Oral Presentation, 4th Workshop on Instrumentation for Parallel Computer Systems, Keystone, CO, April 5-7, 1993

WORLEY, P. H., "Experiences with Instrumenting Message-Passing ("Low Performance") Fortran Programs."

Oral Presentation, Math Department, University of New Mexico, Albuquerque, NM, April 12, 1993

DONGARRA, J. J., "Scalable High-Performance Libraries in Linear Algebra and PVM and HeNCE: Tools for Network-Based Concurrent Computing."

Oral Presentation, New Mexico High Performance Computing Distinguished Lecture Series, Los Alamos National Laboratory, Los Alamos, NM, April 12, 1993

DONGARRA, J. J., "Scalable High-Performance Libraries in Linear Algebra and XNETLIB a Tool for Software Retrieval."

Conference on Sensor Fusion and Aerospace Applications, Optical Engineering/Aerospace Science and Sensing, Orlando, FL, April 12-16, 1993; Proc. Vol. 1956 (1993)

BAKER, J. E., "Image Accuracy and Representational Enhancement Through Low-Level, Multi-Sensor Integration Techniques." (3.38)

BECKERMAN, M., AND F. J. SWEENEY, "Data Fusion Through Simulated Annealing of Registered Range and Reflectance Images," pp. 200-211. (3.44)

SPIE Applications of Artificial Intelligence XI, Orlando, FL, April 12-16, 1993; Proc. Vol. 1964 (1993)

JONES, J. P., "Real-Time Construction and Rendering of Three-Dimensional Occupancy Maps," pp. 249-256. (3.48)

Oral Presentation, Sandia National Laboratory, Albuquerque, NM, April 13, 1993

DONGARRA, J. J., "Scalable High-Performance Libraries in Linear Algebra."

Seminar, Oak Ridge National Laboratory, Physics Division, Oak Ridge, TN, April 16, 1993

GEIST, G. A., "Network Computing with PVM."

American Nuclear Society Topical Meeting on Nuclear Plant Instrumentation, Control and Man-Machine Interface Technologies, Garden Plaza Hotel, Oak Ridge, TN, April 18-21, 1993; Proc. (1993)

SPELT, P. F., "Role of the Operator in Nuclear Power Plants as Determined from a Survey of the North American Nuclear Community," pp. 120-127. (3.96)

WOOD, R. T.,* H. E. KNEE, J. A. MULLENS,* J. K. MUNRO, JR.,* B. K. SWAIL,* AND P. A. TAPP,* "The Integrated Workstation System: A Common, Consistent Link Between Nuclear Plant Personnel and Plant Information and Computerized Resources." (3.91)

Oral Presentation, International High-Performance Computing Conference at the National Center for High Performance Computing, Taipei, Taiwan, April 19, 1993

DONGARRA, J. J., "Scalable High-Performance Libraries in Linear Algebra and XNETLIB a Tool for Software Retrieval."

Oral Presentation, SIAM Conference on Mathematical and Computational Issues in the Geosciences, Houston, TX, April 19-21, 1993

D'AZEVEDO, E. F., AND C. H. ROMINE, "Overview of HPCC Groundwater Activities at the Oak Ridge National Laboratory."

Joint International Conference on Mathematical Methods and Supercomputing in Nuclear Applications, Karlsruhe, Germany, April 19-23, 1993; Proc. (1993)

DIFILIPPO, F. C., M. CARO,* AND T. WILLIAMS,* "Simulation of Pulsed Neutron Source Reactivity Measurements." (4.23)

GEHIN, J. C., AND A. F. HENRY,* "Time-Dependent Discontinuity Factors for Transient Nodal Models," Vol. 1, p. 496. (4.8)

Oral Presentation, NASA-Lewis Research Center, Cleveland, OH, April 20, 1993

DIFILIPPO, F. C., "Scoping Calculations of Power Sources for NEP."

American Nuclear Society Fifth Topical Meeting on Robotics and Remote Handling, Knoxville, TN, April 26-29, 1993; Proc. (1993)

BECKERMAN, M., AND F. J. SWEENEY, "Laser Range Camera Data Fusion." (3.42)

JONES, J. P., "Automatic Code Generation for Distributed Robotic Systems." (3.59)

PIN, F. G., AND Y. WATANABE,* "Mobile Robot Navigation Using Qualitative Reasoning," pp. 523-530. (3.23)

SWEENEY, F. J., D. G. CARROLL,* C. CHEN,* C. CRANE,* R. DALTON,* J. R. TAYLOR,* S. TOSUNOGLU,* T. WEYMOUTH,* AND K. R. WILLIAMS,* "Designs for Remote Inspection of the ALMR Reactor Vessel Auxiliary Cooling System (RVACS)," pp. 431-438. (3.61)

Organization for Economic Cooperation and Development, Nuclear Energy Agency, Advanced Monte Carlo Computer Programs for Radiation Transport, Centre d'Etudes, Saclay, France, April 27-29, 1993

CRAMER, S. N., "Recent Developments and Applications of the MORSE Code." (5.1)

JOHNSON, J. O., AND R. T. SANTORO, "The MASH 1.0 Code System: Utilization of MORSE in the Adjoint Mode." (4.65)

Seminar, University of Tennessee, Math Department, Knoxville, TN, April 28, 1993

DONGARRA, J. J., "Parallel Computing."

Oral Presentation, University of Kentucky, Lexington, KY, April 28, 1993

GEIST, G. A., "PVM 3 Beyond Network Computing."

Oral Presentation, Partial Differential Equations on the Sphere Conference, Global Climate Modeling Project, Oak Ridge, TN, April 28, 1993

WORLEY, P. H., "PSTSWM: A Parallel Algorithm Testbed and Benchmark Code for the Spectral Transform Method."

UT-ORNL Parallel Seminar, University of Tennessee, Knoxville, TN, April 30, 1993

SEIDEL, S. R.,* "Broadcasting on Linear Arrays and Meshes."

Second International Conference on Information and Knowledge Management, Washington, DC, May 1-5, 1993

GLOVER, C. W., N. S. V. RAO, AND E. M. OBLOW, "Hybrid Pattern Recognition System Capable of Self-Modification." (3.50)

Oral Presentation, 3rd Conference on Computational Research on Materials, Morgantown, WV, May 2-4, 1993

SHELTON, W. A., JR., "Panel Discussion on the Current and Future Directions of High Performance Computing."

39th International Instrumentation Symposium, Albuquerque, NM, May 2-6, 1993; Proc. (1993)

KNEE, H. E., "Human Factors Engineering: A Key Element of Instrumentation and Control System Design," pp. 1113-1122. (3.92)

1993 IEEE International Conference on Robotics and Automation, Atlanta, GA, May 2-6, 1993; Proc. Vol. 1 (1993)

BANGS, A. L., "Research and Applications of Cooperating Mobile Robots." (3.55)

JONES, J. P., "Real-Time Construction of Three-Dimensional Occupancy Maps," pp. 52-57. (3.47)

PIN, F. G., AND Y. WATANABE,* "Using Fuzzy Behaviors for the Outdoor Navigation of a Car with Low-Resolution Sensors," pp. 548-553. (3.19)

Oral Presentation, International Workshop on Nuclear Data for Fusion Reactor Technology, Del Mar, CA, May 3-6, 1993

FU, C. Y., "Comparative Cross-Section Calculations Using Exciton Level Densities Based on One and Two Kinds of Fermions."

LARSON, D. C. "Fusion Data Measurement Capabilities at ORELA."

LARSON, D. C., AND D. M. HETRICK,* "Comparison of Recent $^{54,56}\text{Fe}$ Charged-Particle Emission Spectra from 8-15 MeV with ENDF/B-VI."

Oral Presentation, Design of Experiments: Optimality, Construction and Application, Oberwolfach, Germany, May 3-7, 1993

MORRIS, M. D., "An Overview of Some Recent Developments in the Design and Analysis of Computer Experiments."

Oral Presentation, 1993 Parallel Virtual Machine Users' Group Meeting, Knoxville, TN, May 10-11, 1993

DRAKE, J. B., AND B. D. SEMERARO, "A PVM3 Version of the Parallel Community Climate Model."

SEMERARO, B. D., "Parallel Panel Methods: Experience with PVM."

SHELTON, W. A., JR., "Developing Large Scale Material Science Computer Codes by Integrating PVM and the PARAGON."

Theory Institute on Combinatorial Challenges in Computational Differentiation, Argonne National Laboratory, Argonne, IL, May 24-26, 1993

HORWEDEL, J. E.,* "Reverse Automatic Differentiation of Modular Fortran Programs."

Eighth Scandinavian Conference on Image Analysis, Tromso, Norway, May 25-28, 1993

JONES, J. P., O. H. DORUM,* C. S. ANDERSEN,* S. B. JACOBSEN,* M. S. JENSEN,* N. O. S. KIERKEBY,* S. KRISTENSEN, C. B. MADSEN,* H. M. NIELSEN,* E. SORENSEN,* J. J. SORENSEN, AND H. I. CHRISTENSEN,* "Experiments in Mobile Robot Navigation and Range Imaging." (3.26)

Oral Presentation, American Society for Information Sciences, Hyatt Regency Hotel, Knoxville, TN, May 26, 1993

SPELT, P. F., "Virtual Reality: The Cold Fusion of 1993?"

14th Annual Meeting of the Canadian Applied Math Society, York University, North York, Ontario, Canada, May 30-June 3, 1993

NG, E., AND B. W. PEYTON, "Improved Software for Symbolic Factorization." (1.37)

Oral Presentation, Laboratoire LIP-IMAG, Cedex, France, June 9, 1993

DONGARRA, J. J., "An Overview of Our Activities in Linear Algebra and Software Tools."

Oral Presentation, Advanced Computer Research Institute, Cedex, France, June 11, 1993

DONGARRA, J. J., "LAPACK: Algorithms + Software = Performance + Portability."

Oral Presentation, 1993 Householder Symposium, UCLA Lake Arrowhead Conference Center, Los Angeles, CA, June 13-18, 1993

LEE, S. L., "A New and Sharp Upper Bound for Departure from Normality."

Oral Presentation, Nuclear Energy Agency Nuclear Science Committee Working Group Meeting on International Evaluation Cooperation, Aix-en-Provence, France, June 16-18, 1993

FU, C. Y., "A Status Report (March 1993) of Subgroup 1 of the NEANSC Working Group on International Evaluation Cooperation."

LARSON, D. C., "A Status Report of Subgroup 11 of the NEANSC Working Group on International Evaluation Cooperation."

Annual Meeting of the American Nuclear Society, San Diego, CA, June 20-24, 1993; Trans. Am. Nucl. Soc. 68 (1993)

PRIMM, R. T., III, "Establishing Area of Applicability for Benchmarks to Support Storage of Mixed Oxide Waste," pp. 239-241.

Oral Presentation, Workshop on Production of High Quality Parallel Software in Numerical and Scientific Computing, Vienna, Austria, June 22, 1993

DONGARRA, J. J., "LAPACK: Algorithms + Software = Performance + Portability."

61st Military Operations Research Society Symposium, Air Force Institute of Technology, Wright-Patterson Air Force Base, Dayton, OH, June 22-24, 1993

LENHART, S., AND V. PROTOPOPESCU, "Optimal Control for Competitive - Cooperative Systems; Modeling Flexible Coalitions in Tomorrow's Competitive World." (1.60)

SANTORO, R. T., J. O. JOHNSON, AND M. S. SMITH, "Application of the Adjoint Monte Carlo Shielding Code System - MASH - in Nuclear Operations," (oral presentation only).

Oral Presentation, Advanced Seminar on Programming Tools for Parallel Machines, Lecce, Italy, June 24, 1993

DONGARRA, J. J., "Scalable High-Performance Libraries in Linear Algebra."

Oral Presentation, NRC Technical Training Center, Chattanooga, TN, June 24, 1993

KNEE, H. E., "Capabilities and Resources of the Oak Ridge National Laboratory for Establishment of a NRC Human Factors Regulatory Research Facility."

Oral Presentation, International Workshop on Interconnection Networks, Luminy (Marseille), France, July 5, 1993

DONGARRA, J. J., "Tools for Network-Based Concurrent Computing."

Oral Presentation, International Summer Institute on Parallel Computer Architectures, Languages, and Algorithms, Prague, Czech Republic, July 8, 1993

DONGARRA, J. J., "Scalable High-Performance Libraries in Linear Algebra."

Oral Presentation, 1993 SIAM Annual Meeting, Philadelphia, PA, July 8, 1993

SHELTON, W. A., G. A. GEIST, AND G. M. STOCKS,* "The Development of the SCF-KKR-CPA Electronic Structure Method Within a Heterogeneous Distributed Computing Environment."

Oral Presentation, Restoring Our Waters Workshop, Oak Ridge National Laboratory, Oak Ridge, TN, July 13, 1993

BEAUCHAMP, J. J., "Statistics: An Aid to Better Understanding."

Oral Presentation, 1993 SIAM Annual Meeting, Philadelphia, PA, July 15, 1993

SHELTON, W. A., G. A. GEIST, AND G. M. STOCKS,* "The Development of the SCR-KKR-CPA Electronic Structure Method Within a Heterogeneous Distributed Computing Environment."

Oral Presentation, NATO-ARW on Metallic Alloys: Experimental and Theoretical Perspectives, Boca Raton, FL, July 16, 1993

SHELTON, W. A., D. M. C. NICHOLSON,* G. M. STOCKS,* Y. WANG,* W. M. TEMMERMAN,* Z. SZOTEK,* AND B. GINATEMPO,* "Alloy Calculations on Massively Parallel Computers."

NATO Advanced Research Workshop on Metallic Alloys: Experimental and Theoretical Perspectives, Boca Raton, FL, July 16-21, 1993

STOCKS, G. M.,* D. M. C. NICHOLSON,* Y. WANG,* W. A. SHELTON, W. M. TEMMERMAN,* Z. SZOTEK,* AND B. GINATEMPO,* "Alloy Calculations on Massively Parallel Computers." (1.95)

12th International Federation of Automatic Control World Congress, Sydney, Australia, July 19-23, 1993

PIN, F. G., and Y. WATANABE,* "Driving a Car with Sparse and Imprecise Sensor Data Using VLSI Fuzzy Inferencing Chips and Boards." (3.21)

Oral Presentation, Laboratoire LIP-IMAG, Ecole Normale Supérieure de Lyon, Cedex, France, July 22, 1993

DONGARRA, J. J., "Recent Work in Parallel Algorithms for the Eigenvalue Problem."

DONGARRA, J. J., "PVM and MPI: Tools for Concurrent Computing."

Oral Presentation, Institute for Computer Applications in Science and Engineering/Langley Research Center, Short Course on Parallel Computation, Hampton, VA, July 27, 1993

WALKER, D. W., AND G. A. GEIST, "MPI: A Standard Message Passing Interface for Distributed Memory Concurrent Computers."

Oral Presentation, IBM Thomas J. Watson Research Center, Yorktown Heights, NY, July 28-31, 1993

NG, E., J. GILBERT,* and B. W. PEYTON, "An Efficient Algorithm to Compute Row and Column Counts for Sparse Cholesky Factorization."

Oral Presentation, Oak Ridge National Laboratory Workstation Support Seminar, Oak Ridge, TN, July 30, 1993

GEIST, G. A., "Network Computing with PVM."

1993 Joint Statistical Meetings, San Francisco, CA, August 7-12, 1993; Technometrics 36(2) (1994)

DOWNING, D. J., "Comments on 'Use of Conditional Simulation in Nuclear Waste Site Performance Assessment,' by Carol Gotway," p. 147. (1.101)

35th Annual Meeting of the American Association of Physicists in Medicine (AAPM) Washington, DC, August 8-12, 1993

CULLIP, T. J.,* T. A. GABRIEL, AND E. L. CHANEY,* "A Monte Carlo Study of Linac Head Scatter."

Oral Presentation, Joint Statistical Meetings, San Francisco, CA, August 8-12, 1993

OSTROUCHOV, G., "Statistical Modeling Applications on Parallel Computers."

Fifth International Conference on Human-Computer Interaction: Software and Hardware Interfaces, Orlando, FL, August 8-13, 1993; Proc. Vol. 2, G. Salvendy and M. J. Smith, Eds., Elsevier (1993)

SCHRYVER, J. C., AND J. H. GOLDBERG,* "Eye Gaze and Intent: Application in 3D Interface Control," pp. 573-578. (3.90)

Oral Presentation, Molecular Sciences Research Center, Richland, WA, August 9, 1993

SINCOVEC, R. F., "Algorithms and Tools for Solving Grand Challenge Problems on Parallel Computers."

BEM (Boundary Element Methods) 15 Conference, Worcester, MA, August 10-12, 1993

GRAY, L. J., AND L. L. MANNE,* "Hypersingular Integrals at a Corner." (1.54)

Oral Presentation, SHARE81 Summer 1993 Meeting, Washington, DC, August 18, 1993

WALKER, D. W., "Message Passing Interface: The New Parallel Programming Standard?"

International Symposium, on Boundary Element Methods (IABEM-93), University of Braunschweig, Germany, August 23-26, 1993

KANE, J. H.,* L. J. GRAY, AND C. BALAKRISHNA,* "Analytical Treatment of Symmetric Galerkin BIEs." (1.57)

Oral Presentation, U.S. Bureau of the Census, Suitland, MD, August 25, 1993

WRIGHT, T., "Some Simple Ideas on Ranks and Probability Sampling."

Eighth ASTM-EURATOM Symposium on Reactor Dosimetry, Vail, CO, August 29-September 3, 1993; Proc. Harry Farrar IV, E. Parvin Lippincott, J. G. Williams, and D. W. Vehar, Eds. (1994)

BEASLEY, C. O., JR., N. M. LARSON,* J. A. HARVEY, D. C. LARSON, AND G. M. HALE,* "Measurement and Analysis of the Nitrogen Total and Differential Scattering Cross Sections in the Resonance Region," pp. 737-743. (2.1)

INGERSOLL, D. T., J. E. WHITE, R. Q. WRIGHT,* H. T. HUNTER, C. O. SLATER, N. M. GREENE,* AND R. E. MACFARLANE,* "Production and Testing of the Vitamin B6 Fine-Group and the Bugle-93 Broad-Group Neutron/Photon Cross-Section Libraries Derived from ENDF/B-VI Nuclear Data," pp. 660-669. (4.31)

INGERSOLL, D. T., J. E. WHITE, R. Q. WRIGHT,* AND R. W. ROUSSIN, "Generation and Testing of an ENDF/B-VI Multigroup Cross-Section Library for LWR Shielding Applications," (oral presentation only).

PACE, J. V., III, C. O. SLATER, AND M. S. SMITH, "Three-Dimensional Discrete Ordinates Radiation Transport Calculations of Neutron Fluxes for Beginning-of-Cycle at Several Pressure Vessel Surveillance Positions in the High Flux Isotope Reactor," pp. 140-146. (4.33)

ROUSSIN, R. W., J. B. MANNESCHMIDT, AND J. E. WHITE, "Computer Code and Data Libraries for Radiation Transport Available from the Radiation Shielding Information Center," (oral presentation only).

Seventh European Eye Movement Conference, University of Durham, Durham, England, August 31-September 3, 1993

GOLDBERG, J. H.,* AND J. C. SCHRYVER, "Eye-Gaze Determination of User Intent at the Computer Interface." (3.87)

Computational Learning and Machine Learning Workshop, Provincetown, MA, September 10-12, 1993

RAO, N. S. V., AND E. M. OBLOW, "N-Learners Problem: System of PAC Learners." (3.32)

Workshop on RNA 3' Ends: Formation and Function, Oxford, England, September 15-19, 1993

MATIS, S., AND C. MILCAREK,* "Effect of Changes in the Region Near an Immunoglobulin Secretory-Specific Polyadenylation Site on the Strength of the Site and Its Regulation." (3.85)

Physics and Methods in Criticality Safety, Nashville, TN, September 19-23, 1993; Proc. (1993)

PRIMM, R. T., III, "Fissile Material Storage in the Oak Ridge Radiochemical Development Facility," pp. 243-242. (4.35)

VIII International Conference on Finite Elements in Fluids, Barcelona, Spain, September 20-24, 1993

NG, E., B. NITROSO,* AND B.W. PEYTON, "On the Solution of Stokes' Pressure System within N3S Using Supernodal Cholesky Factorization." (1.38)

Oral Presentation, IBM Sup'Eur 93, Vienna Austria, September 27, 1993

DONGARRA, J. J., "Scalable High-Performance Libraries in Linear Algebra."

Oral Presentation, Laboratoire National d'Hydraulique, Electricite de France, Paris, France, September 27, 1993

NG, E., AND B. W. PEYTON, "Sparse Cholesky Factorization Algorithms."

Oral Presentation, Laboratoire National d'Hydraulique, Electricite de France, Paris, France, September 28, 1993

NG, E., "Algorithms for the Direct Solution of Sparse Nonsymmetric Linear Systems."

Oral Presentation, First International Meeting on Vector and Parallel Processing, CICA, Faculdade de Engenharia U.P., Porto, Portugal, October 1, 1993

DONGARRA, J. J., "PVM and MPI: Tools for Concurrent Computing."

Oral Presentation, Intel Supercomputer User's Group Meeting, St. Louis, MO, October 4, 1993

WALKER, D. W., "MPI: A Standard Message Passing Interface for Distributed Memory Environments."

Second International Conference of the Austrian Center for Parallel Computation, Gmunden, Austria, October 4-6, 1993; Proc. Lecture Notes in Computer Science 734, J. Volkert, Ed., (1993)

GEIST, G. A., "PVM 3 Beyond Network Computing," pp. 194-203. (1.13)

Scalable Parallel Libraries Conference, Mississippi State, MS, October 6-8, 1993

CHOI, J.,* J. J. DONGARRA, AND D. W. WALKER, "Parallel Matrix Transpose Algorithms on Distributed Memory Concurrent Computers." (1.27)

37th Annual Meeting: Human Factors and Ergonomics Society, Seattle, WA, October 11-15, 1993

GOLDBERG, J. H.,* AND J. C. SCHRYVER, "Eye-Gaze Control of the Computer Interface: Discrimination of Zoom Intent." (3.88)

Oral Presentation, Specialists' Meeting on Adapting Computer Codes in Nuclear Applications to Parallel Architectures, Madrid, Spain, October 14-15, 1993

KIRK, B. L., AND Y. Y. AZMY, "Advanced Communication Scheme for the Neutron Diffusion Nodal Method on High Performance Computers."

Oral Presentation, Sixth International Conference on Parallel and Distributed Computing Systems, Louisville, KY, October 14-16, 1993

DONGARRA, J. J., "PVM and MPI: Tools for Concurrent Computing."

Oral Presentation, Institute for Mathematics and Its Applications, Minneapolis, MN, October 15, 1993

GRAY, L. J., "Crack Propagation Modeling."

Oral Presentation, Southeastern-Atlantic Differential Equations Conference, University of North Carolina at Wilmington, Wilmington, NC, October 15-16, 1993

LENHART, S. M., V. PROTOPODESCU, AND A. A. SZPIRO,* "Optimal Control for Competing Coalitions."

TMS Symposium on Alloy Modeling and Design, Pittsburgh, PA, October 17, 1993

WANG, Y.,* G. M. STOCKS,* D. M. C. NICHOLSON,* AND W. A. SHELTON, "Spin-Polarized KKR-CPA Calculations for Ferromagnetic CuNi Alloys." (1.99)

Oral Presentation, 4th International Workshop on Fusion Neutronics, Los Angeles, CA, October 20-21, 1993

WHITE, J. E., "Overview of Current RSIC Activities of Interest to Fusion Neutronics."

Hilton Head DNA Sequence Conference, Hilton Head, SC, October 23-27, 1993

GUAN, X., R. MURAL,* S. PETROV, AND E. UBERBACHER, "A Sensitive Sequence Comparison Server for DNA and Proteins."

UBERBACHER, E., J. R. EINSTEIN, S. MATIS, Y. XU, M. SHAH, D. BULEY,* AND R. J. MURAL,* "Gene Recognition and Modeling in the GRAIL System."

The Fourth Keck Symposium on Computational Biology, Pittsburgh, PA, October 24–November 5, 1993

MATIS, S., R. J. MURAL,* AND E. C. UBERBACHER, "Detection of Pre- and Post-Transcriptional Control Sequences in DNA Using Computational Methods." (3.74)

International Symposium on Experimental Robotics, Kyoto, Japan, October 27–29, 1993; Proc. (1993)

REISTER, D. B., M. A. UNSEREN, J. E. BAKER, AND F. G. PIN, "Experimental Investigations of Sensor-Based Surface Following Tasks by a Mobile Manipulator," pp. 110–114. (3.14)

Oral Presentation, University of Tennessee Statistics Department, Knoxville, TN, October 28, 1993

MORRIS, M. D., AND A. D. SOLOMON,* "Design and Analysis for an Inverse Problem of Advective-Dispersive Fluid Flow."

Annual Meeting of the Institute of Nuclear Materials Management, Oak Ridge, TN, October 28–29, 1993

LARSON, D. C., "Use of the Oak Ridge Electron Linear Accelerator (ORELA) for Active Nondestructive Assay (ANDA) and Material Certification Studies."

ICAR '93, The Sixth International Conference on Advanced Robotics, Tokyo, Japan, November 1–2, 1993

PIN, F. G., "On Approximate Reasoning and Minimal Models for the Development of Robust Outdoor Vehicle Navigation Schemes." (3.15)

WATANABE, Y., AND F. G. PIN, "Sensor-Based Navigation of a Mobile Robot Using Automatically Constructed Fuzzy Rules." (3.18)

Oral Presentation, Computer Science Department, University of Toronto, Toronto, Canada, November 2, 1993

DONGARRA, J. J., "PVM and MPI: Tools for Concurrent Computing."

Oral Presentation, IBM, Kingston, New York, November 3, 1993

DONGARRA, J. J., "The Design of a Scalable Linear Algebra Library and IBM's Power 2."

Oral Presentation, Columbia Meeting of the Southeastern Section of the American Physical Society, Columbia, SC, November 4–6, 1993

DRAKE, J. B., "Climate Modeling and the New Generation of Distributed Memory Parallel Computers."

Oral Presentation, International Atomic Energy Agency (IAEA) Advisory Group Meeting on Review of Uncertainty Files and Improved Multigroup Cross Section Files for FENDL, Tokai Research Establishment, JAERI, Tokai, Japan, November 8-12, 1993

LARSON, D. C., AND C. Y. FU, "Potential Improvements to ENDF/B-VI for Structural Materials."

ROUSSIN, R. W., "Recent Activities of CSEWG."

Oral Presentation, 1993 IEEE/Tsukuba International Workshop on Advanced Robotics, Tsukuba, Japan, November 8-9, 1993

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OSTROUCHOV, G., "Two Simple Applications of Parallel Computing in Statistics."

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BURNS, T. J., "CGVIEW Geometry Options."

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CRAMER, S. N., "Introduction to the Monte Carlo Method."

INGERSOLL, D. T., J. E. WHITE, R. W. ROUSSIN, AND C. Y. FU, "DABL69: Broad-Group Neutron/Photon Cross-Section Library for Defense Nuclear Applications."

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JOHNSON, J. O., "DORT A Two-Dimensional Discrete Ordinates Transport Code Input Instructions."

JOHNSON, J. O., "Sample Problem Definition."

LILLIE, R. A., "Theory of Discrete Ordinates."

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GABRIEL, T. A., AND C. ZEITNITZ,* "CALOR and GCALOR: Codes for Detector Design and Analysis."

Oral Presentation, Japanese Convex Users' Group, Kyoto, Japan, December 2, 1993

DONGARRA, J. J., "From Hand-Held to Teraflop Computers: LAPACK - Linear Algebra Software."

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LEE, S. L., S. F. ASHBY,* L. R. PETZOLD,* P. E. SAYLOR, AND E. SEIDEL,* "How to Enforce the Hamiltonian and Momentum Constraints in the Einstein Field Equations."

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RAO, N. S. V., "Fusion Rule Estimation in Multiple Sensor Systems with Unknown Noise Distributions." (3.35)

MADAN, R. N.,* N. S. V. RAO, V. P. BHATKAR,* AND L. M. PATNAIK* (Editors), "Parallel and Distributed Signal and Image Integration Problems." (3.49)

Oral Presentation, Annual American Mathematical Society Meeting on Nonlinear PDEs and Applications, Cincinnati, OH, January 12-15, 1994

LENHART, S. M., V. PROTOPODESCU, AND A. A. SZPIRO,* "Optimal Control for Competing Coalitions."

Oral Presentation, DIMACS Workshop on Interconnection Networks and Mapping and Scheduling Parallel Computations, Rutgers University, New Brunswick, NJ, February 7, 1994

DONGARRA, J. J., "Software Tools for Network Computing."

Oral Presentation, Maui High Performance Computing Center, Maui, HI, February 16, 1994

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LARSON, D. C., "The Oak Ridge Electron Linear Accelerator, An Intense, Pulsed Neutron, Photon and Positron Source and an ORNL User Facility."

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GUAN, X., R. J. MURAL,* AND E. C. UBERBACHER, "Protein Structure Prediction Using Hybrid AI Methods." (3.77)

Oral Presentation, BETECH (Boundary Element Technology) '94, Orlando, FL, March 16-18, 1994

ZARIKIAN, V.,* L. J. GRAY, AND G. PAULINO,* "Local Error Estimation for Boundary Element Calculations."

Oral Presentation, American Mathematical Society Meeting, Lexington, KY, March 18, 1994

DONGARRA, J. J., "Recent Work in Parallel Algorithms for the Linear Algebra."

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SPELT, P. F., AND S. L. JONES,* "Task Automation in a Successful Industrial Telerobot," pp. 88-92. (3.95)

March Meeting of the American Physical Society, Pittsburgh, PA, March 21-25, 1994

CHISHOLM, M. F.,* T. KAPLAN,* AND L. J. GRAY, "Morphology and Stress State of Thin Films," (oral presentation only).

NICHOLSON, D. M. C.,* X. G. ZHANG,* G. M. STOCKS,* Y. WANG,* W. A. SHELTON, Z. SZOTEK, AND W. M. TEMMERMAN,* "Approximate Fermi Functions for Accelerating Density Functional Calculations." (1.91)

SEIFU, D.,* F. J. PINSKI,* W. A. SHELTON, G. M. STOCKS,* AND D. D. JOHNSON,* "Total Energy Ordered and Disordered CuAu." (1.92)

STOCKS, G. M.,* D. M. C. NICHOLSON,* Y. WANG,* W. A. SHELTON, Z. SZOTEK,* AND W. M. TEMMERMAN,* "Towards a Scalable LDA Multiple Scattering Method for Large Systems." (1.97)

WANG, Y.,* G. M. STOCKS,* D. M. C. NICHOLSON,* W. A. SHELTON, X. Y. LIU,* Z. SZOTEK, AND W. M. TEMMERMAN,* "Scalable Large System Multiple Scattering Method: Application to CuZn Alloys." (1.100)

Oral Presentation, Emory Medical School, Atlanta, GA, March 22, 1994

PROTOPODESCU, V., "Chaos and Fractals: Potential Relevance for Medical Applications."

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DONGARRA, J. J., "Recent Work in Parallel Algorithms for the Linear Algebra," (oral presentation only).

NACHTIGAL, N. M., W. A. SHELTON, AND G. M. STOCKS,* "First Principles Simulations of Material Properties," (oral presentation only).

PEYTON, B. W., E. G. NG, AND B. NITROSSO,* "On the Solution of Stokes Pressure System Using Supernodal Cholesky Factorization." (1.40)

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SHELTON, W. A., G. M. STOCKS,* R. G. JORDAN,* Y. LIU,* L. QUI,* D. D. JOHNSON,* F. J. PINSKI,* J. B. STAUNTON,* AND B. GINATEMPO,* "First Principles Simulation of Materials Properties." (1.94)

Oral Presentation, Virginia Polytechnic Institute, Blacksburg, VA, April 1, 1994

PROTOPODESCU, V., "Chaos in Linear Systems: A Mathematical Artifact?"

Oral Presentation, Thinking Machines Corporation, Cambridge, MA, April 5, 1994

GEIST, G. A., "PVM 3.3: New Features, New Directions."

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BAKER, J. E., "Automatic Calibration of Laser Range Cameras Using Arbitrary Planar Surfaces," Vol. 2234, pp. 38-48. (3.40)

BECKERMAN, M., AND F. J. SWEENEY, "Segmentation and Cooperative Fusion of Laser Radar Image Data," Vol. 2233, pp. 88-98. (3.43)

Colorado Conference on Iterative Methods, Breckenridge, CO, April 5-9, 1994

FREUND, R. W.,* AND N. M. NACHTIGAL, "A Look-Ahead Variant of TFQMR." (1.74)

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GRAY, L. J., "Boundary Integral Methods for Crack Propagation Modeling."

Oral Presentation, Numerical Linear Algebra with Applications, Oberwolfach, Germany, April 9-16, 1994

NACHTIGAL, N. M., W. A. SHELTON, AND G. M. STOCKS,* "First Principles Simulations of Material Properties."

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FOSTER, I. T.,* AND D. W. WALKER, "Paradigms and Strategies for Scientific Computing on Distributed Memory," pp. 252-257. (1.9)

STOCKS, G. M.,* D. M. NICHOLSON,* W. A. SHELTON, Y. WANG,* Z. SZOTEK,* AND W. M. TEMMERMAN,* "Towards Scalable Electronic Calculations for Alloys." (1.96)

American Nuclear Society Topical Meeting on Advances in Reactor Physics, Knoxville, TN, April 11-15, 1994; Proc. (1994)

AZMY, Y. Y., "Neutron Transport Methods on Scalable Shared Memory Multiprocessors," Vol. I, pp. 396-405. (4.3)

GEHIN, J. C., J. P. RENIER, AND B. A. WORLEY, "A New Fuel Loading Design for the Advanced Neutron Source," Vol. III, pp. 273-282. (4.27)

KIRK, B. L., AND Y. Y. AZMY, "A New Communication Scheme for the Neutron Diffusion Nodal Method in a Distributed Computing Environment," Vol. I, pp. 298-306. (5.2)

LILLIE, R. A., "ANS Cold Source Neutronics Analysis," Vol. III, p. 355. (4.32)

SMITH, L. A., J. C. GEHIN, B. A. WORLEY, AND J. P. RENIER, "Validation of Multigroup Cross Sections for the Advanced Neutron Source Against the FOEHN Critical Experimental Measurements," Vol. III, pp. 444-452. (4.38)

Oral Presentation, Distinguished IEEE Lecture, University of Iowa, Iowa City, IA, April 14, 1994

DONGARRA, J. J., "Constructing Scalable Numerical Software Libraries for HPC Environments."

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DONGARRA, J. J., "Scalable High-Performance Libraries in Linear Algebra."

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DONGARRA, J. J., A. LUMSDAINE,* X. NIU,* R. POZO,* AND K. A. REMINGTON, "Sparse Matrix Libraries in C++ for High Performance Architectures." (1.32)

American Nuclear Society Eighth International Topical Meeting on Radiation Shielding, Arlington, TX, April 24-28, 1994; Proc. (1994)

AZMY, Y. Y., "Adjacent-Cell Preconditioners for Solving Optically Thick Neutron Transport Problems," Vol. 1, pp. 193-200. (4.1)

BUCHOLZ, J. A.,* "Shielding Analysis of the LMR In-Vessel Fuel Storage Experiments," Vol. 2, pp. 1309-1316. (4.18)

BUCHOLZ, J. A.,* "Overview of Shielding Analyses for the MHTGR From 1986 to 1991," Vol. 1, pp. 316-323. (4.17)

BURNS, T. J., "Implementation and Display of Computer Aided Design (CAD) Models in Monte Carlo Radiation Transport and Shielding Applications," Vol. 1, pp. 468-475. (4.5)

HUNTER, H. T., D. T. INGERSOLL, R. W. ROUSSIN, E. SARTORI,* AND C. O. SLATER, "SINBAD - A Shielding INtegral Benchmark Archive and Database for PCs," Vol. 2, 795-801. (4.28)

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JOB, P. K.,* T. HANDLER,* T. A. GABRIEL, C. O. SLATER, L. S. WATERS,* A. P. T. PALOUNEK,* AND C. ZEITNITZ,* "Neutron Fluence Calculations for the SDC Detector and the Results of Codes Comparison," Vol. 2, pp. 980-984. (4.54)

JOHNSON, J. O., R. T. SANTORO, AND M. S. SMITH, "Application of the MASH 1.0 Code System to Radiological Warfare Radiation Threats," Vol. 1, pp. 531-538. (4.66)

PEREZ, C. L.,* AND J. O. JOHNSON, "Vulnerability Assessment of a Space Based Weapon Platform Electronic System Exposed to a Thermonuclear Weapon Detonation," Vol. 1, pp. 611-618. (4.68)

RHOADES, W. A., "The TORSED and TORSET Codes for Coupling Three-Dimensional TORT Calculations," Vol. 1, pp. 551-557. (4.14)

RHOADES, W. A., J. M. BARNES,* AND R. T. SANTORO, "An Explanation of the Hiroshima Activation Dilemma," Vol. 1, pp. 238-244. (4.69)

SLATER, C. O., "Analysis of the JASPER Axial Shield Experiment," Vol. 2, pp. 1271-1278. (4.37)

SLATER, C. O., R. A. LILLIE, AND T. A. GABRIEL, "Shielding Optimization Studies for the Detector Systems of the Superconducting Super Collider," Vol. 2, pp. 972-979. (4.58)

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MATIS, S., M. SHAH, R. MURAL,* E. C. UBERBACHER, "Detection of Human RNA Polymerase II Promoters Using Artificially Intelligent Methods." (3.75)

Oral Presentation, Modulation of Signal Transduction and Gene Expression, Bethesda, MD, April 25-27, 1994

UBERBACHER, E. C., "Annotation of Genomic DNA Sequence Using the GRAIL Neural Network System."

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PIN, F. G., AND S. M. KILLOUGH,* "Omnidirectional Holonomic Platforms." (3.6)

RAO, N. S. V., "Stochastic Approximation Methods for Fusion-Rule Estimation in Multiple Sensor Systems," pp. 161-168. (3.36)

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GABRIEL, T. A., "Overview of New, Upgraded, or Proposed High Energy Facilities in the United States and Canada." (4.48)

Oral Presentation, Sixth Meeting of the NEANSC Working Party on International Evaluation Cooperation, Oak Ridge, TN, May 4-6, 1994

FU, C. Y., "Status Report of Subgroup 16 of the NEANSC Working Party on International Evaluation Cooperation."

FU, C. Y., D. C. LARSON, D. M. HETRICK,* H. VONACH,* J. KOPECKY,* S. IJIMA,* N. YAMAMURO,* T. ASAMI,* S. CHIBA,* G. MAINO,* AND I. MENGONI,* "Report of Subgroup 1 of the NEANSC Working Party on International Evaluation Cooperation."

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MERLO, A. P.,* AND P. H. WORLEY, "Analyzing PICL Trace Data with MEDEA," pp. 445-464. (1.16)

1994 IEEE International Conference on Robotics and Automation, San Diego, CA, May 8-13, 1994; Proc. (1994)

PIN, F. G., P. F. R. BELMANS, J.-C. CULIOLI,* D. D. CARLSON,* AND F. A. TULLOCH,* "A New Solution Method for the Inverse Kinematic Joint Velocity Calculations of Redundant Manipulators." pp. 96-102. (3.1)

International Conference on Nuclear Data for Science and Technology, Gatlinburg, TN, May 9-13, 1994

FU, C. Y., "Neutron Emission Spectra Calculated with Exciton Level Densities Based on One and Two Kinds of Fermions," (2.9)

LARSON, N. M.,* "Recent Improvements in the R-Matrix Analysis Code SAMMY," (oral presentation only).

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PACE, J. V., III, "Overview of the Nuclear Data Related to the Hiroshima Dosimetry Discrepancy." (4.67)

ROUSSIN, R. W., AND E. MENAPACE,* "NEA NSC WP International Evaluation Cooperation Subgroup 7/Multigroup Cross-Section Processing: Progress and New Directions." (5.4)

ROUSSIN, R. W., E. MENAPACE,* S. GANESAN,* M. GREENE,* A. HASAGAWA,* R. MACFARLANE,* V. MANOKHIN,* M. MATTES,* G. PANINI,* H. TAKANO,* J. WHITE, AND R. WRIGHT,* "International Evaluation Cooperation Subgroup 7/Multigroup Cross-Section Processing: Progress and New Directions," (oral presentation only).

ROUSSIN, R. W., P. G. YOUNG,* AND R. MCKNIGHT,* "Current Status of ENDF/B-VI." (5.7)

SPENCER, R. R., J. H. TODD,* N. M. LARSON,* AND L. W. WESTON,* "The ORNL Neutron-Capture Cross Section Facility." (2.7)

WHITE, J. E., R. Q. WRIGHT,* D. T. INGERSOLL, R. W. ROUSSIN, N. M. GREENE,* AND R. E. MACFARLANE,* "VITAMIN-B6: A Fine-Group Cross Section Library Based on ENDF/B-VI for Radiation Transport Applications." (5.5)

WRIGHT R. Q.,* J. E. WHITE, AND D. T. INGERSOLL, "Fast and Thermal Reactor Data Testing of ENDF/B-VI." (4.41)

WUNSTORF, R.,* W. M. BUGG,* C. C. PARKS,* T. A. GABRIEL, T. A. LEWIS,* AND J. K. DICKENS, "Experimental and Calculated Radionuclide Production by Photonuclear Reactions Using Bremsstrahlung Photons Produced by 150 MeV Electrons." (4.59)

Annual Meeting of the Mechanical Working Group of the Interagency Advanced Power Group (IAPG), Arlington, VA, May 10-11, 1994

HAALAND, C. M., "Four-Piston Double-Duct Liquid Metal MHD Engine and AC Generator." (4.71)

Oral Presentation, Genome Mapping and Sequencing, Cold Spring Harbor, NY, May 11-15, 1994

MURAL, R. J.,* M. SHAH, X. GUAN, S. PETROV, AND E. C. UBERBACHER, "GenQuest: A Sensitive Sequence Comparison Server for DNA and Proteins."

SHAH, M., J. R. EINSTEIN, S. MATIS, Y. XU, X. GUAN, D. BULEY,* R. J. MURAL,* AND E. C. UBERBACHER, "Gene Recognition and Modeling in the GRAIL System."

Oral Presentation, 5th Research Coordination Meeting on Validation of Safety Related Physics Calculations for Low Enriched Gas Cooled Reactors, Villigen, Switzerland, May 16-18, 1994

DIFILIPPO, F. C., "Experiments Analysis with Monte Carlo Methods. Benchmarking MCNP."

Oral Presentation, 1994 U.S. Department of Energy Defense Programs Packaging Workshop, Knoxville, TN, May 16-19, 1994

BIGELOW, J. E.,* C. W. ALEXANDER,* J. V. PACE, III, AND C. M. SIMMONS,* "A New Shipping Container for an Intense Neutron Emitter."

Department of Energy Defense Programs Packaging Workshop, Hyatt Regency, Knoxville, TN, May 16-20, 1994; Proc. Conf-9405109 (1994)

PRIMM, R. T., III, AND D. A. TOLLEFSON,* "Validation Calculations in Support of Transportation Safety Analyses." (4.36)

Oral Presentation, National Symposium on Americans with Disabilities from Diverse Cultural Communities, 1994 Annual National Conference, Atlanta, GA, May 17, 1994

BOWMAN, K. O., "Employment Opportunities in Science for Persons with Disabilities."

Vision Interface '94, Banff, Alberta, Canada, May 18-20, 1994

DORUM, O. H.,* A. HOOVER,* AND J. P. JONES, "Calibration and Control for Range Imaging in Mobile Robot Navigation." (3.41)

Oral Presentation, NASA High Performance Computing Semi-Lagrangian Transport Methods Workshop, NASA Goddard Space Flights Center, May 19, 1994

DRAKE, J. B., "Communication Strategies for Semi-Lagrangian Transport in Parallel Climate Models."

Oral Presentation, PVM Users Group Meeting, Garden Plaza Hotel, Oak Ridge, TN, May 19-20, 1994

KOHL, J. A., "XPVM: A Graphical Console and Monitor for PVM."

PAPADOPOULOS, P. M., "Enhancing PVM Group Performance - Milestones and Speed Bumps."

Scalable High Performance Computing Conference, Knoxville, TN, May 23-25, 1994; Proc. IEEE Computer Society Press (1994)

WORLEY, P. H., AND I. T. FOSTER,* "Parallel Spectral Transform Shallow Water Model: A Runtime-Tunable Parallel Benchmark Code," pp. 207-214. (1.86)

KOHL, J. A., "XPVM: A Graphical Console and Monitor for PVM." (1.15)

Workshop on Environments and Tools for Parallel Scientific Computing, Walland, TN, May 26-27, 1994

CHOI, J.,* J. J. DONGARRA, AND D. W. WALKER, "The Design of a Parallel, Dense Linear Algebra Software Library: Reduction to Hessenberg, Tridiagonal, and Bidiagonal Form." (1.25)

KOHL, J. A., AND T. L. CASAVANT,* "Equate Relationships in the IMPROV Program Visualization Environment." (1.45)

WALKER, D. W., J. CHOI,* AND J. J. DONGARRA, "Issues in the Design of Scalable Software Libraries for Distributed Memory," (oral presentation only).

6th International Conference on Computing and Information, Peterborough, Ontario, Canada, May 26-28, 1994

XU, Y., "Dynamic Subtrees: A New Data Structure for Manipulating Trees." (3.82)

Oral Presentation, Georgia Institute of Technology Spring Quarter Seminar Series, Atlanta, GA, May 27, 1994

PACE, J. V., III, "A Review of the Hiroshima Dosimetry Discrepancy."

AIR '94, Application of Artificial Intelligence and Robotics to Nuclear Plants, Tokai-mura, Naka-gun, Ibaraki, Japan, May 29-June 2, 1994

SPELT, P. F., C. CRANE,* L. FENG,* M. ABIDI,* AND S. TOSUNOGLU,* "A Wall-Crawling Robot for Reactor Vessel Inspection in Advanced Reactors." (3.63)

Oral Presentation, Parallel Tools Consortium, NASA Ames Research Center, Moffett Field, CA, June 8-10, 1994

KOHL, J. A., AND T. L. CASAVANT,* "The IMPROV Custom Animation Environment for Parallel Program Visualization."

IEEE Infocom '94: 13th Joint Conference on IEEE Computer and Communication Societies, Toronto, Canada, June 12-16, 1994

RAO, N. S. V., K. J. MALY,* S. OLARIU,* S. DHARANIKOTA,*
L. ZHANG,* AND D. GAME,* "Average Waiting Time Profiles of Uniform
DQDB Model." (3.65)

Oral Presentation, Nuclear Sister Laboratory Consultations, Kuala Lumpur, Malaysia, June 12-16, 1994

PRIMM, R. T., III, "Overview of Technical Capabilities Existing at Oak Ridge National Laboratory with Emphasis on Reactor Physics."

Fifth SIAM Conference on Applied Linear Algebra, Snowbird, UT, June 15-18, 1994; Proc. John G. Lewis (1994)

FREUND, R. W.,* AND N. M. NACHTIGAL, "QMRPACK and Applications." (1.75)

LEE, S. L., "Bounds for Eigenvalues for Departure from Normality, with Applications," pp. 509-511. (1.78)

NG, E., "A Comparison of Some Direct Methods for Solving Sparse Nonsymmetric Linear Systems." (1.35)

PEYTON, B. W., E. NG, AND J. GILBERT,* "Computing Row and Column Counts for Sparse QR Factorization." (1.43)

Oral Presentation, Workshop on Parallel Scientific Computing, Lyngby, Denmark, June 19-23, 1994

GEIST, G. A., "Cluster Computing: The Wave of the Future?"

Computer Science Colloquium, Sandia National Laboratory, Albuquerque, NM, June 20, 1994

PEYTON, B. W., E. G. NG, AND B. NITROSSO,* "On the Solution of Stokes Pressure System Using Supernodal Cholesky Factorization." (1.40)

Oral Presentation, Workshop on Parallel Scientific Computing - PARA '94, Danish Technical University, Lyngby, Denmark, June 21, 1994

DONGARRA, J. J., "Constructing Numerical Software Libraries for HPCC Environments."

Oral Presentation, The Federal Highway Administration Overview of the Development of an In-Vehicle Signing Specification, Washington, DC, June 21, 1994

KNEE, H. E., "Development of an In-Vehicle Signing Specification."

Seventh SIAM Conference on Discrete Mathematics, Albuquerque, NM, June 22-25, 1994

PEYTON, B. W., "Chordal-Graph Algorithms for Sparse Cholesky Factorization." (1.39)

Intel Supercomputer Users Group Meeting, San Diego, CA, June 26-29, 1994

SEMERARO, B. D., "Parallel Fast Fourier Transforms for Non Power of Two Data." (1.82)

1994 ASA Conference on Radiation and Health, Nantucket, MA, June 26-July 1, 1994

MITCHELL, T. J., G. OSTROUCHOV, E. L. FROME, AND G. D. KERR,* "A Method for Estimating Occupational Radiation Dose to Individuals, Using Weekly Dosimetry Data." (1.118)

IEEE World Congress on Computational Intelligence, Orlando, FL, June 26-July 2, 1994; Proc. IEEE International Conference on Neural Networks, Vol. 2 (1994)

RAO, N. S. V., V. R. R. UPPULURI,* AND E. M. OLOW, "On Stochastic Approximation Algorithms for Classes of PAC Learning Problems," pp. 791-796. (3.33)

Oral Presentation, High-Performance Computing: Technology and Applications Advanced Workshop, Cetraro, Italy, June 28, 1994

DONGARRA, J. J., "ScaLAPACK, Its Building Blocks, and PVM."

IEEE International Conference on Neural Networks, Orlando, FL, June 28-July 2, 1994; Proc. Vol. V (1994)

NEIS, E.,* F. W. STARR,* T. HANDLER,* T. A. GABRIEL, C. W. GLOVER, AND S. SAINI,* "Using Neural Networks as an Event Trigger in Elementary Particle Physics Experiments," pp. 3056-3060. (4.57)

Seminar at the Mathematics and Computer Science Department, University of Odense, Odense, Denmark, July 4, 1994

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Oral Presentation, BaBar Detector Collaboration Meeting, Stanford Linear Accelerator Center, Stanford, CA, July 7-12, 1994

GABRIEL, T. A., "Background and Trigger Studies for the BaBar Detector."

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Oral Presentation, International Conference on the Human Genome Project, Washington, DC, October 2-5, 1994

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Oral Presentation, IBM European Supercomputer Users Meeting, Supeur 94, Amsterdam, October 3, 1994

DONGARRA, J. J., "Constructing Scalable Numerical Software Libraries for
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DONGARRA, J. J., "PVM and MPI: Tools for Concurrent Computing."

Oral Presentation, Workshop on Debugging and Performance Tuning for Parallel Computing Systems, Chatham, MA, October 4, 1994

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Oral Presentation, Work on Large Systems on Parallel Computers, Wuppertal, Germany, October 6, 1994

DONGARRA, J. J., "Recent Work in Parallel Algorithms for the Linear
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Oral Presentation, Midwest Differential Equations Conference, Norman, OK, October 7, 1994

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1994 Scalable Parallel Libraries Conference, Mississippi State University, Starkville, MS, October 12-14, 1994

WALKER, D. W., "An MPI Version of the BLACS." (1.22)

Oral Presentation, Swiss Scientific Computing Center, Lugano, Switzerland, October 17, 1994

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Oral Presentation, Convex European Users' Group Meeting, Krakow, Poland, October 19, 1994

DONGARRA, J. J., "Benchmarking Parallel Machines."

Oral Presentation, Differential Equations Conference, University of Tennessee, Knoxville, TN, October 21-22, 1994

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38th Annual Meeting of the Human Factors and Ergonomics Society, Nashville, TN, October 24-28, 1994; Proc. (1994)

KNEE, H. E., P. F. SPELT, M. M. HOUSER,* AND W. E. HILL,* "Operator Role Definition: An Initial Step in the Human Factors Engineering Design of the Advanced Neutron Source (ANS)," Vol. 2, pp. 1013-1017. (3.93)

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SPELT, P. F., AND S. L. JONES,* "Operator-Centered Control of a Semi-Autonomous Industrial Robot." (3.94)

Dagstuhl Seminar 9443 on Environment Modeling and Motion Planning, Dagstuhl, Germany, October 24-28, 1994

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Cross Section Evaluation Working Group, Oak Ridge, TN, October 25-27, 1994

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ROUSSIN, R. W., "Summary of NEANSC Working Party - International Evaluation Cooperation Meeting, May 5-6, 1994, Oak Ridge, Tennessee," (oral presentation only).

Oral Presentation, University of Wisconsin, Madison, WI, October 31, 1994

NG, E. G., "Direct Solution of Sparse Linear Systems: Algorithms, Codes, and Performance."

International Dedicated Conference on Robotics, Motion and Machine Vision, Aachen, Germany, October 31-November 4, 1994

RAO, N. S. V., "Unknown-Terrains Navigation of a Mobile Robot Using an Array of Sonars." (3.25)

Oral Presentation, Second IAEA RCM Meeting on Improvement of Measurements, Calculations and Evaluations of Neutron-Induced Helium Production Cross Sections, Beijing, China, November 1-4, 1994

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Robotics Industry Forum and Annual Meeting, Orlando, FL, November 2-4, 1994

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Nuclear Engineering Seminar, Georgia Institute of Technology, Atlanta, GA, November 4, 1994

INGERSOLL, D. T., "Design and Neutronics Issues for the Advanced Neutron Source."

Oral Presentation, The Ninth International Symposium on Computer and Information Sciences ISCIS IX, Antalya, Turkey, November 7-9, 1994

DONGARRA, J. J., "Software Tools and Templates for Developing a Software Library for High-Performance Computers."

Oral Presentation, Conference on Beryllium Disease Research Triangle Park, NC, November 8-10, 1994

FROME, E. L., M. H. SMITH,* R. L. NEUBERT,* AND S. P. COLYER,* "Statistical Methods for the Blood Lymphocyte Proliferation Test."

OECD NEANSC Specialists' Meeting on Measurement, Calculation and Evaluation of Photon Production Data, Bologna, Italy, November 8-11, 1994

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1994 Winter Meeting of the American Nuclear Society Tutorial Review of Solution Methods and Applications of the One-Group Transport Equation, Washington, DC, November 13-17, 1994; Trans. Am. Nucl. Soc. 71 (1994)

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DOE Contractor's Meeting, Santa Fe, NM, November 13-17, 1994

PETROV, S., M. SHAH, L. HAUSER,* R. MURAL,* AND E. C. UBERBACHER, "Informatics Support for Mapping in Mouse-Human Homology Regions." (3.81)

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IAEA First Research Coordination Meeting on Measurement, Calculation and Evaluation of Photon Production Data, Bologna, Italy, November 14-17, 1994

DICKENS, J. K., "Precision Measurement of the ^{56}Fe Cross Section for the $E_\gamma=846\text{-keV}$ Transition and for E_n Between Threshold and 4 MeV." (2.2)

Seminar, National Institute of Standards and Technology, November 16, 1994

MORRIS, M. D., "Some Recent Developments in the Design and Analysis of Computer Experiments, and an Input Screening Example."

Oral Presentation, Radiation Sciences Simulation and Modeling Conference, Williamsburg, VA, November 19-December 1, 1994

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JOHNSON, J. O., "MASH The Nuclear Vulnerability Assessment Code of the U.S. Army."

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LIU, C. L.,* J. N. LEOEUF,* R. F. WOOD,* D. B. GEOHEGAN,* J. M. DONATO, K. R. CHEN,* AND A. A. PURETZKY,* "Modeling of Thermal, Electronic, Hydrodynamic, and Dynamic Deposition Processes for Pulsed-Laser Deposition of Thin Films." (1.62)

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Oral Presentation, Michigan State University, East Lansing, MI, December 13, 1994

DONGARRA, J. J., "ScaLAPACK, Its Building Blocks, and PVM."

Oral Presentation, 33rd IEEE Conference on Decision and Control, Lake Buena Vista, FL, December 14-16, 1994

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