DOE Grant #DE-FG02-03ER25549

Second SIAM Conference on Computational Science and Engineering

February 10-12, 2003

San Diego, California

The Second SIAM Conference on Computational Science and Engineering was held in San Diego from February 10-12, 2003. Total conference attendance was 553. This is a 23% increase in attendance over the first conference. The focus of this conference was to draw attention to the tremendous range of major computational efforts on large problems in science and engineering, to promote the interdisciplinary culture required to meet these large-scale challenges, and to encourage the training of the next generation of computational scientists.

Computational Science & Engineering (CS&E) is now widely accepted, along with theory and experiment, as a crucial third mode of scientific investigation and engineering design. Aerospace, automotive, biological, chemical, semiconductor, and other industrial sectors now rely on simulation for technical decision support. For federal agencies also, CS&E has become an essential support for decisions on resources, transportation, and defense.

CS&E is, by nature, interdisciplinary. It grows out of physical applications and it depends on computer architecture, but at its heart are powerful numerical algorithms and sophisticated computer science techniques. From an applied mathematics perspective, much of CS&E has involved analysis, but the future surely includes optimization and design, especially in the presence of uncertainty. Another mathematical frontier is the assimilation of very large data sets through such techniques as adaptive multi-resolution, automated feature search, and low-dimensional parameterization.

The themes of the 2003 conference included, but were not limited to:
Advanced Discretization Methods
Computational Biology and Bioinformatics
Computational Chemistry and Chemical Engineering
Computational Earth and Atmospheric Sciences
Computational Electromagnetics
Computational Fluid Dynamics
Computational Medicine and Bioengineering
Computational Physics and Astrophysics
Computational Solid Mechanics and Materials
CS&E Education
Meshing and Adaptivity
Multiscale and Multiphysics Problems
Numerical Algorithms for CS&E
Discrete and Combinatorial Algorithms for CS&E
Inverse Problems
Optimal Design, Optimal Control, and Inverse Problems
Parallel and Distributed Computing
Problem-Solving Environments
Software and Middleware Systems
Uncertainty Estimation and Sensitivity Analysis
Visualization and Computer Graphics

DISCLAIMER

Conference Format

The conference featured 11 invited plenary presentations, 86 mini-symposia, 32 contributed paper sessions, and a poster session featuring 26 presenters. In total, 514 presentations were made at the meeting. There also was special session commemorating the 100th anniversary of the birth of John von Neumann. Prior to the conference, three tutorials on timely and important themes were presented. The subjects of these tutorials were, respectively, adaptive methods for PDEs, uncertainty quantification, and scientific visualization.

The eleven plenary presentations were given by leading computational scientists drawn from a number of disciplines and organizations, including government laboratories and industry. Each presentation was extremely well attended and well received.

A New Era in Computational Science

Francine D. Berman, University of California, San Diego, NPACI

Computational Science and Engineering Aspects of Wildland Fire Modeling

Janice L. Coen, National Center for Atmospheric Research

Computational Proteomics: Prediction of Protein Function on a Genome-Scale

Mark Gerstein, Yale University

Architecture and Algorithms

William D. Gropp, Argonne National Laboratory

Combinatorial Scientific Computing: The Role of Discrete Algorithms in Computational Science and Engineering

Bruce Hendrickson, Sandia National Laboratories

Variational and Multiscale Methods in Turbulence with Particular Emphasis on Large Eddy Simulation

Thomas J.R. Hughes, University of Texas, Austin

High Performance Computing for Image Guided Therapy

Ron Kikinis, Brigham and Women's Hospital and Harvard Medical School

A Numerical Toolkit for Microsystem (MEMS) Design: System Modeling, Device Model Creation, and Point Solvers

Tom Korsmeyer, Coventor, Inc.

Science Discoveries using Computational Astrophysics
Michael L. Norman, University of California, San Diego

The Fast Flow Dynamics of Polymer Solutions As Calculated Using Implicit Configurational Time Stepping Schemes
Eric S.G. Shaqfeh, Stanford University

Arteries and Algorithms: Computational Modelling of the Human Vascular System
Spencer Sherwin, Imperial College, University of London

The overall conference program was well received. In an evaluation handed out to attendees, 90% agreed that the program and invited speakers were excellent. The conference program is archived on the SIAM website at http://www.siam.org/meetings/cse03/index.htm.

Conference Organization
The conference was organized by Steven F. Ashby (Co-chair) Lawrence Livermore National Laboratory, Isabelle Charpentier, Institut d'Informatique et Mathematiques Appliques de Grenoble, John Drake, Oak Ridge National Laboratory, Omar Ghattas (Co-chair), Carnegie Mellon, Gene H. Golub, Stanford University, George M. Homsy, University of California, Santa Barbara, Christopher R. Johnson, University of Utah, David E. Keyes (Co-chair), Old Dominion University, Michael Levitt, Stanford University, Linda R. Petzold (Co-chair), University of California, Santa Barbara, Michael Ortiz, California Institute of Technology, John Shadid, Sandia National Laboratories, Shang-Hua Teng, Akamai/Boston University, and Mary F. Wheeler, University of Texas, Austin.

SIAM conducted this conference with support from the Department of Energy, the National Science Foundation, and the Office of Naval Research. This support is deeply appreciated and was acknowledged during the meeting.

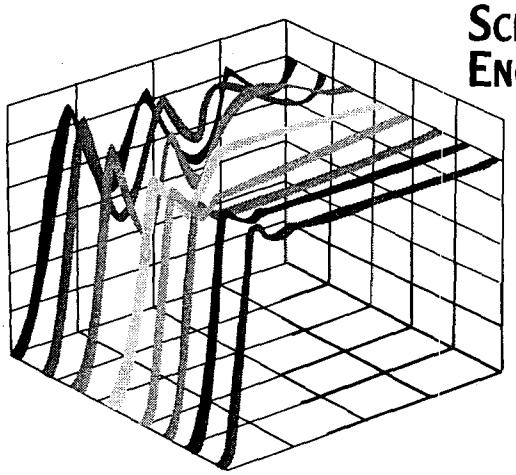
Student Support
SIAM made available a limited amount of support for students to attend the conference. The priority for funding was student speakers, students, post docs, and others, in that order. Several students received travel awards under this program.

Summary
This meeting was an extraordinary success, as evidenced by both the large attendance and the large increase in attendance and presentations over the first conference. Many attendees remarked that this kind of meeting was long overdue and that SIAM was the right professional society to organize it. The organizers were particularly happy to see that a number of computer scientists, domain scientists, and engineers attended, in addition to a large number of computational and applied mathematicians.

Submitted by
William G. Kolata
SIAM Technical Director

Final Program and Abstracts

SIAM Conference on COMPUTATIONAL SCIENCE AND ENGINEERING



February 10 - 13, 2003

Hyatt Regency Islandia Hotel & Marina San Diego, CA

Sponsored by the SIAM Activity Group on Computational Science and Engineering.

The SIAM Activity Group on CS&E fosters collaboration and interaction among applied mathematicians, computer scientists, domain scientists and engineers in those areas of research related to the theory, development, and use of computational technologies for the solution of important problems in science and engineering. It seeks to promote and facilitate CS&E as an academic discipline, and simulation as a peer to theory and experiment in the process of scientific discovery.

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www.siam.org/meetings/cse03/

siam® Society for Industrial and Applied Mathematics

Table of Contents

Organizing Committee

Steven F. Ashby (Co-chair), Lawrence Livermore National Laboratory

Isabelle Charpentier, Institut d'Informatique et Mathematiques Appliquees de Grenoble

John Drake, Oak Ridge National Laboratory

Omar Ghattas (Co-chair), Carnegie Mellon University

Gene H. Golub, Stanford University

George M. Homsy, University of California, Santa Barbara

Christopher R. Johnson, University of Utah

David E. Keyes (Co-chair), Old Dominion University

Michael Levitt, Stanford University

Linda R. Petzold (Co-chair), University of California, Santa Barbara

Michael Ortiz, California Institute of Technology

John Shadid, Sandia National Laboratories

Shang-Hua Teng, Akamai/Boston University

Mary F. Wheeler, University of Texas, Austin

General Information

SIAM Registration Desk

The SIAM registration desk is located in the Regency Annex. It is open at the following times:

Saturday, February 8
4:00 PM - 7:00 PM

Sunday, February 9
8:00 AM - 6:00 PM

Monday, February 10
7:30 AM - 5:30 PM

Tuesday, February 11
8:00 AM - 5:30 PM

Wednesday, February 12
8:00 AM - 5:30 PM

Thursday, February 13
8:00 AM - 2:00 PM

Hotel Address

Hyatt Regency Islandia Hotel & Marina

1441 Quivira Road

San Diego, California 92109

Hotel Telephone Number

The telephone number of the Hyatt Regency Islandia Hotel & Marina is (619) 224 1234. The hotel operator can either connect a caller with the SIAM registration desk for a message to be taken and posted to the SIAM message board or forward a caller to an attendee's room to leave a message.

Corporate Members & Sponsor

SIAM corporate members provide their employees with knowledge about, access to, and contacts in the applied mathematics and computational sciences community through their membership benefits. Corporate membership is more than just a bundle of tangible products and services; it is an expression of support for SIAM and its programs. SIAM is pleased to acknowledge its corporate members. In recognition of their support, non-member attendees who are employed by the following organizations are entitled to the SIAM member registration rate.

Corporate Sponsor

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IDA Center for Communications Research, Princeton

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Pacific Northwest National Laboratory, operated for the Department of Energy by Battelle

Schlumberger-Doll Research

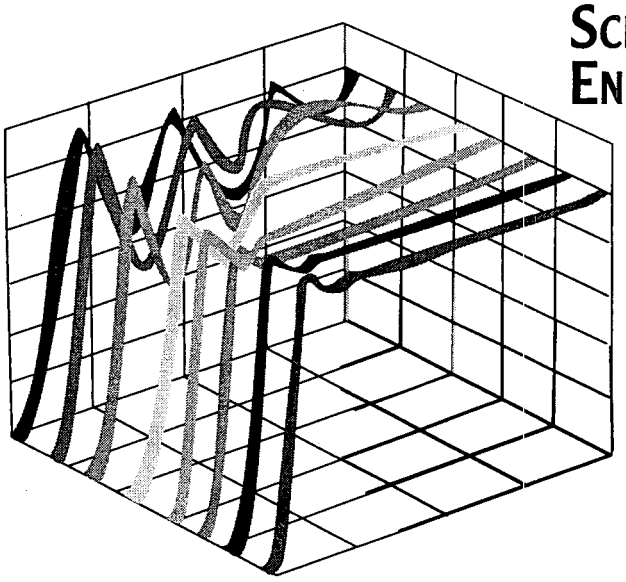
Telcordia Technologies

Xerox Corporation PARC

*List current at time of printing.

CSE03
Program-At-A-Glance

SIAM Conference on **COMPUTATIONAL SCIENCE AND ENGINEERING**



February 10 - 13, 2003

Hyatt Regency Islandia
Hotel & Marina
San Diego, CA

CSE03 Program-at-a-Glance

Saturday & Sunday February 8 & 9

5:00 PM - 8:00 PM
Registration
Regency Annex

Sunday, February 9

8:00 AM - 6:00 PM
Registration
Regency Annex

8:00 AM - 6:00 PM
E-Mail
Regency Annex

9:00 AM - 5:00 PM
Concurrent Sessions
SC1 *Mission Ballroom A*
SC2 *Mission Ballroom B*
SC3 *Mission Ballroom C*

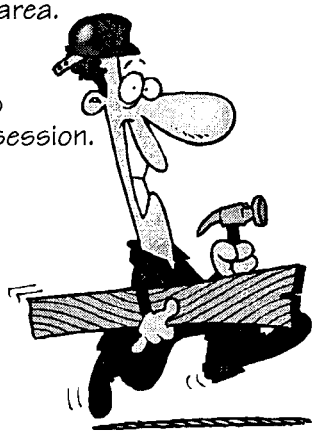
10:00 AM - 10:30 AM
Coffee Break
Regency Annex

12:00 PM - 1:30 PM
Short Course Luncheon
Regency Ballroom A

3:00 PM - 3:30 PM
Coffee Break
Regency Annex

6:00 PM - 9:00 PM
Welcome Reception
Islandia Restaurant

UNDER CONSTRUCTION
This program is subject to change. Check the "Program Updates" posted on the bulletin board located in the registration area. Changes are posted once daily, prior to the opening session.



Monday February 10

7:30 AM - 5:30 PM
Registration
Regency Annex

8:00 AM - 6:00 PM
E-Mail
Regency Annex

8:15 AM - 8:30 AM
Welcoming Remarks
Omar Ghattas, Carnegie Mellon University
Regency Ballroom

8:30 AM - 9:15 AM
IP1 High Performance Computing for Image Guided Therapy
Ron Kikinis, Brigham and Women's Hospital and Harvard Medical School
Regency Ballroom

9:15 AM - 10:00 AM
IP2 The Fast Flow Dynamics of Polymer Solutions As Calculated Using Implicit Configurational Time Stepping Schemes
Eric S.G. Shaqfeh, Stanford University
Regency Ballroom

10:00 AM - 10:30 AM
Coffee Break
Regency Annex

10:30 AM - 12:30 PM
Concurrent Sessions
MS1 *Regency Ballroom A*
MS2 *Regency Ballroom B*
MS3 *Regency Ballroom C*
MS4 *Mission Ballroom A*
MS5 *Mission Ballroom B*
MS6 *Mission Ballroom C*
MS7 *Island Ballroom A*
MS8 *Island Ballroom B*
MS9 *Garden Room A*
MS10 *Garden Room C*
MS11 *Garden Room D*
MS12 *Garden Room F*

12:30 PM - 2:00 PM
Lunch Break
Attendees on Own

2:00 PM - 2:45 PM
IP3 A New Era in Computational Science
Fran Berman, NPACI and University of California, San Diego
Regency Ballroom

2:45 PM - 3:15 PM
Coffee Break
Regency Annex

Monday February 10

3:15 PM - 5:15 PM
Concurrent Sessions
MS13 *Regency Ballroom A*
MS14 *Regency Ballroom B*
MS15 *Regency Ballroom C*
MS16 *Mission Ballroom A*
MS17 *Mission Ballroom B*
MS18 *Mission Ballroom C*
MS19 *Island Ballroom A*
MS20 *Island Ballroom B*
MS21 *Garden Room A*
MS22 *Garden Room C*
MS23 *Garden Room D*
MS24 *Garden Room F*

5:15 PM - 5:20 PM
Intermission

5:20 PM - 6:20 PM
Concurrent Sessions
CP1 *Regency Ballroom A*
CP2 *Regency Ballroom B*
CP4 *Mission Ballroom A*
CP5 *Mission Ballroom B*
CP6 *Mission Ballroom C*
CP7 *Island Ballroom A*
CP8 *Island Ballroom B*
CP9 *Garden Room C*
CP10 *Garden Room D*
CP11 *Garden Room F*

5:20 PM - 6:40 PM
CP3 *Regency Ballroom C*

8:00PM - 10:00PM
John Von Neumann's 100th Birthday Celebration Symposium
Regency Ballroom

Program-At-A-Glance

Quick Guide to
SIAM Conference on
Computational Science
and Engineering

OPEN HERE

Non SIAM Members Join SIAM Now and SAVE!

If you register for the Computational Science and Engineering Conference as a member, you save $90! SIAG/CSE members save an additional $10! Join SIAM now and enjoy a 2003, 12-month membership for just $108. For postgraduates, a one-year membership is only $54 and full-time students dues are $23.

SIAM members receive subscriptions to SIAM Review and SIAM News, and enjoy substantial discounts on SIAM books, journal subscriptions and conference registrations.

SIAM Audio-visual Policy

Standard AV Set-Up in Meeting Rooms Computers will not be ordered for any speakers. If Power Point or another type of presentation utilizing computer is planned, the speaker must bring his/her own computer.

If you have questions regarding availability of equipment in the meeting room of your presentation, please see a SIAM staff member at the registration desk.

Hotel Check-in and Check-out Times

Check in time is 4:00PM

Checkout time is 12:00PM

E-mail Access

Located in the Regency Annex during the following times:

Sunday	8:00 AM - 6:00 PM
Monday	8:00 AM - 6:00 PM
Tuesday	8:00 AM - 6:00 PM
Wednesday	8:00 AM - 6:00 PM
Thursday	8:00 AM - 2:00 PM

Registration Fee Includes

Two Coffee Breaks

Room set-ups and audio-visual equipment

Admission to all Technical Sessions

Welcome Reception

Poster Session and Dessert Reception

Job Postings

There is a dedicated bulletin board located in the registration area for job postings. Academic and corporate employers who wish to solicit applications or interview during the conference should post information here. Attendees who wish to review job opportunities should check this board.

Important Notice to Poster Presenters

Poster presenters are requested to set up their poster material in Regency Annex. Presenters may set up their posters on Monday or Tuesday between the hours of 8:00 AM and 5:00 PM. **All materials must be posted by 8:00 PM Tuesday, the official start time of the session.** Posters will remain on display through 10:30 AM on Thursday. Poster displays must be removed by 2:00 PM on Thursday, February 13, 2003. Posters remaining after this time will be discarded. SIAM is not responsible for discarded posters.

Get-togethers

Welcome Reception

Sunday, February 9

6:00PM - 9:00PM

Islandia Restaurant

John Von Neumann's 100th Birthday Celebration Symposium

Monday, February 10

8:00PM - 10:00PM

Regency Ballroom

Poster Session

Tuesday, February 11

8:00PM - 10:00PM

Regency Annex

Business Meeting

Wednesday, February 12

6:30PM - 7:30PM

Regency A & B

Cash & Carry Breakfast and Lunch for SIAM Meeting Attendees

KOI pond area of the gardens.

Monday, 2/10 through Thursday, 2/13

7:30AM - 8:30AM

The Hyatt Islandia is offering breakfast items; coffee, juice, danish or bagle, at the cost of $7.00 plus tax.

12:30PM - 1:30PM

The Hyatt Islandia is offering lunch items; sandwich, fruit, dessert, drink, at the cost of $12.00 plus tax.

The hotel restaurants are also open to serve you if you would prefer to have a sit down meal. The cash and carry meals have been arranged for your convenience.

Short Courses

SC1 Adaptive Methods for PDE-solution

Organizers:

David Brown
Center for Applied Scientific Computing
Lawrence Livermore National Laboratory

Lori Freitag
Mathematics and Computer Science Division
Argonne National Laboratory

Lecturers:

Phillip Colella
Lawrence Berkeley National Laboratory

James Glimm
SUNY Stony Brook, Brookhaven National Laboratory

Mark Shephard
Rensselaer Polytechnic Institute

SC2 Uncertainty Quantification

Organizers:

Roger Ghanem
Johns Hopkins University

Steve Wojtkiewicz
Sandia National Laboratories

Lecturers:

Roger Ghanem
Johns Hopkins University

Steve Wojtkiewicz
Sandia National Laboratories

SC3 SIAM Short Course on Scientific Visualization

Organizer:

Chris Johnson
University of Utah

Lecturers:

Greg Abram
IBM Data Explorer

Will Schroeder
Kitware Inc.

David Weinstein
Scientific Computing and Imaging Institute

SIAM/ACM Prize in Computational Science and Engineering

SIAM Establishes New Prize in CS&E

At its July 2002 meetings, the SIAM Council and Board of Trustees gave final approval to establishing a new prize in the area of computational science and engineering. SIAM and the ACM jointly award this prize.

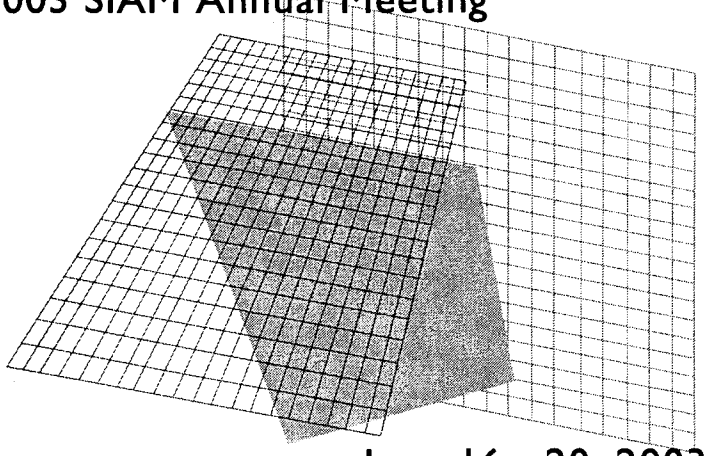
The SIAM/ACM Prize in Computational Science and Engineeering recognizes outstanding contributions to the development and use of mathematical and computational tools and methods for the solution of science and engineering problems.

The nomination process is open from now until March 14, 2003. Information about nominations, as well as the prizespecifications, are available on SIAM's website.

This prize has a substantial endowment from funds remaining from the SIAM Institute for Scientific Computing. These fundswere legally transferred entirely to the prize fund, and should endow this prize in perpetuity.

Mark Your Calendar!

First Joint Meeting of CAIMS & SIAM
24th Annual Meeting of CAIMS / SCMAI
2003 SIAM Annual Meeting



June 16 - 20, 2003
Queen Elizabeth Hotel
Montreal, QC • Canada

Invited Plenary Speakers

Monday, February 10

8:30 AM - 9:15 AM

IP1 High Performance Computing for Image Guided Therapy
Ron Kikinis, Brigham and Women's Hospital and Harvard Medical School

9:15 AM - 10:00 AM

IP2 The Fast Flow Dynamics of Polymer Solutions As Calculated Using Implicit Configurational Time Stepping Schemes
Eric S.G. Shaqfeh, Stanford University

2:00 PM - 2:45 PM

IP3 A New Era in Computational Science
Fran Berman, NPACI and University of California, San Diego

Tuesday, February 11

8:30 AM - 9:15 AM

IP4 Computational Proteomics: Prediction of ProteinFunction of Genome-Scale
Mark Gerstein, Yale University

9:15 AM - 10:00 AM

IP5 Architecture and Algorithms
William D. Gropp, Argonne National Laboratory

2:00 PM - 2:45 PM

IP6 Computational Science and Engineering Aspects of Wildland Fire Modeling
Janice Coen, National Center for Atmospheric Research

All Invited Plenary presentations will be given in the Regency Ballroom

Invited Plenary Speakers

Wednesday, February 12

8:30 AM - 9:15 AM

IP7 The Evolving Numerical Toolkit for Micro Machined Device (MEMS) Design: Fast Integral Equation Solvers, Coupled Domain Techniques, and Model Reduction

Jacob White, Massachusetts Institute of Technology

9:15 AM - 10:00 AM

IP8 Variational and Multiscale Methods in Turbulence with Particular Emphasis on Large Eddy Simulation

Thomas J.R. Hughes, University of Texas, Austin

2:00 PM - 2:45 PM

IP9 Combinatorial Scientific Computing: The Role of Discrete Algorithms in Computational Science and Engineering

Bruce Hendrickson, Sandia National Laboratories

Thursday, February 13

8:30 AM - 9:15 AM

IP10 Arteries and Algorithms: Computational Modelling of the Human Vascular System

Spencer Sherwin, Imperial College, London, United Kingdom

9:15 AM - 10:00 AM

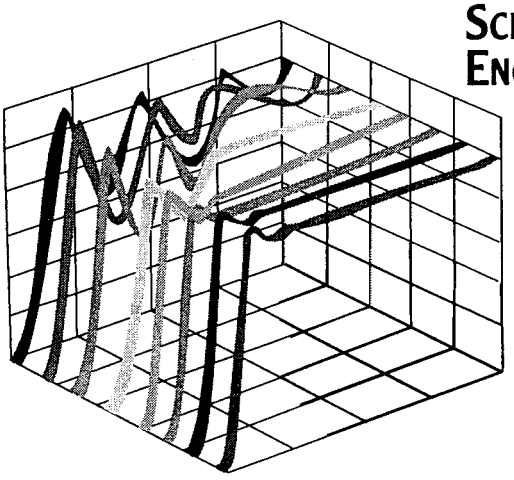
IP11 Science Discoveries using Computational Astrophysics

Michael Norman, University of California, San Diego

All Invited Plenary presentations will be given in the Regency Ballroom

Program

SIAM Conference on COMPUTATIONAL SCIENCE AND ENGINEERING



February 10 - 13, 2003

Hyatt Regency Islandia
Hotel & Marina
San Diego, CA

Saturday, February 8

Registration

5:00 PM-8:00 PM

Regency Annex

Sunday, February 9

Registration

8:00 AM - 6:00 PM

Regency Annex

Concurrent Short Courses
9:00 AM - 5:00 PM

SC1 SIAM Short Course on Adaptive Methods for PDE-solution

Mission Ballroom A

Organizers:

David Brown, Lawrence Livermore National Laboratory

Lori Freitag, Argonne National Laboratory

Lecturers:

Phillip Colella
Lawrence Berkeley National Laboratory

James Glimm
SUNY Stony Brook, Brookhaven National Laboratory

Mark Shephard
Rensselaer Polytechnic Institute

SC2 SIAM Short Course on Uncertainty Quantification

Mission Ballroom B

Organizers:

Steve Wojtkiewicz, Sandia National Laboratories

Roger Ghanem, Johns Hopkins University

Lecturers:

Roger Ghanem
The Johns Hopkins University

Steve Wojtkiewicz
Sandia National Laboratories

SC3 SIAM Short Course on Scientific Visualization

Mission Ballroom C

Organizer:

Chris Johnson
University of Utah

Lecturers:

Greg Abrams
IBM T.J. Watson Laboratory

Will Schroeder
Kitware

David Weinstein
Scientific Computing and Imaging Institute

Coffee Break
10:00 AM - 10:30 AM
Regency Annex

Luncheon
12:00 PM - 1:30 PM
Regency Ballroom A

Coffee Break
3:00 PM - 3:30 PM
Regency Annex

Welcome Reception
6:00 PM - 9:00 PM
Islandia Restaurant

Monday, February 10

Registration

7:30 AM-5:30 PM

Regency Annex

Welcoming Remarks

8:15 AM-8:30 AM

Room: Regency Ballroom

Omar Ghattas, Carnegie Mellon University

IP1

High Performance Computing for Image Guided Therapy

8:30 AM-9:15 AM

Regency Ballroom

Chair: Chris Johnson, University of Utah

Most tissues in the human body are not transparent. This is one of the fundamental limitations of conventional surgery. The objective of image guided therapy (IGT) is to overcome this limitation through the use of volumetric diagnostic imaging. All imaging modalities available in a modern radiology department have been used for IGT procedures. In its most advanced implementation, IGT requires "on-line" processing of intraoperatively acquired image data. Preoperative images need to be modified to incorporate intraoperative changes.

The computer science component of IGT is addressed with algorithms from the fields of applied mathematics, computer vision, computer graphics, and systems engineering. For working solutions, segmentation, registration and sophisticated rendering techniques have to be combined into complex software systems. It takes years to develop the appropriate algorithmic approaches and to implement them into practical systems. High performance computing (HPC) can be used in IGT as a "time machine", giving scientists and engineers access to future levels of computational performance today. This requires the integration of proper parallelization and network communication technologies.

The presentation will introduce the application domain and algorithms and will give examples for the successful execution of IGT concepts in real surgical and interventional procedures using magnetic resonance imaging.

Ron Kikinis
Brigham & Womens Hospital and Harvard Medical School

IP2

The Fast Flow Dynamics of Polymer Solutions As Calculated Using Implicit Configurational Time Stepping Schemes

9:15 AM-10:00 AM

Regency Ballroom

Chair: Gene H. Golub, Stanford University

Polymer solution dynamics in flows far from equilibrium involves a host of interesting nonlinear dynamics in systems containing thousands of degrees of freedom per molecular chain. These dynamics are critical to understanding many important applications such as fiber spinning, coating, or drag reduction. Typically these flows are calculated beginning with a bead-spring model for the polymer which involves constraining forces which become singular in the limit as the flow tends to pull the chain beyond some finite extensibility. Solvers for these configurational dynamics can be of two types: stochastic solvers or Brownian dynamics which try to reproduce a configurational path or field and preaveraged solvers which within closure approximations allow an average moment of the configurational field to be determined directly. For both solvers, time stepping near the singularity in the constraining force becomes very important for fast flows. I will discuss a series of algorithms that have been developed to implicitly time-step these equations and demonstrate that the savings in computer time per simulation can be more than an order of magnitude over explicit or predictor-corrector techniques. I will then demonstrate the usefulness of these techniques via calculations involving three important examples: fast stress relaxation of polymers following strong extensional flow, critical fluctuations of polymers in mixed flows near the shear flow boundary, and polymer-induced turbulent drag reduction.

Eric S.G. Shaqfeh
Stanford University

Coffee Break

10:00 AM-10:30 AM

Regency Annex

Monday, February 10

MS1

Mathematical and Computational Challenges in Drug Discovery

10:30 AM-12:30 PM

Room: Regency Ballroom A

Computational drug discovery is an actively growing field of research. As academic researchers and biotech and pharmaceutical companies solve more protein structures, attention is now focusing on the design and selection of small molecule drug candidates. Among the challenges in this field are efficient techniques for screening chemical databases for "druglike" compounds, and the design of scoring functions which can select the energetically preferred binding modes of drug candidates with target proteins.

Organizer: Daniel L. Pick

10:30-10:55 Median Partitioning for Diversity Selection, Compound Classification, and Virtual Screening
Jurgen Bajorath and *Jeffrey W. Godden*, Albany Molecular Research Inc.

11:00-11:25 Scoring Methods in Virtual Ligand Screening
Daniel L. Pick

11:30-11:55 The Poisson-Boltzmann Equation: How to use Greek Symbols with Chemists and get Away with It
Anthony Nicholls, OpenEye Scientific Software, Inc.

12:00-12:25 Wavelet Transforms in Protein Structure Determination
Arno Paehler, Syrrx, Inc

Monday, February 10

MS2 (For Part II, see MS 26)

Computational Modeling of MEMS and BioMEMS

10:30 AM-12:30 PM

Regency Ballroom B

The mini-symposium deals with the computational modeling of MEMS and BioMEMS performance and characterization. Specific areas to be addressed in this mini-symposia are silicon micro-cantilevers for bio-sensing applications, computational models for microfluidics-specific applications, design tools for processes in bio-microsystems (BioMEMS), modeling of permeation layers (gels) in microarrays and BioMEMS. Further, this mini-symposia will act as a platform for information exchange for the more broader audience of BioMEMS industry, academia, and CAD software developers for MEMS.

Organizer: Samuel K. Kassegne
University of California, San Diego

Organizer: Kamal Sarkar
Nanogen, Inc.

10:30-10:55 Computational Modeling of MEMS and BioMEMS
Narayana Aluru, University of Illinois, Urbana-Champaign

11:00-11:25 Design and Analysis of Microcantilevers for Biosensing Applications
Cengiz Osman, University of California, Riverside

11:30-11:55 Unified Computational Models for Microfluidics-Specific Applications
Athonu Chatterjee, Corning-IntelliSense

12:00-12:25 Two-Beam Optical Trap System for Detecting Index of Refraction and Size of Colloids and Live Cells
Richard Flynn, University of California, San Diego

Monday, February 10

MS3

Interaction of Flow with Dynamic Boundaries

10:30 AM-12:30 PM

Regency Ballroom C

Understanding the interaction of a fluid with a deforming time-dependent "dynamic boundary" is a key problem of biological fluid dynamics. Much progress has been made in numerical and analytical methods for such flows. However, recent experiments of flexible filaments in a 2D soap film flow display a range of phenomena not attainable by current simulation techniques. This is a prototypical fluid-structure interaction problem which presents many of the difficulties observed in studies of dynamic boundary flows.

In this minisymposium, we discuss applications of novel high-order accurate methods developed by the speakers for computing and understanding fluid dynamic interactions with elastic and time-dependent boundaries.

Organizer: Petri Fast
Lawrence Livermore National Laboratory

10:30-10:55 Deforming filaments in a Viscous Flow using Overset Grids
Petri Fast, Lawrence Livermore National Laboratory

11:00-11:25 Applying the Free-Lagrange, Moving Adaptive Mesh Method to Solving Time and Space Dependent Systems Biology Problems
Harold E. Trease, Pacific Northwest National Laboratory

11:30-11:55 Direct Simulations of Suspensions of Long Slender Filaments
Anna-Karin Tornberg, Courant Institute of Mathematical Sciences, New York University

12:00-12:25 How an Elastic Body Reduces its Drag
Jun Zhang, Silas Alben, and *Michael J. Shelley*, Courant Institute of Mathematical Sciences, New York University

Monday, February 10

MS4 (For Part II, see MS 16)

Recent Advances in Computational Earthquake Ground Motion Modeling

10:30 AM-12:30 PM

Mission Ballroom A

This minisymposium will review recent advances in various aspects of large-scale earthquake ground motion modeling in large basins: (1) the finite element method as an efficient tool for forward modeling of earthquake ground motion; (2) modeling of the earthquake source as a dynamic rupture process; and (3) modern inversion techniques to better characterize the properties of the geological structure and the earthquake source.

The problems that will be addressed, while of specific interest to computational seismologists, are representative of many other PDE-based simulations. Thus, we expect that the presentations will be of interest also to mathematicians and computational scientists and engineers from other disciplines.

Organizer: Steven Day
San Diego State University

Organizer: Jacobo Bielak
Carnegie Mellon University

10:30-10:55 Octree-based Finite Element Ground Motion Modeling in Large Basins
Omar Ghattas, Eui-Joong Kim, and *Jacobo Bielak*, Carnegie Mellon University; and Jianlin Wang, Synopsis, Inc.

11:00-11:25 Self-Consistent Models of Earthquake Ruptures in the Los Angeles Area
Thomas Heaton and *Brad Aagard*, California Institute of Technology

11:30-11:55 Large-Scale Parallel 3-D Simulation of Seismic Wave Propagation using the Earth Simulator
Takashi Furumura, University of Tokyo, Japan

12:00-12:25 A Dynamic-Stochastic Model for the Earthquake Rupture Process
P. Mai, Institute of Geophysics, Switzerland; and M. Guatteri and *Gregory Beroza*, Stanford University

Monday, February 10

MS5 (For Part II, see MS 17)

Uncertainty Quantification I

10:30 AM-12:30 PM

Mission Ballroom B

The vision of computational experiments predicting the outcomes of physical tests is already a driving force and an accepted model for the future of scientific computing. The emerging field of Uncertainty Quantification addresses issues that are paramount to the validation of model-based predictions and their use as surrogates or supplements to physical tests.

This minisymposium reviews current research in various aspects of Uncertainty Quantification. These include modeling issues, numerical algorithms, result interpretation, and applications.

Organizer: Steven F. Wojtkiewicz
Sandia National Laboratories

Organizer: Roger Ghanem
Johns Hopkins University

10:30-10:55 Distribution-Free Uncertainty Quantification
Steven F. Wojtkiewicz, Sandia National Laboratories

11:00-11:25 Quantification and Management of Uncertainty in the Aerothermal Design of Aircraft Engines
David l. Darmofal, Massachusetts Institute of Technology

11:30-11:55 Representing Geometric Uncertainty via Hermite Polynomial Chaos
Robert Walters, Virginia Polytechnic Institute & State University

12:00-12:25 PDV Arithmetic in Uncertainty Computation
Mac Hyman and *Weiye Li*, Los Alamos National Laboratory

Monday, February 10

MS6 (For Part II, see MS 30)

Challenges in Material Interfaces

10:30 AM-12:30 PM

Mission Ballroom C

Polycrystalline and thin film materials are systems where interface behavior and texture can dominate their processing and behavior. Orientations and arrangements within the material and its network of boundaries are implicated in properties across wide scales, such as, functional properties, like conductivity in microprocessors, and lifetime properties, like fracture toughness in structures. Simulation is becoming an important tool to understand both these properties and processing requirements. This includes compelling evidence of the predictability and robustness of statistical properties of large systems. In this minisymposium we discuss the challenges inherent in this program.

Organizer: Shlomo Ta'asan
Carnegie Mellon University

Organizer: David Kinderlehrer
Carnegie Mellon University

10:30-10:55 The Fine Structure of Dislocation Pile-Ups near Grain Boundaries and Resulting Macroscopic Scaling Relations
Michael Ortiz, California Institute of Technology; and Sergio Conti, Max Planck Institute, Leipzig, Germany

11:00-11:25 Simulation of Epitaxial Growth with Strain
Russel Caflisch, University of California, Los Angeles

11:30-11:55 Structures of Local Minimizers of a One-Dimensional Higher Order Variational Problem
Aaron Yip, Purdue University

12:00-12:25 Level Set Computations of Faceted Polycrystalline Thin Films
Peter Smereka, University of Michigan

Monday, February 10

MS7 (For Part II, see MS 19)

Fast and Efficient Methods for PDE and Applications

10:30 AM-12:30 PM

Island Ballroom A

The need to harness the maximum potential of available high performance computers has led to the development of fast and efficient methods for partial differential equations and systems of linear equations arising from the discretization of PDE. These numerical methods have wide applicability, and different classes of partial differential equations arising from increasingly realistic and complicated problems in every field of computational simulation, have emerged. This minisymposium will address the recent developments and future directions for such methods.

Organizer: Prabir Daripa
Texas A&M University

Organizer: Satyendra K. Tomar
University of Twente, Netherlands

10:30-10:55 An Overview of Some Fast Algorithms for Elliptic PDEs
Prabir Daripa, Texas A&M University

11:00-11:25 Sub-Stepping and Semi-Lagrangian Formulations of the Spectral/HP Element Navier-Stokes Equations
Dongbin Xiu, Brown University; and *Spencer Sherwin*, Imperial College, London, United Kingdom

11:30-11:55 An Efficient and Exponentially Accurate Parallel h-p Spectral Element Method for Elliptic Problems on Polygonal Domains - The Mixed Boundary Conditions
Pravir Dutt, IIT Kanpur, India; and *Satyendra K. Tomar*, University of Twente, Netherlands

12:00-12:25 An Efficient Cell-Centered Finite Volume Solver For Navier Stokes Equations On Vector Parallel Processors
B. V. Rathish Kumar, IIT Kanpur, India

Monday, February 10

MS8

Plasma Physics and Computer Science: A Partnership for Advancing the Understanding of Magnetically Confined Plasmas

10:30 AM-12:30 PM

Island Ballroom B

Progress in understanding the physics of magnetic fusion is dependent on plasma modeling and simulation, and on the analysis of data from large experimental facilities. Success in these tasks requires the effective use of the state-of-the-art computers, networks, and collaboration technologies, as well partnerships between physicists and computer scientists. This minisymposium will describe scientific and computational issues in order to promote a joint understanding of the issues, and to foster more effective collaborations. The first three talks will outline the content and importance of the physics issues they address; the current status of the research and the role of computational science in the advancement of the physics; and future directions. The last talk will discuss modeling and simulation, scientific visualization, and collaboration technologies as network services.

Organizer: Lee Berry
Oak Ridge National Laboratory

10:30-10:55 Radio Frequency Field Interactions in Magnetized Plasmas
Lee Berry, Oak Ridge National Laboratory

11:00-11:25 3D Extended MHD Calculations of Magnetically Confined Plasma
Stephen Jardin, Princeton Plasma Physics Laboratory

11:30-11:55 Micro-turbulence and its Impact on Plasma Confinement
William Nevins, Lawrence Livermore National Laboratory

12:00-12:25 The National Fusion Collaboratory
David Schissel, General Atomics

Monday, February 10

MS9

Application Design Issues for New and Emerging Supercomputer Architectures

10:30 AM-12:30 PM

Garden Room A

After years of decline, one can argue that high-end supercomputing architectures are becoming more diverse and worthy of the prefix ``super." Continued improvement in clustered designs, customized networks, and the advent of innovative new architectures make this an exciting time for supercomputing applications. In this minisymposium each speaker will give an overview of a supercomputing architecture followed by a discussion of application design issues for that architecture. Four basic architectures are discussed, exemplified by the following four platforms: the Cray SV2, the Earth Simulator, ASCI Red and ASCI White.

Organizer: Michael A. Heroux
Sandia National Laboratories

10:30-10:55 An Overview of Some Design Issues for High-end Supercomputers
Michael A. Heroux, Sandia National Laboratories

11:00-11:25 How to use Hybrid MPI-OpenMP on IBM SP Systems
Edmond T. Chow, Lawrence Livermore National Laboratory

11:30-11:55 Cray X1: Extreme Performance for the Most Demanding Applications
Kristyn Maschhoff, Cray, Inc.

12:00-12:25 Solid Earth Simulation Using GeoFEM Platform on the *Earth Simulator*
Kengo Nakajima, Research Organization for Information Science and Technology, Japan

Monday, February 10

MS10 (For Part II, see MS 22)

Algorithms for Optimal Design and Control of Systems Governed by Time-Dependent PDEs I

10:30 AM-12:30 PM

Garden Room C

This minisymposium will focus on computational aspects of optimization of systems governed by unsteady PDEs. Areas of specific interest include applications to computational mechanics/physics especially in 3D with large design spaces, algorithms to ensure and accelerate convergence, and parallelization strategies.

Organizer: George Biros
Courant Institute of Mathematical Sciences, New York University

Organizer: Martin Berggren
Sandia National Laboratories

Organizer: Bart Van Bloomen Waanders
Sandia National Laboratories

10:30-10:55 Application of Advanced Large-Scale Minimization Algorithms for Inverse Problems and Data Assimilation.
Ionel Michael Navon, Florida State University; Dacian N. Daescu, University of Minnesota, Minneapolis; and Aleksey Alekseev, RSC ENERGIA Corporation, Russia

11:00-11:25 A Reduced Sqp Method for the Shape Optimization of Turbine and Compressor Blades
Georg Bock, IWR - University of Heidelberg, Germany

11:30-11:55 Order-Reduction in a Wavelet Basis for a Problem of Data Assimilation in Oceanology
Isabelle Charpentier, Institut d'Informatique et Mathematiques Appliquees, France; and Ioana Paun, Institut de Recherche Mathématique Avancée de Strasbourg, France

12:00-12:25 Managing Pod Models for Optimal Control Problems
Ekkehard W. Sachs, University of Trier, Germany and Virginia Tech

Monday, February 10

MS11 (For Part II, see MS 35)

Undergraduate Computational Science and Engineering

10:30 AM-12:30 PM

Garden Room D

These two minisymposia have been organized to continue the discussion of undergraduate Computational Science and Engineering programs. The scope is broad. Presentations will cover programs and curricula at various levels; assessment techniques, tools and resources; course and information resources; and there will be some time set aside for open discussion to facilitate getting others more involved in the discussion and the ongoing development of undergraduate CSE.

Organizer: Kris Stewart
San Diego State University

Organizer: Peter R. Turner
Clarkson University

10:30-10:55 Scientific Visualization in Undergraduate Computational Science Education
Angela B. Shiflet, Wofford College; and Steve Cunningham, California State University, Stanislaus

11:00-11:25 Building Assessment into the Development of Undergraduate Computational Science Curricula
Kris Stewart, San Diego State University

11:30-11:55 A Computational Science Curriculum For A Liberal Arts Environment
Ignatios E. Vakalis, Capital University

12:00-12:25 A Computational Science Case Study: Classification of Hybrids using Genetic Markers and maximum-likelihood estimates
Alex Buerkle and *Andrew Phillips*, University of Wisconsin, Eau Claire

Monday, February 10

MS12 (For Part II, see MS 48)

Mesh Quality Improvement

10:30 AM-12:30 PM

Garden Room F

Methods for improving the quality of unstructured meshes are needed to reduce discretization error and improve solver efficiency in computational simulations. Correct problem formulation, robust and efficient numerical improvement algorithms, and studies showing the effect of mesh quality are all of current interest.

A crucial preliminary step in Computational Science and Engineering is mesh generation and improvement. This minisymposium will provide conference attendees with an overview of the latest research in this important area.

Organizer: Patrick Knupp
Sandia National Laboratories

Organizer: Lori Freitag
Argonne National Laboratory

10:30-10:55 MESQUITE: The Mesh Quality Improvement Toolkit
Patrick Knupp, Michael Brewer, and Darryl Melander, Sandia National Laboratories; and Thomas Leurent and *Lori Freitag*, Argonne National Laboratory

11:00-11:25 Mesh Untangling
Mikhail Shashkov and Rao V. Garimella, Los Alamos National Laboratory; and Pavel Vachal, Czech Technical University, Prague, Czech Republic

11:30-11:55 What Is a Good Linear Finite Element? Interpolation, Conditioning, Anisotropy, and Quality Measures
Jonathan R. Shewchuk, University of California, Berkeley

12:00-12:25 Toward a Theory of Preconditioners for Mesh Quality Improvement
Patrick Knupp, Sandia National Laboratories

Lunch Break

12:30 PM-2:00 PM

Attendees on Own

• *Cash and carry lunch for SIAM Meeting attendees is available in the Koi Pond area of the gardens.*

Monday, February 10

IP3

A New Era in Computational Science

2:00 PM-2:45 PM

Room: Regency Ballroom

Chair: Steven F. Ashby, Lawrence Livermore National Laboratory

At the dawn of the 21st century, computational and data management infrastructure has become a first-class tool for science and engineering. Some of the most difficult problems in science are being addressed by the integration of computation and science -- computational science. The next decade in computational science promises to enable fundamental advances in biology, physics, chemistry, astronomy, and a host of disciplines through the coordination of computation, data management, access to instrumentation, knowledge synthesis, and the use of new devices.

At the center of many of the advances will be Grid Computing. The Grid has provided a way to link computation, data, networking, instruments and other resources together to solve today's complex and critical problems. In this talk, we describe a new era of computational science and the challenges of building the information infrastructure needed to enable science and engineering discoveries of the future.

Fran Berman
NPACI and University of California, San Diego

Coffee Break

2:45 PM-3:15 PM

Regency Annex

Monday, February 10

MS13

Stochasticity in the Simulation of Cellular Behavior and Genetic Regulation

3:15 PM-5:15 PM

Room: Regency Ballroom A

It is now universally recognised that stochasticity is an inherent property of cellular behaviour and regulation. One of the most important markers in this area was the development of the stochastic simulation algorithm (SSA) due to Gillespie. This is essentially an exact procedure for numerically simulating chemically reacting systems, where there may be relatively few molecules of some key chemical species present. However, despite recent improvements it remains computationally inefficient for most practical simulations. Thus an important field of research is to develop new simulation algorithms that can overcome some of these difficulties. This minisymposium will explore the role of stochasticity in cellular models, and the development of a computational framework for simulation of multiscale stochastic chemically reacting systems.

Organizer: Linda R. Petzold
University of California, Santa Barbara

Organizer: Kevin Burrage
University of Queensland, Australia

3:15-3:40 Meaningful Noise in Biological Systems
Lars Keld Nielsen, University of Queensland, Australia

3:45-4:10 Stochastic Chemical Kinetics
Daniel Gillespie, Consultant

4:15-4:40 A Computational Framework for the Efficient Simulation of Stochastic Chemical Kinetics (Part I)
Linda R. Petzold, University of California, Santa Barbara; Muruhan Rathinam, University of Maryland, Baltimore County; and Kevin Burrage and Tianhai Tian, University of Queensland, Australia

5:15-5:15 A Computational Framework for the Efficient Simulation of Stochastic Chemical Kinetics (Part II)
Muruhan Rathinam, University of Maryland, Baltimore County; Linda R. Petzold, University of California, Santa Barbara; and Tianhai Tian and *Kevin Burrage*, University of Queensland, Australia

Monday, February 10

MS14

Modeling of Transport Phenomena in Nano-Technology

3:15 PM-5:15 PM

Regency Ballroom B

Development of new computational fluid dynamics tools and implementation of existing CFD tools to a new branch of engineering named ``nanotechnology" is a goal of the current minisimphosium. One example of nanotechnology is the topic of this minisymposium. Nanotubes are carbon sheets wrapped into cylinders, which have only a few nano-meters in diameter but up to a milli-meter long. Nanotubes could be used as semiconductors in electronic industry, light-weight highly elastic fibrous material for aerospace industry, and as lightweight packing material for fuel cells and drug delivery.

CFD for nano-technology means use of various mathematical models ranging from continous fluid mechanics to molecular dynamics. Currently, nano-tubes are produced using HiPco process, laser ablation (LA), and chemical vapor deposition (CVD) processes. Modeling of HiPco requires refined models of jet turbulence suitable for high-angle of incidence jets while LA modeling needs models and numerical methods suitable for periodic explosion of plasma-type plume and interface rolling. On the contrary, CVD process requires modeling of low-Reynolds feedstock gas flow around growing nanotubes that calls for high-Knudsen number models of fluid flow.

Similar diversity of needed models and computational tools exists in micro-combustion and in enforcement of polymer materials by mixing melted polymers with nano-tubes. The right choice of models and tools is a goal of this Minisymposium.

Organizer: Alex Povitsky
Concordia University, Canada

3:15-3:40 Modeling of Transport Phenomena in Carbon Nanotube Synthesis
Diomar Lobao, CERCA and Concordia University, Canada; and Jilin Zhang and *Alex Povitsky*, Concordia University, Canada

3:45-4:10 Numerical Modeling of Small-Scale Heat Recirculating Burners
Craig Eastwood, University of Southern California

Monday, February 10

MS14 *(continued)*

Modeling of Transport Phenomena in Nano-Technology

3:15 PM-5:15 PM

Regency Ballroom B

4:15-4:40 Modeling of Active Propulsion in Capillaries
Jeffrey Wright, University of San Diego

4:45-5:10 Modified Characteristic Scheme for Quantum Hydrodynamic Simulation of Nanoscale Heterostructures
Ming Cheng and *Min Shen*, Clarkson University

Monday, February 10

MS15 (For Part II, see MS 39)

Progress in Implicit Large Eddy Simulation (ILES)

3:15 PM-5:15 PM

Regency Ballroom C

Using modern high-resolution numerical methods to implicitly model turbulence is playing a greater role in many applications from astrophysics to engineering. This two-session mini-symposium will examine the frontiers of physical and mathematical theory supporting these techniques, addressing both, successes and pressing research needs of current implicit subgrid scale (SGS) modeling practices. Finite volume formulations based on various nonlinear discrete equations will be examined, and their relevant differences in the ILES context will be investigated. The main focus is to improve our understanding of how interesting desirable SGS physics can be built implicitly into the numerical scheme or discrete set of equations.

Organizer: William J. Rider
Los Alamos National Laboratory

Organizer: Fernando Grinstein
Naval Research Laboratory

3:15-3:40 From Numerical Analysis to Implicit Subgrid Turbulence Models
Len Margolin and *William J. Rider*, Los Alamos National Laboratory

3:45-4:10 Recent Progress on MILES for High-Re Flows
Christer Fureby, FOI, Sweden; and *Fernando Grinstein*, Naval Research Laboratory

4:15-4:40 On the Transition between DNS and LES Simulations of Turbulence
Len Margolin and *Andrzej A. Wyszogrodzki*, Los Alamos National Laboratory; and Piotr Smolarkiewicz, NCAR

4:45-5:10 Treatment of Small Scale Vortices as Solitary Waves: a New Approach to LES.
John Steinhoff, University of Tennessee Space Institute

Monday, February 10

MS16 (For Part I, see MS 4)

Recent Advances in Computational Earthquake Ground Motion Modeling

3:15 PM-5:15 PM

Mission Ballroom A

This minisymposium will review recent advances in various aspects of large-scale earthquake ground motion modeling in large basins: (1) the finite element method as an efficient tool for forward modeling of earthquake ground motion; (2) modeling of the earthquake source as a dynamic rupture process; and (3) modern inversion techniques to better characterize the properties of the geological structure and the earthquake source.

The problems that will be addressed, while of specific interest to computational seismologists, are representative of many other PDE-based simulations. Thus, we expect that the presentations will be of interest also to mathematicians and computational scientists and engineers from other disciplines.

Organizer: Steven Day
San Diego State University

Organizer: Jacobo Bielak
Carnegie Mellon University

3:15-3:40 Numerical and Scale-Model Simulation of Earthquake Rupture
R. Anooshehpoor, University of Nevada, Reno; and S. Gonzales and *Steven Day*, San Diego State University

3:45-4:10 Seismic Methods for Imaging Basin Properties
Hianming Hu, Min Zhou, and *Gerald Schuster*, University of Utah; and Yonghe Sun, Amerada Hess Corporation

4:15-4:40 Fully Non-Linear Inversion of Dynamic Earthquake Rupture Parameters
R. Madariaga, Ecole Normale Supérieure, France; and S. Peyrat and *Kim Olsen*, University of California, Santa Barbara

4:45-5:10 Large-Scale Source and Material Inversion for Earthquake Ground Motion Modeling
Ioannis Epanomeritakis, Carnegie Mellon University; and Jacobo Bielak, Volkan Akcelik, and *Omar Ghattas*, Carnegie Mellon University

Monday, February 10

MS17 (For Part I, see MS 5) (For Part III, see MS 29)

Uncertainty Quantification II

3:15 PM-5:15 PM

Mission Ballroom B

The vision of computational experiments predicting the outcomes of physical tests is already a driving force and an accepted model for the future of scientific computing. The emerging field of Uncertainty Quantification addresses issues that are paramount to the validation of model-based predictions and their use as surrogates or supplements to physical tests.

This minisymposium reviews current research in various aspects of Uncertainty Quantification. These include modeling issues, numerical algorithms, result interpretation, and applications.

Organizer: Steven F. Wojtkiewicz
Sandia National Laboratories

Organizer: Roger Ghanem
Johns Hopkins University

3:15-3:40 Dynamic Systems Subjected to a Class of Equivalent Inputs
Mircea Grigoriu, Cornell University

3:45-4:10 Equation-Free Multiscale Computation
Yannis Kevrekidis, Princeton University

4:15-4:40 Variable Reduction in Mechanical Models of a Heat Bath
Raz Kuperfman, Hebrew University, Jerusalem, Israel

4:45-5:10 Iterative solvers for Wave Propagation in Random Media
Didier Clouteau, Ecole Centrale Paris, France; and Rémi Lafargue, Ecole Centrale de Paris, France

Monday, February 10

MS18 (For Part II, see MS 42)

Nonconvex Variational Methods in Computational Solid Mechanics I

3:15 PM-5:15 PM

Mission Ballroom C

Variational methods are at the core of several breakthroughs in nonlinear solid mechanics. Noteworthy examples are the development of return mapping algorithms in computational plasticity, and the application of relaxation techniques from nonconvex variational calculus to model martensitic phase transformations.

A possibility to combine the successes in these two fields has recently emerged. For example, constitutive updates for crystal plasticity based on (nonconvex) incremental potentials have been proposed, and complex dislocation structures have been studied based on such potentials. Moreover, relaxation of nonconvex potential has established itself as a powerful technique for the development of multiscale models of complex material behavior.

The goal of the minisymposium is to review these recent advances, and to assess their potential as robust computational tools. The intended audience consists of mathematicians, materials scientists, engineers, and computational scientists with an interest in computational solid mechanics.

Organizer: Michael Ortiz
California Institute of Technology

Organizer: Antonio Desimone
Max Planck Institute for Mathematics in the Sciences, Germany

3:15-3:40 Quasiconvexity and Multiscale Methods in the Modelling of Soft Elasticity of Nematic Elastomers
Antonio Desimone, Max Planck Institute for Mathematics in the Sciences, Germany

3:45-4:10 Evolution of Deformation-Induced Microstructures
Darcy Hughes and *Sylvie Aubry*, Sandia National Laboratories

4:15-4:40 The Application of Quasiconvex Relaxation in Shape Memory Alloys
Sanjay Govindjee, University of California, Berkeley

4:45-5:10 Homogenization and Microstructure Development in Non-Convex Standard Dissipative Solids
Christian Miehe, Universität Stuttgart, Germany

Monday, February 10

MS19

Fast and Efficient Methods for PDE and Applications II

3:15 PM-5:15 PM

Island Ballroom A

The need to harness the maximum potential of available high performance computers has led to the development of fast and efficient methods for partial differential equations and systems of linear equations arising from the discretization of PDE. These numerical methods have wide applicability, and different classes of partial differential equations arising from increasingly realistic and complicated problems in every field of computational simulation have emerged. This minisymposium will address the recent developments and future directions for such methods.

Organizer: Prabir Daripa
Texas A&M University

Organizer: Satyendra K. Tomar
University of Twente, Netherlands

3:15-3:40 Algorithms for Terascale Computations of PDEs
David E. Keyes, Old Dominion University and ICASE

3:45-4:10 Scalable Parallel Direct Solution of General Sparse Systems of Linear Equations
Anshul Gupta, IBM T.J. Watson Research Center

4:15-4:40 New Error Estimators and Adaptive Schemes for Updated Lagrangian Formulations
Abani K. Patra, State University of New York, Buffalo; and Viswanath Ramakkagari, RPI

4:45-5:10 Scalable Solution of CFD Problems on Unstructured Meshes
William D. Gropp, Argonne National Laboratory

Monday, February 10

MS20 (For Part II, see MS 44)

Computational Electromagnetics I: Discretization

3:15 PM-5:15 PM

Island Ballroom B

Numerical solution of Maxwell's equations is a critical component in many indistrial and scientific applications. The main focus of this minisimposium will be on recent advances in discretization and efficient iterative solution of Maxwell's equations. It is now well understood that succesful discrete models reflect fundamental topological properties of Maxwell's equations described by the formalism of exterior calculus, differential forms and De Rham cohomology. The speakers will present a wide range of methods that exploit these connections in the context of finite volume, finite difference and finite element settings. The second part of the minisimposium will deal with the challenges that must be overcome in order to solve efficiently the ensuing algebraic systems.

Organizer: Pavel Bochev
Sandia National Laboratories

Organizer: R Lehoucq
Sandia National Laboratories

Organizer: R Tuminaro
Sandia National Laboratories

3:15-3:40 An Overview of Compatible Discretizations in Electromagnetics
Pavel Bochev, Sandia National Laboratories

3:45-4:10 Higher Order Covolume Techniques for Vector Field Problems
Kathryn Trapp and *Roy Nicolaides*, Carnegie Mellon University

4:15-4:40 Mimetic Discretizations for Maxwell's Equations and the Equations of Magnetic Diffusion
James M. Hyman and *M. Shaskov*, Los Alamos National Laboratory

4:45-5:10 Stability and Conservation Properties of Transient Electromagnetic Simulations Using FIT
Rolf Schuhmann, Technische Universitaet Darmstadt, Germany

Monday, February 10

MS21 (For Part II, see MS 45)

Computational Science in Component-Based Environments

3:15 PM-5:15 PM

Garden Room A

Component environments are emerging as tools to help computational scientists manage the complexity of the software systems they develop. A goal of component-based design is to allow software modules to interact in a well-defined and controlled manner, hiding low-level details of the implementation of each component from others. The component approach facilitates a collaborative, community-oriented approach to the development of large-scale software systems and a component-rich environment greatly simplifies experimentation software of any scale. This minisymposium will present a range of computational science research performed using component-based environments, and discuss some of the distinctive features of the component approach.

Organizer: David E. Bernholdt
Oak Ridge National Laboratory

3:15-3:40 Components for Scientific Computing: An Introduction
David E. Bernholdt, Oak Ridge National Laboratory

3:45-4:10 CCA-Component Based Simulation of Flows on Adaptively Refined Structured Meshes
Habib N. Najm, Sophia Lefantzi, and *Jaideep Ray*, Sandia National Laboratories

4:15-4:40 The BioPSE Software System: Releasing and Supporting An Open Source Problem Solving Environment
David Weinstein, University of Utah

4:45-5:10 Creating Grid-Enabled Applications Through Cactus and GridLab
John Shalf, Lawrence Livermore National Laboratory; and Gabrielle Allen, Edward Seidel, and Thomas Goodale, Max Planck Institute for Gravitation Physics, Potsdam, Germany

Monday, February 10

MS22 (For Part I, see MS 10)

Algorithms for Optimal Design and Control of Systems Governed by Time-Dependent PDEs II

3:15 PM-5:15 PM

Garden Room C

This minisymposium will focus on computational aspects of optimization of systems governed by unsteady PDEs. Areas of specific interest include applications to computational mechanics/physics especially in 3D with large design spaces, algorithms to ensure and accelerate convergence, and parallelization strategies.

Organizer: Martin Berggren
Sandia National Laboratories

Organizer: George Biros
Courant Institute of Mathematical Sciences, New York University

3:15-3:40 Shape Optimization of an Acoustic Horn
Martin Berggren, Sandia National Laboratories; and Erik Bängtsson and Daniel Noreland, Uppsala University, Sweden

3:45-4:10 Linear and Nonlinear Optimal Control in Spatial Boundary Layers
Martin Berggren, Sandia National Laboratories; Markus Högberg and *Mattias Chevalier*, FOI - The Swedish Defence Research Agency, Sweden; and Dan Henningson, Royal Institute of Technology, Stockholm

4:15-4:40 Towards a Comprehensive Framework for the Regularization of Adjoint Analysis in Multiscale Pde Systems
Bartosz Protas, University of California, San Diego; and *Thomas R. Bewley*, Stanford University

4:45-5:10 Reduced Order Modelling for Optimal Control of Wake Flows Using Pod
S. S. Ravindran, University of Alabama, Huntsville

Monday, February 10

MS23 (For Part II, see MS 47)

Combinatorial Algorithms in Scientific Computing

3:15 PM-5:15 PM

Garden Room D

Although scientific computing is generally viewed as the province of differential equations and numerical analysis, combinatorial techniques have long played a crucial role. This minisymposium will showcase several areas in which combinatorial insights can be usefully applied to scientific computing problems. Examples include sparse direct methods, preconditioning, geometric discretization methods, and parallel algorithms. The minisymposium will not only provide an opportunity for researchers to present their most recent results, but also provide a forum for dialogue between applications scientists and algorithm developers.

Organizer: John Gilbert
University of California, Santa Barbara

Organizer: Bruce Hendrickson
Sandia National Laboratories

Organizer: Ali Pinar
Lawrence Berkeley Laboratory

3:15-3:40 Computing a Nice Basis: Matroids and Matchings
Edmond T. Chow, Lawrence Livermore National Laboratory; Alex Pothen, Old Dominion University and Sandia National Laboratories; and Ali Pinar, Lawrence Berkeley Laboratory

3:45-4:10 Combinatorial Preconditioners and Support Theory
Bruce Hendrickson and Erik G. Boman, Sandia National Laboratories

4:15-4:40 Fill Reduction Algorithm Using Diagonal Markowitz Scheme with Local Symmetrization
Esmond G. Ng and Sherry Li, Lawrence Berkeley National Laboratory; and Patrick Amestoy, ENSEEIHT, Toulouse, France

4:45-5:10 Modifying a Sparse Cholesky Factorization
William W. Hager and Tim Davis, University of Florida

Monday, February 10

MS24 (For Part II, see MS 36)

Advanced Meshing and Discretization Strategies in Application Solution

3:15 PM-5:15 PM

Garden Room F

This minisymposium will provide conference attendees with an overview of the latest research and software developments in the area of meshing and discretization. A large number of toolkits exist in these areas, and we highlight their use in a variety of application areas ranging from computational fluid dynamics and biological models to accelerator design and high energy fusion modeling. By showcasing many different meshing and discretization strategies, we will provide a broad overview of the variety of techniques and software available to application scientists.

Organizer: David L. Brown
Lawrence Livermore National Laboratory

Organizer: Lori Freitag
Argonne National Laboratory

3:15-3:40 Solving Elliptic PDEs on Overlapping Grids with Multigrid
Bill Henshaw, Lawrence Livermore National Laboratory

3:45-4:10 Spectral Element Methods for the Shallow Water Equations
Paul F. Fischer, Argonne National Laboratory

4:15-4:40 High Resolution Algorithms for Fluid Mixing
Andrea Marchese, Ning Zhao, Xaiolin Li, Zhiliang Xu, and *James Glimm*, State University of New York, Stony Brook; and Myoungyoun Kim, Brookhaven National Laboratory

4:45-5:10 A Discontinuous Galerkin Method for Radiative Transfer
Valmor de Almeida, Oak Ridge National Laboratory

Intermission

5:15 PM-5:20 PM

Monday, February 10

CP1

Optimization in Biology

5:20 PM-6:20 PM

Regency Ballroom A

Chair: Genetha Gray, Sandia National Laboratories

5:20-5:35 Scalable Parallel Branch-and-Bound for Protein Structure Prediction
Nihar R. Mahapatra, *Amruth Sivalenka,* and Sandeep Namilikonda, State University of New York, Buffalo

5:40-5:55 Using Optimization in Biological Research
Tamara G. Kolda and *Genetha Gray*, Sandia National Laboratories

6:00-6:15 Nondifferentiable Optimization Methods for Protein Docking
Ben Rosen and *Roummel F. Marcia*, University of California, San Diego; and Julie Mitchell, San Diego Supercomputer Center

Monday, February 10

CP2

Schemes for Complex Flows I

5:20 PM-6:20 PM

Regency Ballroom B

Chair: William J. Rider, Los Alamos National Laboratory

5:20-5:35 The Accuracy and Efficiency of Shock Capturing Methods for Shocks: High-Resolution Godunov Methods, Weighted Eno Schemes and Neo-Godunov Methods
Jeffery Greenough, Lawrence Livermore National Laboratory; and *William J. Rider*, Los Alamos National Laboratory

5:40-5:55 A Numerical Method for the Coupling Radiation-Hydrodynamics
Jean-Francois Ripoll, Stanford University

6:00-6:15 A High-Resolution Constrained Transport Method for Magnetohydrodynamic Flows
James A. Rossmanith, University of Michigan

Monday, February 10

CP3

Computational Biology I

5:20 PM-6:40 PM

Regency Ballroom C

Chair: Jesus A. Izaguirre, University of Notre Dame

5:20-5:35 A Linearly Scalable Hybrid Monte Carlo for Sampling the Conformational Space of Proteins
Jesus A. Izaguirre and *Scott Hampton*, University of Notre Dame

5:40-5:55 Automatic Empirical Optimization of Fast Electrostatics Algorithms
Alice Ko and *Jesus A. Izaguirre*, University of Notre Dame

6:00-6:15 CompuCell, a Multi Model Framework for Simulation of Morphogenesis
Jesus A. Izaguirre and *Rajiv Chaturvedi*, University of Notre Dame

6:20-6:35 Parallel Solution of the Poisson-Boltzmann Equation for Evaluating Nanoscale Biomolecular Electrostatic Properties
Simpson Joseph, Michael J. Holst, and J Andrew McCammon, University of California, San Diego; and David Sept and *Nathan A. Baker*, Washington University, St. Louis

Monday, February 10

CP4

Multilevel Methods

5:20 PM-6:20 PM

Mission Ballroom A

Chair: Abani K. Patra, State University of New York, Buffalo

5:20-5:35 Multi-Level Preconditioners for Adaptive *hp* Finite Element Simulations
Andrew Bauer and *Abani K. Patra*, State University of New York, Buffalo

5:40-5:55 Scalability of P_1 Nonconforming Multigrid
David E. Keyes, Old Dominion University and ICASE; and *Kab Seok Kang*, Old Dominion University

6:00-6:15 How Close Can We Approach Singular Points in Nonlinear Eigenvalue Problems
S.-L. Chang, Southern Taiwan University of Technology, Taiwan; and J.-Y. Jiang and *Cheng-Sheng Chien*, National Chung-Hsing University, Taiwan

Monday, February 10

CP5

Solvers for Electromagnetics and Circuits

5:20 PM-6:20 PM

Mission Ballroom B

Chair: Vivek Sarin, Texas A&M University

5:20-5:35 Novel Algorithms for Inductance Extraction
Hemant Mahawar, Weiping Shi, and *Vivek Sarin*, Texas A&M University

5:40-5:55 Preconditioning Techniques for Large Dense Matrices From Electromagnetic Wave Scattering Simulations
Cai-Cheng Lu, Jeonghwa Lee, and *Jun Zhang*, University of Kentucky

6:00-6:15 On Consistent Initial Value Assignment for Electronic Circuit Cad Simulation Tools
Kamyar Hazaveh Hesarmaskan, Ryerson University, Canada; and Greg Reid, University of Western Ontario, Canada

Monday, February 10

CP6

Parallel Adaptive PDE Solvers

5:20 PM-6:00 PM

Mission Ballroom C

Chair: To Be Determined

5:20-5:35 Parallel Performance of An Adaptive-Mesh Reactive Hydrodynamics Simulation Code
Mike Zingale, University of California, Santa Cruz; Frank Timmes, Bruce Fryxell, Andrew Siegel, Alan Calder, Paul Ricker, and *Jonathan Dursi*, University of Chicago; Peter MacNeice, NASA Goddard Space Flight Center; and Kevin Olson, University of Maryland, Baltimore County and NASA Goddard Space Flight Center

5:40-5:55 Benchmarking Applications with Irregular, Dynamically Changing Memory Access
Rob F. Van Der Wijngaart, Rupak Biswas, and *Huiyu Feng*, NASA Ames Research Center

Monday, February 10

CP7

Inverse Problems

5:20 PM-6:20 PM

Island Ballroom A

Chair: Alexandra Tolstoy, ATolstoy Sciences

5:20-5:35 Light Aircraft Noise for the Estimation of Ocean Depth in Shallow Water
M.J. Buckingham, Scripps Institution of Oceanography; and *Alexandra Tolstoy*, ATolstoy Sciences

5:40-5:55 Solving Inverse Acoustic Scattering Problems Using Shape Sensitivity Analysis
Gonzalo R. Feijoo, Sandia National Laboratories

6:00-6:15 New Adjoint-Based Methods for Targeted Observations in Atmospheric Modeling
Dacian N. Daescu, University of Minnesota, Minneapolis; and Ionel Michael Navon, Florida State University

Monday, February 10

CP8

Discrete Algorithms

5:20 PM-6:20 PM

Island Ballroom B

Chair: William Mitchell, National Institute of Standards and Technology

5:20-5:35 Through-Vertex Paths in 2D and 3D Simplicial Grids
William F. Mitchell, National Institute of Standards and Technology

5:40-5:55 A New Implementation of the Space Filling Curve Load-Balancing Algorithm
Andrew Bauer, State University of New York, Buffalo; and Karen D. Devine, Carter Edwards, and Robert Heaphy, Sandia National Laboratories

6:00-6:15 A Comprehensive Evaluation of Parallel Algorithms for the Linear Assignment Problem
Nihar R. Mahapatra and *Amruth Sivalenka*, State University of New York, Buffalo

Monday, February 10

CP9

Multiscale Simulations

5:20 PM-6:20 PM

Garden Room C

Chair: Sorin M. Mitran, University of North Carolina

5:20-5:35 Coupled Continuum and Molecular Simulation of Dilute Polymer Solutions in Turbulent Flow
Sorin M. Mitran, University of North Carolina

5:40-5:55 Loosely Coupled Multiscale Modeling of Growth of Carbon Nanotubes
Don Noid, Jack Wells, Zhenyu Zhang, Richard Wood, Bobby Sumpter, and *Sreekanth Pannala*, Oak Ridge National Laboratory

6:00-6:15 A Simulation Software Architecture for Interacting Discrete and Continuous Phases of Matter
Omar Santiago and *Damian W. Rouson*, City University of New York, City College

Monday, February 10

CP10

Parallel Iterative Solvers

5:20 PM-6:20 PM

Garden Room D

Chair: Daniel B. Szyld, Temple University

5:20-5:35 A Nested Iterative Scheme for Indefinite Linear Systems in Particulate Flows
Ahmed Sameh and *Abdelkader Baggag*, Purdue University

5:40-5:55 Variations on distributed Schur Complement techniques in pARMS
Yousef Saad and *Masha Sosonkina*, University of Minnesota, Duluth

6:00-6:15 Inexact Krylov Subspace Methods
Valeria Simoncini, Istituto di Analisi Numerica del CNR, Italy; and *Daniel B. Szyld*, Temple University

John von Neumann's 100th Birthday Celebration Symposium

8:00 PM - 10:00 PM
Regency Ballroom

Organizers:
Gene Golub, *Stanford University* and
Joseph Grcar, *Lawrence Berkeley National Laboratory*

Invited Speakers:
William Aspray, *Indiana University*
Peter Lax, *Courant Institute of Mathematical Science, New York University*
G. W. (Pete) Stewart, *Institute for Advanced Computer Studies (UMIACS), University of Maryland*
Marina v.N. Whitman, *University of Michigan, School of Business, Gerald R. Ford School of Public Policy*

Monday, February 10

CP11

Scalable Parallel Linear Solvers

5:20 PM-6:20 PM

Garden Room F

Chair: Kendall H. Pierson, Sandia National Laboratories

5:20-5:35 Recursive Use of Domain Decomposition Methods for Solving Linear Systems of Equations
Kendall H. Pierson, Sandia National Laboratories

5:40-5:55 Massively Parallel Large-Scale Pool Fire Simulations
Philip Smith, Rajesh Rawat, and *Wing K. Yee*, University of Utah; and Homer Walker, Worcester Polytechnic Institute

6:00-6:15 Parallel Preconditioning Using Blocked Incomplete Cholesky Factorization and Selective Inversion.
Esmond G. Ng, Lawrence Berkeley National Laboratory; and Padma Raghavan and *Keita Teranishi*, Pennsylvania State University

Tuesday, February 11

Registration

8:00 AM-5:30 PM

Regency Annex

Announcements

8:15 AM-8:30 AM

Regency Ballroom

Linda R. Petzold, University of California, Santa Barbara

Tuesday, February 11

IP4

Computational Proteomics: Prediction of Protein Function on a Genome-Scale

8:30 AM-9:15 AM

Regency Ballroom

Chair: Linda R. Petzold, University of California, Santa Barbara

My talk will address a major post-genomic challenge: trying to predict protein function on a genomic scale. I will approach both of this through analyzing the properties and attributes of proteins in a database framework. The work on predicting protein function will discuss the strengths and limitations of a number of approaches: (i)using sequence similarity; (ii) using structural similarity; (iii) clustering microarray experiments; and (iv) data integration. The last approach involves systematically combining information from the other three and holds the most promise for the future. For the sequence analysis, I will present a similarity threshold above which functional annotation can be transferred, and for the microarray analysis, I will present a new method of clustering expression timecourses that finds "time-shifted" relationships.

Mark Gerstein
Yale University

Tuesday, February 11

IP5

Architecture and Algorithms

9:15 AM-10:00 AM

Regency Ballroom

Chair: David E. Keyes, Old Dominion University and ICASE

Any algorithm seeks to find a balance between requirements of accuracy, software complexity, and performance. In the early days of computers, floating point operations were by far the most expensive operation, leading to an analysis of algorithmic efficiency that focuses on floating-point operations. Modern computers, however, can perform hundreds of floating point operations in the time it takes to read one word from main memory. This talk will illustrate the need for new criteria for evaluating numerical algorithms and discuss some of the opportunities for developers of new algorithms.

William D. Gropp
Argonne National Laboratory

Coffee Break

10:00 AM-10:30 AM

Regency Annex

Tuesday, February 11

MS25

Computational Modeling in Proteomics

10:30 AM-12:30 PM

Room: Regency Ballroom A

Now that the genomes of many organisms have been sequenced, a major challenge is the characterization of the proteins (numbering in the hundreds of thousands) and protein complexes that drive cellular function. High-throughput technologies such as mass spectrometry and NMR are being developed to characterize the sequence, structure, and function of proteins. A related computational effort is the study of which proteins interact with each other, and the characterization of protein interaction networks. The Department of Energy's new Genomes to Life program is an active sponsor of this work. The speakers in this session will discuss some of the developments in the newly emerging field of computational proteomics. Related work on how protein interaction data is used in cell-level modeling will be discussed by speakers in mini-symposia MS37 and MS61.

Organizer: Steve Plimpton
Sandia National Laboratories

Organizer: Alex Pothen
Old Dominion University and Sandia National Laboratories

10:30-10:55 Hybrid Methods for Protein Structure Determination: Application of Computational Methods and Sparse Experimental Data
Ying Xu, Oak Ridge National Laboratory

11:00-11:25 Enumerating and Counting Protein Folds using Distance Information
Alex Slepoy, Malin Young, Mark Rintoul, and *Jean-Loup Faulon*, Sandia National Laboratories

11:30-11:55 Enhancing Protein Secondary Structure Prediction by Sequence-to-Structure Alignments
Jarek Meller, Children's Hospital Research Foundation and University of Cincinnati; Aleksey Porollo, Children's Hospital Research Foundation; and *Rafal Adamczak*, University of Cincinnati

12:00-12:25 Graph and Hypergraph Models of Protein Interaction Networks
Alex Pothen, Old Dominion University and Sandia National Laboratories

Tuesday, February 11

MS26 (For Part I, see MS 2)

Computational Modeling of MEMS and BioMEMS

10:30 AM-12:30 PM

Regency Ballroom B

The mini-symposium deals with the computational modeling of MEMS and BioMEMS performance and characterization. Specific areas to be addressed in this mini-symposia are silicon micro-cantilevers for bio-sensing applications, computational models for microfluidics-specific applications, design tools for processes in bio-microsystems (BioMEMS), modeling of permeation layers (gels) in microarrays and BioMEMS. Further, this mini-symposia will act as a platform for information exchange for the more broader audience of BioMEMS industry, academia, and CAD software developers for MEMS.

Organizer: Samuel K. Kassegne
University of California, San Diego

Organizer: Kamal Sarkar
Nanogen, Inc.

10:30-10:55 Simulation-Based Process Design Tool For Biomicrosystems
Metin Ozen, CFD Research Corporation

11:00-11:25 Design Methodology for Inkjet Applications
Ken Greiner, Coventor, Inc.

11:30-11:55 Challenges in Computational Modeling of Permeation Layers in BioMEMS
Samuel Kassegne, University of California; and *Kamal Sarkar*, Nanogen, Inc.

12:00-12:25 Computational Bionanotechnology
Jon Sauer, Eagle Research & Development

Tuesday, February 11

MS27 (For Part II, see MS 51)

Computational Methods for Simulation of Flows with Dynamic Interfaces I

10:30 AM-12:30 PM

Regency Ballroom C

This minisymposium is centered around algorithms for modeling multifluid and flow-solid interactions involving dynamic interfaces. It will focus on the formulation and implementation of the various algorithms used to simulate these challenging problems.

The speakers will cover a wide range of methods and techniques. Methods that scale to large-scale complex 3D problems are of particular interest.

Organizer: Noel J. Walkington
Carnegie Mellon University

10:30-10:55 Phase Field/Level Set Methods for Problems Involving Elasticity
Noel J. Walkington, Carnegie Mellon University

11:00-11:25 Direct Numerical Simulation of the Motion of Settling Ellipsoids in Newtonian and non-Newtonian Fluids
Roland Glowinski and *Tsorng-Whay Pan*, University of Houston

11:30-11:55 Immersed Interface Methods for Fluid Dynamics Problems
Randy LeVeque, Washington University

12:00-12:25 Direct Numerical Simulations of Complex Multiphase Flows
Nabeel Al-Rawahi, Sultan Qaboos University, Oman; and Asghar Esmaeeli and *Gretar Tryggvason*, Worcester Polytechnic Institute

Tuesday, February 11

MS28

Simulation of Transport/ Reaction Systems: Algorithms and Applications

10:30 AM-12:30 PM

Mission Ballroom A

Many important engineering and scientific systems are governed by the complex nonlinear interactions of transport and chemical reactions. Examples include materials processing, combustion, catalysis, biological cell and fuel cell systems. The models for transport/reaction systems consist of coupled nonlinear PDEs with multiple time scales, often over complex geometries. This session will include discussions of the numerical methods for solving these models and results from the analysis of some important transport/ reaction systems.

Organizer: John Shadid
Sandia National Laboratories

Organizer: Andrew Salinger
Sandia National Laboratories

10:30-10:55 Stabilized Finite Element Methods for Simulation of Transport/reaction Systems
Andrew Salinger and *John Shadid*, Sandia National Laboratories

11:00-11:25 An Adaptive Projection Algorithm for Low Mach Number Reacting Flow
John B. Bell, Lawrence Berkeley National Laboratory

11:30-11:55 Numerical Simulation of Heat and Mass Transport and Heterogeneous and Homogeneous Chemical Reactions in Catalytic Monoliths
Steffen Tischer and *Olaf Deutschmann*, University of Heidelberg, Germany

12:00-12:25 Simulating Surface Reaction and Bulk Transport in Solution Crystal Growth
Jeff Derby, University of Minnesota

Tuesday, February 11

MS29 (For Part II, see MS 17) (For Part IV, see MS 41)

Uncertainty Quantification III

10:30 AM-12:30 PM

Mission Ballroom B

The vision of computational experiments predicting the outcomes of physical tests is already a driving force and an accepted model for the future of scientific computing. The emerging field of Uncertainty Quantification addresses issues that are paramount to the validation of model-based predictions and their use as surrogates or supplements to physical tests.

This mini-symposium reviews current research in various aspects of Uncertainty Quantification. These include modeling issues, numerical algorithms, result interpretation, and applications.

Organizer: Steven F. Wojtkiewicz
Sandia National Laboratories

Organizer: Roger Ghanem
Johns Hopkins University

10:30-10:55 A Computational Framework for the Quantitative Representation and Approximation of Uncertainty
Roger Ghanem, Johns Hopkins University

11:00-11:25 Efficient Iterative Algorithms for the Stochastic Finite Element Method with Application to Scattering
Dianne P. O'Leary and *Howard C. Elman*, University of Maryland, College Park; Oliver Ernst, TU Bergakademie Freiberg, Germany; and Michael Stewart, Georgia State University

11:30-11:55 Using Sensitivities in the Calculation of Uncertainties for 3-D Time-Dependent Neutral Particle Transport
Peter Brown, Keith Grant, and *Carol S. Woodward*, Lawrence Livermore National Laboratory

12:00-12:25 A Posteriori Error Estimation for Ordinary Differential Equations
Yang Cao and *Linda R. Petzold*, University of California, Santa Barbara

Tuesday, February 11

MS30 (For Part I, see MS 6)

Challenges in Material Interfaces

10:30 AM-12:30 PM

Mission Ballroom C

Polycrystalline and thin film materials are systems where interface behavior and texture can dominate their processing and behavior. Orientations and arrangements within the material and its network of boundaries are implicated in properties across wide scales, such as, functional properties, like conductivity in microprocessors, and lifetime properties, like fracture toughness in structures. Simulation is becoming an important tool to understand both these properties and processing requirements. This includes compelling evidence of the predictability and robustness of statistical properties of large systems. In this minisymposium we discuss the challenges inherent in this program.

Organizer: Shlomo Ta'asan
Carnegie Mellon University

Organizer: David Kinderlehrer
Carnegie Mellon University

10:30-10:55 Grain Boundary Mobility
David Srolovitz, Princeton University

11:00-11:25 Crossover From Dislocation- to Grain-Boundary Based Deformation in Nanocrystalline Materials by Molecular-Dynamics Simulation
Dieter Wolf, Argonne National Laboratory

11:30-11:55 3D Curvature Driven Grain Growth Simulation
Jeehyun Lee, Carnegie Mellon University

12:00-12:25 Topology Change in a Moving Finite Elements Grain Growth Simulation
Andrew Kuprat, Los Alamos National Laboratory

Tuesday, February 11

MS31 (For Part II, see MS 19)

Fast and Efficient Methods for PDE and Applications III

10:30 AM-12:30 PM

Island Ballroom A

The need to harness the maximum potential of available high performance computers has led to the development of fast and efficient methods for partial differential equations and systems of linear equations arising from the discretization of PDE. These numerical methods have wide applicability, and different classes of partial differential equations arising from increasingly realistic and complicated problems in every field of computational simulation have emerged. This minisymposium will address the recent developments and future directions for such methods.

Organizer: Prabir Daripa
Texas A&M University

Organizer: Satyendra K. Tomar
University of Twente, Netherlands

10:30-10:55 High-Performance Spectral Element Algorithms with Applications in Biofluid Dynamics
Paul F. Fischer, Argonne National Laboratory

11:00-11:25 Efficient Numerical Methods for Porous Media Flow Applications
Richard E. Ewing, Texas A&M University

11:30-11:55 Discontinuous Galerkin Methods for Water Waves
Jaap van der Vegt and *Satyendra K. Tomar*, University of Twente, Netherlands

12:00-12:25 Applications of Some Fast Algorithms for Elliptic PDEs
Prabir Daripa, Texas A&M University

Tuesday, February 11

MS32

A New Initiative in Fusion Simulation

10:30 AM-12:30 PM

Island Ballroom B

The Fusion Simulation Project (FSP) is an ambitious new DOE Office of Science initiative to accurately model magnetically confined plasma discharges for fusion energy. This requires integrating multiple physics domains(extended MHD, gyrokinetics and transport, external drives, and turbulence) and involves time and length scales ranging over several decades in size. New mathematical methods and software architectures for creating and tying together models and codes are needed; this minisymposium outlines the associated technical issues and seeks to enlist potential FSP participants.

Organizer: James P. Corones
Krell Institute

10:30-10:55 An Overview of the Fusion Simulation Project
Jill Dahlburg, General Atomics

11:00-11:25 Issues Related to Integrated Modeling in Fusion Science
Dalton Schnack, SAIC Corporation

11:30-11:55 Preconditioning Implicit Methods for Coupled Physics Models
David E. Keyes, Old Dominion University and ICASE

12:00-12:25 Software Architecture Issues in Integrated Fusion Simulation
Randall B. Bramley, Indiana University

Tuesday, February 11

MS33 (For Part II, see MS 57)

A Toolkit Approach to Parallel Application Development

10:30 AM-12:30 PM

Garden Room A

Implementing parallel applications can be complicated and time consuming. Fortunately, software toolkits are available to simplify application development. These toolkits (often available as open-source software) provide services such as partitioning, solvers, optimization, mesh management and visualization. Their designs place minimal requirements on developers, making them easy to use in applications. Compared to large-scale frameworks for parallel applications, the toolkit approach enables greater flexibility, customization and experimentation. The mini-symposium speakers have developed software following this toolkit philosophy. They represent many areas of scientific computing. They will describe their software's design and capabilities, and discuss its use in applications.

Organizer: Karen D. Devine
Sandia National Laboratories

Organizer: Michael Heroux
Sandia National Laboratories

10:30-10:55 Zoltan: Parallel Data Services and Dynamic Load Balancing
Bruce Hendrickson, Robert Heaphy, Courtenay Vaughan, Erik G. Boman, Robert Preis, and *Karen D. Devine,* Sandia National Laboratories; and William Mitchell, National Institute of Standards and Technology

11:00-11:25 The Unified Parallel Software Project
Richard Barrett, Los Alamos National Laboratory

11:30-11:55 PYRAMID's Link in Tool Chain Development for Unstructured Adaptive Methods
Charles D. Norton, Jet Propulsion Laboratory, California Institute of Technology

12:00-12:25 A Toolkit for the Management of Mesh and Solution Information in a Parallel Distributed Environment
Mark Beall, Simmetrix, Inc.

Tuesday, February 11

MS34

Addressing the Challenges of Simulation-Based Design Optimization

10:30 AM-12:30 PM

Garden Room C

Complex engineering design optimization problems---especially problems governed by computational simulations---rarely lend themselves to straightforward formulation and solution by conventional methods of nonlinear programming. In this minisymposium, we discuss the challenging analytical and computational aspects of simulation-based design problems, as well as techniques for solving some classes of these problems. The techniques include exploiting problem structure, alternative problem formulation, the use of various approximations and multi-physics models to address the cost of expensive simulations (e.g., the solution of differential equations), and the use of computational infrastructures. We also examine alternatives to conventional nonlinear programming for posing and solving design optimization problems.

Organizer: Natalia Alexandrov
NASA Langley Research Center

Organizer: Robert Michael Lewis
College of William & Mary

10:30-10:55 Outstanding Issues in Simulation-Based Design Optimization I
Michael Lewis, College of William & Mary; and *Natalia Alexandrov*, NASA Langley Research Center

11:00-11:25 Outstanding Issues in Simulation-Based Design Optimization II
Michael Lewis, College of William & Mary; and Natalia Alexandrov, NASA Langley Research Center

11:30-11:55 Case Studies in Computational Engineering Design Optimization: Challenges and Solutions
Michael S. Eldred and *Anthony A. Giunta*, Sandia National Laboratories

12:00-12:25 Cellular Automata for Simultaneous Evolution of Simulation and Design of Structural Systems
Zafer Gurdal, Virginia Polytechnic Institute & State University

Tuesday, February 11

MS35 (For Part I, see MS 11)

Undergraduate Computational Science and Engineering

10:30 AM-12:30 PM

Garden Room D

These two minisymposia have been organized to continue the discussion of undergraduate Computational Science and Engineering programs. The scope is broad. Presentations will cover programs and curricula at various levels; assessment techniques, tools and resources; course and information resources; and there will be some time set aside for open discussion to facilitate getting others more involved in the ongoing development of undergraduate CSE.

Organizer: Kris Stewart
San Diego State University

Organizer: Peter R. Turner
Clarkson University

10:30-10:55 CSE in the Calculus Sequence
Robert White, North Carolina State University

11:00-11:25 The Bachelor of Science Degree in Computational Science at SUNY Brockport
Osman Yasar, State University of New York, Stony Brook

11:30-11:55 The Computational Science Minor program at UW-Eau Claire
Paul Thomas, Andrew Phillips, and *Marc R. Goulet*, University of Wisconsin, Eau Claire

12:00-12:25 Resources and Open Discussion
Peter R. Turner, Clarkson University

Tuesday, February 11

MS36 (For Part I, see MS 24)

Advanced Meshing and Discretization Strategies in Application Solution

10:30 AM-12:30 PM

Garden Room F

This minisymposium will provide conference attendees with an overview of the latest research and software developments in the area of meshing and discretization. A large number of toolkits exist in these areas, and we highlight their use in a variety of application areas ranging from computational fluid dynamics and biological models to accelerator design and high energy fusion modeling. By showcasing many different meshing and discretization strategies, we will provide a broad overview of the variety of techniques and software available to application scientists.

Organizer: David L. Brown
Lawrence Livermore National Laboratory

Organizer: Lori Freitag
Argonne National Laboratory

3:15-3:40 An Improved Discretization Library for the Trellis Simulation System
Jean-Francois Remacle, Dibyendu Datta, and *Mark S. Shephard*, Rensselaer Polytechnic Institute

3:45-4:10 Building a Computational Biology Simulation Framework by Using Unstructured, Hybrid Mesh Generation and Discretization Tools
Lynn Trease and *Harold E. Trease*, Pacific Northwest National Laboratory

4:15-4:40 Title Not Available At Time of Publication
Phillip Colella, Lawrence Berkeley National Laboratory

4:45-5:10 Hybrid Continuum-Atomistic Simulations for Multiscale Hydrodynamics
Rich Hornung, Lawrence Livermore National Laboratory; Sanith Wijesinghe, Massachusetts Institute of Technology; and Alejandro Garcia, Lawrence Livermore National Laboratory and San Jose State University

Lunch Break

12:30 PM-2:00 PM

Attendees on Own

• *Cash and carry lunch for SIAM Meeting attendees is available in the Koi Pond area of the gardens.*

Tuesday, February 11

IP6

Computational Science and Engineering Aspects of Wildland Fire Modeling

2:00 PM-2:45 PM

Regency Ballroom

Chair: Mary F. Wheeler, University of Texas, Austin

Wildland fire is a timely application that presents many substantial scientific, computational, and operational challenges. Current field tools for diagnosing expected fire behavior are simple algorithms that can be run on calculators. Researchers and fire managers alike envision a future when we might rely on complex simulations driven by remote sensing data on fire location and land surface properties, as components of planning, education, evacuation, and wildfire mitigation decision support systems.

Many of the challenges that must be faced are common to other CS&E applications. Others are peculiar to this application, in that many of the fundamental physical processes are not understood, some have a stochastic nature and may never be deterministically modeled, nowcasting of convective precipitation (often a factor in fire behavior) may show skill only on the order of a few hours, the need to include geographic spatial data such as roads, streams, etc., due to the physical role it plays in fire behavior, and the difficulty of gathering data for verification and initialization in this dangerous environment. And despite the need for intense computations, for use as an operational application, it must proceed at better than real time.

Simulations of a coupled atmosphere-fire model will be presented. This presentation will provide insight into the current state of the science and the challenges that lay ahead.

Janice Coen
National Center for Atmospheric Research

Coffee Break

2:45 PM-3:15 PM

Regency Annex

Tuesday, February 11

MS37 (For Part II, see MS 61)

Computational Cell Biology

3:15 PM-5:15 PM

Regency Ballroom A

This mini-symposium concentrates on the relatively new and emerging discipline of computational cell biology, where quantitative computer models are used to simulate various aspects of the structure and function of Eucaryotic and Procaryotic cells. Several levels of complexity exist in generating these "virtual" cell models that progress from simulating well mixed, time-dependent, reaction kinetics to fully 3-D, spatially resolved, time-dependent, reaction/diffusion/advection models. The speakers will cover computational cell biology models, codes and environments for simulating intra- and extra-cellular processes. Specific subjects to be covered include models, algorithms, data management, code development, parallel computing, and biologist/code interfaces relevant to computational cell biology.

Organizer: Petri Fast
Lawrence Livermore National Laboratory

Organizer: Harold E. Trease
Pacific Northwest National Laboratory

3:15-3:40 The Virtual Microbial Cell Simulator (VMCS): A Computational Simulation Hierarchy for Modeling the Systems Biology of Microbial Cells
Harold E. Trease, Pacific Northwest National Laboratory

3:45-4:10 Optimized Monte Carlo Methods for Large-scale Microphysiological Modeling
Thomas M. Bartol, The Salk Institute; and Joel Stiles, Pittsburgh Supercomputing Center

4:15-4:40 A Three-dimensional Overset Grid Model of Ca^{2+} Waves in *Xenopus Laevis* Eggs
Petri Fast, Lawrence Livermore National Laboratory

4:45-5:10 The Virtual Cell Project
Les Loew, University of Connecticut

Tuesday, February 11

MS38

Modeling and Simulation of the Electrophysiology of the Heart

3:15 PM-5:15 PM

Regency Ballroom B

Simulating normal and abnormal cardiac electrical rhythms and the effects of external shocks for converting fibrillation is a significant scientific challenge. New methods for these large multi-scale computations and their applications to problems in bioengineering and medicine will be presented in this minisymposium.

Organizer: Andrew D. McCulloch
University of California, San Diego

Organizer: Glenn T. Lines
University of Oslo, Norway

3:15-3:40 Coupling Ventricular Mechanics to Models of Cardiac Electrophysiology
Mary Ellen Belik, Taras Usyk, and *Andrew D. McCulloch*, University of California, San Diego

3:45-4:10 Parallel Solution Strategies for the Bidomain Equations
Glenn T. Lines, University of Oslo, Norway; and Xing Cai, Simula Research Laboratory, Norway

4:15-4:40 Simulation of Shock-Induced Electrical Behavior in the Heart
Natalia A. Trayanova, Tulane University

4:45-5:10 Scroll Wave Stability in the Anatomical Heart
James Weiss, *Alan Garfinkel*, Junzhong Yang, Fagen Xie, Zhilin Qu, and Alan Garfinkel, University of California, Los Angeles

Tuesday, February 11

MS39 (For Part I, see MS 15)

Progress in Implicit Large Eddy Simulation (ILES)

3:15 PM-5:15 PM

Regency Ballroom C

Using modern high-resolution numerical methods to implicitly model turbulence is playing a greater role in many applications from astrophysics to engineering. This two-session mini-symposium will examine the frontiers of physical and mathematical theory supporting these techniques, addressing both, successes and pressing research needs of current implicit subgrid scale (SGS) modeling practices. Finite volume formulations based on various nonlinear discrete equations will be examined, and their relevant differences in the ILES context will be investigated. The main focus is to improve our understanding of how interesting desirable SGS physics can be built implicitly into the numerical scheme or discrete set of equations.

Organizer: William J. Rider
Los Alamos National Laboratory

Organizer: Fernando Grinstein
Naval Research Laboratory

3:15-3:40 A Spectral Vanishing Viscosity Method for LES Applied toTurbulent Channel Flows.
George E. Karniadakis, J. Xu, and *R.M. Kirby*, Brown University

3:45-4:10 Requirements for and Potential Benefits of Subgrid-Scale Turbulence Models for Compressible Fluid Dynamics Codes such as PPM
Sarah Anderson, David Porter, and *Paul Woodward*, University of Minnesota

4:15-4:40 Implicit Subgrid-Scale Modeling by Adaptive Local Deconvolution
Nikolaus Adams, Technische Universität Dresden, Germany

4:45-5:10 MILES of the Flow Past a 6:1 Prolate Spheroid
Christer Fureby, FOI, Sweden

Tuesday, February 11

MS40

Modeling and Simulation of Large Scale Granular Flows

3:15 PM-5:15 PM

Mission Ballroom A

Over the last few years great strides have been made in developing sound mathematical models of granular flows (see for e.g. the work of Hutter or more recently Iverson and Denlinger). Accurate numerical modeling of such flows is of great importance in conducting the realistic simulations necessary for a variety of purposes ranging from public safety planning to a fundamental understanding of the mechanisms. The speakers have expertise in the modeling of the physics and large scale numerical solutions of such problems.

Organizer: Abani K. Patra
State University of New York, Buffalo

Organizer: Bruce Pitman
State University of New York, Buffalo

3:15-3:40 Recent Developments in the Mathematical Modeling of Geophysical Mass Flows
Bruce Pitman, State University of New York, Buffalo

3:45-4:10 Coupled Continuous and Discontinuous Galerkin Methods
Vadym Azinger and *Clint Dawson*, University of Texas, Austin

4:15-4:40 Determination of Granular Free Surfaces
Pierre Gremaud, North Carolina State University

4:45-5:10 Developing High Resolution Simulations of Geophysical Mass Flows Using Solution Adaptive Methods
Abani K. Patra, Andrew Bauer, and *Constantin Nichita*, State University of New York, Buffalo

Tuesday, February 11

MS41 (For Part III, see MS 29) (For Part IV, see MS 53)

Uncertainty Quantification IV

3:15 PM-5:15 PM

Mission Ballroom B

The vision of computational experiments predicting the outcomes of physical tests is already a driving force and an accepted model for the future of scientific computing. The emerging field of Uncertainty Quantification addresses issues that are paramount to the validation of model-based predictions and their use as surrogates or supplements to physical tests.

This mini-symposium reviews current research in various aspects of Uncertainty Quantification. These include modeling issues, numerical algorithms, result interpretation, and applications.

Organizer: Steven F. Wojtkiewicz
Sandia National Laboratories

Organizer: Roger Ghanem
Johns Hopkins University

3:15-3:40 Uncertainty Quantification for Numerical Simulations
James Glimm, State University of New York, Stony Brook

3:45-4:10 The Role of UQ in the Structural Dynamics Model Validation
Tom Paez and *John Red-Horse*, Sandia National Laboratories; and Roger Ghanem, Johns Hopkins University

4:15-4:40 The Application Of Stochastic Differential Equations To Problems Of Contaminant Transport In Porous Media
Thomas F. Russell and *David Dean*, University of Colorado, Denver

4:45-5:10 Stochastic Projection Method for Low-Mach-Number Flow
Habib N. Najm and Matthew Reagan, Sandia National Laboratories; Roger Ghanem and *Omar M. Knio*, Johns Hopkins University; and Olivier Le Maitre, Universite d'Evry Val d'Essone, Evry, France

Tuesday, February 11

MS42 (For Part I, see MS 18)

Nonconvex Variational Methods in Computational Solid Mechanics II

3:15 PM-5:15 PM

Mission Ballroom C

Variational methods are at the core of several breakthroughs in nonlinear solid mechanics. Noteworthy examples are the development of return mapping algorithms in computational plasticity, and the application of relaxation techniques from nonconvex variational calculus to model martensitic phase transformations.

A possibility to combine the successes in these two fields has recently emerged. For example, constitutive updates for crystal plasticity based on (nonconvex) incremental potentials have been proposed, and complex dislocation structures have been studied based on such potentials. Moreover, relaxation of nonconvex potential has established itself as a powerful technique for the development of multiscale models of complex material behavior.

The goal of the minisymposium is to review these recent advances, and to assess their potential as robust computational tools.

Organizer: Michael Ortiz
California Institute of Technology

Organizer: Antonio Desimone
Max Planck Institute for Mathematics in the Sciences, Germany

3:15-3:40 An Application of Gamma Convergence to the Problem of Accelerated Dynamics
Michael Ortiz, California Institute of Technology

3:45-4:10 Adaptive Variational Approximation of a Class of Geometric PDE
Michael J. Holst, University of California, San Diego

4:15-4:40 Metastability and Microstructure in Structural Phase Transformations
Mitchell Luskin, University of Minnesota

4:45-5:10 Formation of Microstructure in 2D Elastic Solids
Johannes Zimmer, California Institute of Technology

Tuesday, February 11

MS43

Bifurcation Analysis Software and Applications

3:15 PM-5:15 PM

Island Ballroom A

A number of publicly available bifurcation analysis codes have been developed to aid the simulation community in analyzing the behavior predicted by their numerical models. The authors of four such codes will present their software, including the targeted class of numerical models, the available algorithms, the user interface, and future research and software directions. The talks will also present an analysis of physical systems using their bifurcation tools.

Organizer: Andrew Salinger
Sandia National Laboratories

3:15-3:40 LOCA: A Stability Analysis Library for Large-Scale Applications
Roger Pawlowski, Louis Romero, and *Andrew Salinger*, Sandia National Laboratories

3:45-4:10 AUTO2000 and Continuation of Periodic Orbits in the Circular Restricted Three Body Problem
Randy Paffenroth, California Institute of Technology

4:15-4:40 DDE-BIFTOOL, a Software Package for the Bifurcation Analysis of Delay Differential Equations
Tatyana Luzyanina, Giovanni Samaey, Koen Engelborghs, and *Dirk Roose*, Katholieke Universiteit Leuven, Belgium

4:45-5:10 Bifurcation Analysis for Time-steppers
Shihe Xin and *Laurette S. Tuckerman*, LIMSI-CNRS, France

Tuesday, February 11

MS44 (For Part I, see MS 20)

Computational Electromagnetics II: Fast Solvers

3:15 PM-5:15 PM

Island Ballroom B

Numerical solution of Maxwell's equations is a critical component in many indistrial and scientific applications. The main focus of this minisimposium will be on recent advances in discretization and efficient iterative solution of Maxwell's equations. It is now well understood that succesful discrete models reflect fundamental topological properties of Maxwell's equations described by the formalism of exterior calculus, differential forms and De Rham cohomology. The speakers will present a wide range of methods that exploit these connections in the context of finite volume, finite difference and finite element settings. The second part of the minisimposium will deal with the challenges that must be overcome in order to solve efficiently the ensuing algebraic systems.

Organizer: Pavel Bochev
Sandia National Laboratories

Organizer: R Lehoucq
Sandia National Laboratories

Organizer: R Tuminaro
Sandia National Laboratories

3:15-3:40 Algebraic Multigird for the Maxwell's Equations
Jonathan Hu, Allen C. Robinson, Pavel Bochev, and *R Tuminaro*, Sandia National Laboratories

3:45-4:10 Element Agglomeration Coarsenings Applied to Non--Traditional Unstructured Finite Element Problems
P Vassilevski, Lawrence Livermore National Laboratory

4:15-4:40 Some Iterative Techniques for Time Harmonic Maxwell Equations
Jay Gopalakrish, University of Florida

4:45-5:10 Back-tracking Ax = b, Reformulation and Preconditioning for Maxwell's Equations
Eldad Haber, Emory University

Tuesday, February 11

MS45 (For Part I, see MS 21)

Computational Science in Component-Based Environments II

3:15 PM-5:15 PM

Garden Room A

This is the second part of the "Computational Science in Component-Based Environments" minisymposium.

Organizer: David E. Bernholdt
Oak Ridge National Laboratory

3:15-3:40 High Throughput Genome Analysis Environment
Philip Locascio, Oak Ridge National Laboratory

3:45-4:10 A Migration Framework for Legacy Scientific Applications
Skip Egdorf and *Teri Roberts*, Los Alamos National Laboratory

4:15-4:40 yourSky as a Prototype for the National Virtual Observatory Component Architecture
David Curkendall and *Joseph C. Jacob*, California Institute of Technology

4:45-5:10 A Common Component Architecture (CCA) Study
Charles D. Norton and *Daniel S. Katz*, Jet Propulsion Laboratory, California Institute of Technology; and E. Robert Tisdale, NASA, Jet Propulsion Laboratory

Tuesday, February 11

MS46

High-Level Software for Parallel PDE Simulation and Optimization

3:15 PM-5:15 PM

Garden Room C

Efficient algorithms for parallel PDE simulation and PDE-constrained nonlinear optimization are key in many areas of computational science and engineering. However, exploration of a research idea can involve months of software development. High-level software can facilitate rapid development of code and consequently rapid exploration of ideas for algorithms or models of physical phenomena. In this minisymposium, we will present results of research done using Sundance and TSF, a system of high-level components that can be used to build efficient parallel simulation codes. Applications include physics-based preconditioners for Navier-Stokes flow, multiphysics interface problems, and PDE-constrained inverse problems.

Organizer: Kevin Long
Sandia National Laboratories

3:15-3:40 Sundance: a High-Level System for Parallel PDE Simulation and Optimization
Kevin Long, Sandia National Laboratories

3:45-4:10 Solving Multiphysics and Interface Problems with Sundance
George Biros, Courant Institute of Mathematical Sciences, New York University

4:15-4:40 Source Inversion for Chemical Attack Using PDE-Constrained Optimization
Volkan Akcelik, Carnegie Mellon University

4:45-5:10 Solving Incompressible Navier-Stokes via Parallel Block Preconditioning
Victoria Howle, Sandia National Laboratories

Tuesday, February 11

MS47 (For Part I, see MS 23)

Combinatorial Algorithms in Scientific Computing

3:15 PM-5:15 PM

Garden Room D

Although scientific computing is generally viewed as the province of differential equations and numerical analysis, combinatorial techniques have long played a crucial role. This minisymposium will showcase several areas in which combinatorial insights can be usefully applied to scientific computing problems. Examples include sparse direct methods, preconditioning, geometric discretization methods, and parallel algorithms. The minisymposium will not only provide an opportunity for researchers to present their most recent results, but also provide a forum for dialogue between applications scientists and algorithm developers.

Organizer: Bruce Hendrickson
Sandia National Laboratories

Organizer: John Gilbert
University of California, Santa Barbara

Organizer: Ali Pinar
Lawrence Berkeley Laboratory

3:15-3:40 Provably Good Boundary Recovery for Delaunay Tetrahedral Meshes
Jonathan R. Shewchuk, University of California, Berkeley

3:45-4:10 Locality and Load Balance in *O(N)* Quantum Chemistry
Chee Kwan Gan and *Matt Challacombe*, Los Alamos National Laboratory

4:15-4:40 Moebius Transformation in Scientific Computing
Marshall W. Bern, Xerox Corporation; and David Eppstein, University of California, Irvine

4:45-5:10 Common Refinement of Nonmatching Meshes for Accurate and Conservative Data Transfer
Michael Heath and Xiangmin Jiao, University of Illinois, Urbana-Champaign

Tuesday, February 11

MS48 (For Part I, see MS 12)

Mesh Quality Improvement

3:15 PM-5:15 PM

Garden Room F

Methods for improving the quality of unstructured meshes are needed to reduce discretization error and improve solver efficiency in computational simulations. Correct problem formulation, robust and efficient numerical improvement algorithms, and studies showing the effect of mesh quality are all of current interest.

A crucial preliminary step in Computational Science and Engineering is mesh generation and improvement. This minisymposium will provide conference attendees with an overview of the latest research in this important area.

Organizer: Patrick Knupp
Sandia National Laboratories

Organizer: Lori Freitag
Argonne National Laboratory

3:15-3:40 Newton Methods for Mesh Quality Optimization
Patrick Knupp, Sandia National Laboratories; Suzanne M. Shontz, Cornell University; and Lori Freitag and *Todd S. Munson*, Argonne National Laboratory

3:45-4:10 Mesh Quality Improvement for Accelerator Design
Patrick Knupp, Sandia National Laboratories; and Kwok Ko and *Nathan Folwell*, Stanford Linear Accelerator Center

4:15-4:40 A Mesh Warping Algorithm based on Weighted Laplacian Smoothing
Stephen A. Vavasis and *Suzanne M. Shontz*, Cornell University

4:45-5:10 Quality Improvement of Geodesic Grids
Patrick Knupp and Mike Brewer, Sandia National Laboratories; and David Randall and *Todd Ringler*, Colorado State University

Intermission

5:15 PM-5:20 PM

Tuesday, February 11

CP12

Computational Biology II

5:20 PM-6:20 PM

Regency Ballroom A

Chair: Monica Hanslien, Simula Research Laboratory, Norway

5:20-5:35 Stability Conditions for Numerical Methods Applied to Stiff Systems of Reaction Diffusion Equations
Monica Hanslien, Simula Research Laboratory, Norway

5:40-5:55 Numerical Methods for Electrophysiology Models of Cardiac Cells
Joakim Sundnes and *Trygve K. Nilssen*, Simula Research Laboratory, Norway

6:00-6:15 Cycling Behavior in Coupled Cell Systems
Antonio Palacios and *Patrick A. Longhini*, San Diego State University

Tuesday, February 11

CP13

Schemes for Complex Flows II

5:20 PM-6:20 PM

Regency Ballroom B

Chair: Paul J. Dellar, University of Oxford, United Kingdom

5:20-5:35 Modeling Continua with Implicit Evolution Equations
Paul J. Dellar, University of Oxford, United Kingdom

5:40-5:55 Removal of Spurious Modes with a Chebyshev Collocation Method
Henar Herrero, Universidad de Castilla-La Mancha, Spain; and Ana Mancho, University of Bristol, United Kingdom

6:00-6:15 A Newton-Krylov Based Solver for Finite Rate Chemistery CFD Modeling
J.-Y. Chen, University of California, Berkeley; and David Wang, Mark Cremer, and *Michael Bockelie*, Reaction Engineering International

Tuesday, February 11

CP14

Electromagnetics

5:20 PM-6:20 PM

Regency Ballroom C

Chair: Georg Hebermehl, Weierstrass Institute for Applied Analysis and Stochastics, Germany

5:20-5:35 Eigen Mode Computation for High Dimensional Problems of Microwave and Laser Structures
Thorsten Tischler, Wolfgang Heinrich, and Horst Zscheile, Ferdinand-Braun-Institut fuer Hoechstfrequenztechnik, Germany; and Rainer Schlundt, Friedrich-Karl Huebner, and *Georg Hebermehl*, Weierstrass Institute for Applied Analysis and Stochastics, Germany

5:40-5:55 Fast High-Order FEM Solutions for Dielectric Waveguides
Zoltan Cendes and *Din-Kow Sun*, Ansoft Corporation

6:00-6:15 Accurate and Unconditionally Stable Algorithms That Solve the Time Evolution of Electromagnetic, Elastodynamic and Acoustic Wavefields
Kristel Michielsen, Hans De Raedt, Thilo Figge, and *Sebastiaan Kole*, University of Groningen, Netherlands

Tuesday, February 11

CP15

Contact Algorithms

5:20 PM-6:20 PM

Mission Ballroom A

Chair: Mark F. Adams, Sandia National Laboratories

5:20-5:35 Multigrid Algorithms for Solving Constrained Linear Systems
Mark F. Adams, Sandia National Laboratories

5:40-5:55 Parallel Finite Element Computation of Contact-Impact Problems with Large Deformations
Fehmi Cirak, California Institute of Technology

6:00-6:15 Numerical Solution of Saddle Point Problems Arising from Linear Elasticity with Intersecting Slide Constraints
Charles Tong, Lawrence Livermore National Laboratory

Tuesday, February 11

CP16

Sensitivity Analysis

5:20 PM-6:00 PM

Mission Ballroom B

Chair: Adrian Sandu, Michigan Technological University

5:20-5:35 Discrete Adjoints for Stiff Systems
Dacian N. Daescu, University of Minnesota, Minneapolis; and *Adrian Sandu*, Michigan Technological University

5:40-5:55 Parameter Sensitivity Analysis of Stochastic Simulation Codes
Eric Hukkanen, Richard C. Alkire, Richard Braatz, and *Timothy Drews*, University of Illinois, Urbana-Champaign

Tuesday, February 11

CP17

Wavelet Methods for Differential Equations

5:20 PM-6:20 PM

Mission Ballroom C

Chair: Ian Gladwell, Southern Methodist University

5:20-5:35 Wavelet Collocation for Ode Boundary Value Problems
Bentley Garrett and *Ian Gladwell*, Southern Methodist University

5:40-5:55 Smoothing and the Discrete Wavelet Transform: The PDE Connection
Raghu K. Machiraju and *Gheorghe Craciun*, Ohio State University; and David Thompson, Mississippi State University

Tuesday, February 11

CP18

Stochastic PDEs

5:20 PM-6:00 PM

Island Ballroom A

Chair: David J. Horntrop, New Jersey Institute of Technology

5:20-5:35 Simulation for Mesoscopic Models
David J. Horntrop, New Jersey Institute of Technology; Markos A. Katsoulakis, University of Massachusetts, Amherst; and Dionisios Vlachos, University of Delaware

5:40-5:55 Adaptive Solution of Nonlinear Stochastic Problems
Andreas Keese and *Hermann G. Matthies*, Technical University Braunschweig, Germany

Tuesday, February 11

CP19

Interface Problems

5:20 PM-6:20 PM

Island Ballroom B

Chair: Arturo Fernandez, Worcester Polytechnic Institute

5:20-5:35 Effects of Electrostatic Forces on the Phase Distribution in Droplet Suspension. Three-Dimensional Numerical Simulations
Arturo Fernandez, Worcester Polytechnic Institute

5:40-5:55 Coalescence of Unequal Particles by Surface Diffusion
Wen Zhang, Oakland University; Pavlo Sachenko and Joachim Schneibel, Oak Ridge National Laboratory; and Ian Gladwell, Southern Methodist University

6:00-6:15 Solving Differential-Difference Equations and Their Application to Crystalline Growth
Christopher E. Elmer, New Jersey Institute of Technology; Antony Humphries and Kate Abell, University of Sussex, United Kingdom; and Erik Van Vleck, University of Kansas

Tuesday, February 11

CP20

Methods for Particle Simulations

5:20 PM-6:20 PM

Garden Room C

Chair: Ashok Srinivasan, Florida State University

5:20-5:35 Computational Techniques for Efficient Carbon Nanotube Simulation
Ashok Srinivasan, Florida State University; and Namas Chandra, Florida A & M University

5:40-5:55 Adaptive Treecode Algorithms for Particle Simulations
Robert Krasny and *Hans E. Johnston*, University of Michigan

6:00-6:15 Targeted Langevin Stabilization of Molecular Dynamics
Jesus A. Izaguirre and *Qun Ma*, University of Notre Dame

Tuesday, February 11

CP21

Problem Solving Environments

5:20 PM-6:20 PM

Garden Room D

Chair: Deborah A. Payne, Pacific Northwest National Laboratory

5:20-5:35 The Architecture of a Problem-Solving Environment for Computational Biology and Bioinformatics
George Chin, Heidi Sofia, Deborah Gracio, Eric Stephan, Kyle Klicker, and *Deborah A. Payne*, Pacific Northwest National Laboratory

5:40-5:55 A Framework for Check-Pointed Fault-Tolerant Out-of-Core Linear Algebra
Eduardo F. D'Azevedo, Oak Ridge National Laboratory; and Piotr Luszczek, University of Tennessee, Knoxville

6:00-6:15 A High-Level Approach to the Synthesis of High-Performance Codes for Quantum Chemistry
Daniel Cociorva, Russell Pitzer, P Sadayappan, and Gerald Baumgartner, Ohio State University; Robert Harrison, University of Tennessee and Oak Ridge National Laboratory; J Ramanujam, Louisiana State University; So Hirata, Pacific Northwest National Laboratory; *David E. Bernholdt*, Oak Ridge National Laboratory; and Marcel Nooijen, Princeton University

Tuesday, February 11

CP22

Domain Decomposition Methods

5:20 PM-6:00 PM

Garden Room F

Chair: Xiao-Chuan Cai, University of Colorado

5:20-5:35 A Scalable One-Level Schwarz Algorithm for the Unsteady Nonlinear Radiation Diffusion Problem
Serguei Ovtchinnikov and *Xiao-Chuan Cai*, University of Colorado

5:40-5:55 Alternating Explicit Implicit Domain Decomposition for Parabolic Equations
Yu Zhuang, Texas Tech University

Tuesday, February 11

Poster and Dessert Reception

8:00 PM-10:00 PM

Regency Annex

Optimization of Systems Governed by Pdes: Parallel Algorithms and Applications to Parameter Estimation, Optimal Control, and Optimal Design
Volkan Akcelik, Carnegie Mellon University; George Biros, Courant Institute of Mathematical Sciences, New York University; Alexandre Cunha, Carnegie Mellon University; Ioannis Epanomeritakis, Carnegie Mellon University; Omar Ghattas, Carnegie Mellon University; Kevin Long and Bart van Bloeman Waanders, Sandia National Laboratories

Effect of Slat Gap Width on the Performance of A Naca 0012 Airfoil: A Numerical Study
Khalid N. Alammar, King Abdulaziz City for Science and Technology, Saudi Arabia

Improving the Performance of Pde-Based Simulations by Using Multi-Method Solvers
Sanjukta Bhowmick and Padma Raghavan, Pennsylvania State University; Lois C. McInnes and Boyana Norris, Argonne National Laboratory

Parallel Multiresolution Octree-Based Simulation of Earthquake Ground Motion in Heterogeneous Basins
Omar Ghattas, Carnegie Mellon University; Eui-Joong Kim, Carnegie Mellon University; Jacobo Bielak, Carnegie Mellon University; Jianlin Wang,Synopsis, Inc.

A Method of Using Neumann Functions to Analyze Waveguides with Arbitrary Cross Section
Nguyen Hoang Hai, Hanoi University of Technology, Vietnam; Akira Yonesu, Yamashiro Yasumasa, and Masao Kodama, University of the Ryukyus, Japan

The Numerical Calculation of Electromagnetic Fields by Using Watson's Transformation Methods
Nguyen Hoang Hai, Hanoi University of Technology, Vietnam; Akira Yonesu, Yamashiro Yasumasa, and Masao Kodama, University of the Ryukyus, Japan

Numerical Method for Time Reversal of Waves in Random Media
Mansoor A. Haider, Jean-Pierre Fouque, and Kurang Mehta, North Carolina State University

Geometric Completion of Circuit Dae Using Numeric-Symbolic Methods
Kamyar Hazaveh Hesarmaskan, Ryerson University, Canada; Greg Reid, University of Western Ontario, Canada

Microstructural Simulation of Blood Flow on Parallel Computers
Judy Hill, Carnegie Mellon University

High-End Computer System Performance: Science and Engineering
Paul D. Hovland, Argonne National Laboratory; David Bailey, Erich Strohmaier, and Dan Quinlan, Lawrence Berkeley National Laboratory; Bronis deSupinski, Lawrence Livermore National Laboratory; Jeffrey S. Vetter, Lawrence Livermore National Laboratory; Patrick H. Worley, Oak Ridge National Laboratory; Thomas Dunigan, Oak Ridge National Laboratory; Boyana Norris, Argonne National Laboratory; Jack J. Dongarra, University of Tennessee, Knoxville; Dan Reed, University of Illinois; Jeff Hollingsworth, University of Maryland; Allan Snavely, San Diego Supercomputer Center

The Estimation of Missing Data for Acute and Chronic Stress Arena, Duration and Stress Ratings
Paul Johnson, University of California, San Francisco

The Modeling of Acute and Chronic Stress
Paul Johnson, University of California, San Francisco

Projection-Based Parallel Delaunay Meshing Algorithms
Clemens Kadow, Carnegie Mellon University

Terascale Optimal Pde Simulations
David E. Keyes, Old Dominion University and ICASE

Robust Algebraic Multigrid
Scott P. Maclachlan and Marian Brezina, University of Colorado, Boulder; Robert Falgout, Lawrence Livermore National Laboratory; Tom Manteuffel, Steve McCormick, and John Ruge, University of Colorado, Boulder

Large-Scale Methods for Calculating Exact Cumulative Reaction Probabilities
Michael Minkoff, Al Wagner, and Ron Shepherd, Argonne National Laboratory

Least-Squares Finite Element Methods for Hyperbolic Pdes
Luke Olson, Hans De Sterck, Tom Manteuffel, and Steve McCormick, University of Colorado, Boulder

Parallel Bipartite Matching for Sparse Matrix Computations
Jason Riedy, University of California, Berkeley

Managing Biological Concept Maps With The Heuristic Entity Relationship Building Environment (herbe)
Eric Stephan, George Chin, and Heidi Sofia, Pacific Northwest National Laboratory

Computational Simulation Environments
Dave A. Swensen, Martin Denison, and Chris Montgomery, Reaction Engineering International; Dav de St. Germain, University of Utah; Mike Maguire andMichael Bockelie, Reaction Engineering International

Uncertainty in Numerical Prediction Models: the Lack of Convergence of the Lorenz Equations
Joao C. Teixeira, UCAR/VSP, Naval Research Laboratory

Automatic Performance Tuning of Sparse Matrix Kernels
Richard Vuduc, James W. Demmel, and Katherine Yelick, University of California, Berkeley

Robust Optimal Design for Biological Systems Via the Laplace Approximation
Mitchell J. Watrous, Bradley Bell, Mike Dodds, Andrew Hooker, and Paolo Vicini, University of Washington

First-Order System Least Squares for Geometrically Nonlinear Elasticity
Chad Westphal, Tom Manteuffel, Steve McCormick, and Jens Schmidt, University of Colorado, Boulder

Wednesday, February 12

Registration
8:00 AM-5:30 PM
Regency Annex

Announcements
8:15 AM-8:30 AM
Regency Ballroom
Steven F. Ashby, Lawrence Livermore National Laboratory

IP7
The Evolving Numerical Toolkit for Micromachined Device (MEMS) Design: Fast Integral Equation Solvers, Coupled-Domain Techniques, and Model Reduction
8:30 AM-9:15 AM
Regency Ballroom
Chair: Shanghua Teng, Boston University & Akamai Technologies

The technical and capital investment in VLSI technology has made it possible to put more than a million transistors on a square centimeter of silicon, and that investment has also been making it possible to fabricate devices with micron-scale moving parts. These micromachined devices, often referred to as MEMS, are appearing in an ever broading range of applications including wristwatch-sized communicators, pipe and tire sensors, credit-card sized chemical analysis systems, and medical diagnostic equipment. In order to design these complicated systems, engineers need easily evaluated models of the micromachined devices. Although most micromachined-device models are still generated in a time-consuming manual fashion, the trend is to generate the models numerically. In this talk we will describe how micromachined models are being generated by combining fast integral equations methods, coupled-domain techniques, and model-order reduction algorithms.

Jacob White
Massachusetts Institute of Technology

IP8
Variational and Multiscale Methods in Turbulence with Particular Emphasis on Large Eddy Simulation
9:15 AM-10:00 AM
Regency Ballroom
Chair: Michael Ortiz, California Institute of Technology

We describe recent progress in the formulation and development of Large Eddy Simulation procedures utilizing variational methods in place of traditional filtering techniques and employing multiscale decompositions of underlying function spaces. The approach provides a framework for simultaneously addressing theoretical issues concerning the foundation of Large Eddy Simulation procedures and practical modeling issues. Computations employing the simplest instantiations of the ideas are presented for homogeneous isotropic flows and wall-bounded flows and in all cases very good results are obtained.

Thomas J.R. Hughes
University of Texas, Austin

Coffee Break
10:00 AM-10:30 AM
Regency Annex

Wednesday, February 12

MS49

10:30 AM-12:30 PM

Regency Ballroom A

This session was merged with MS61 Computational Cell Biology. MS 61 is scheduled for Wednesday, February 12, 2002, 3:15 PM - 5:15 PM.

Wednesday, February 12

MS50

Large, Multi-Scale Modeling in Computational Chemistry and Engineering

10:30 AM-12:30 PM

Room: Regency Ballroom B

The focus of this mini-symposium is recent developments in modeling large, multi-scale problems in chemical engineering and computational chemistry. A related secondary theme is the underlying research in computational tools for solving these models. Of particular interest are methodologies that combine knowledge of physics and mathematics to develop novel algorithms for solving physical problems. Four of the most active researchers from the engineering and science communities will present the latest developments of their work in large, multi-scale modeling.

Organizer: Mark A. Stadtherr
University of Notre Dame

Organizer: Angelo Lucia
University of Rhode Island

10:30-10:55 Large Scale Optimization in Molecular Modeling
Praveen Depa and *Angelo Lucia*, University of Rhode Island

11:00-11:25 Interval Computing Approach in Computational Chemistry and Engineering
Youdong Lin and *Mark A. Stadtherr*, University of Notre Dame; and Hongkun Liang, Quest Pharmaceutical Services

11:30-11:55 Coarse, Equation-Free Computation
Yannis Kevrekidis, Princeton University

12:00-12:25 Novel Techniques for Bridging Time and Length Scales in Molecular Dynamics
Mark E. Tuckerman, Courant Institute of Mathematical Sciences, New York University

Wednesday, February 12

MS51 (For Part I, see MS 27) (For Part III, see MS 75)

Computational Methods for Simulation of Flows with Dynamic Interfaces II

10:30 AM-12:30 PM

Regency Ballroom C

The minisymposium is cenerted around algorithms for modeling multifluid and flow-solid interactions involving dynamic interfaces. This symposium will focus on the formulation and implementation of the various algorithms used to simulate these challenging problems.

The speakers will cover a wide range of methods and techniques. Methods that scale to large-scale complex 3D problems are of particular interest.

Organizer: Noel J. Walkington
Carnegie Mellon University

Organizer: George Biros
Courant Institute of Mathematical Sciences, New York University

Organizer: Xiaolin Li
State University of New York, Stony Brook

10:30-10:55 Simplifying the Front Tracking Method to Track Complex Interface in High Dimensions
Xiaolin Li, State University of New York, Stony Brook

11:00-11:25 Robust Modeling Techniques for Free-Surface Flows in Complex Geometries
Feby Abraham and *Marek Behr*, Rice University

11:30-11:55 A Fully Conservative Ghost Fluid Method for Shocks, Contacts, and Detonations in Compressible Flows
Ron Fedkiw, Stanford University

12:00-12:25 Overset Grid Methods for Simulating Interfaces in Motion
Petri Fast, Lawrence Livermore National Laboratory

Wednesday, February 12

MS52 (For Part II, see MS 76)

Computational Methods for the Simulation of Heavily-Loaded Gas-Particle Flows

10:30 AM-12:30 PM

Mission Ballroom A

There are many instances of dense particle-fluid flow, ranging from industrial processes to geologic events. These are described by a wide variety of mathematical models. Attempts to simulate these processes quantitatively, by accurate solution of models, have led to the development of a variety of computational methods. Some of these approaches are novel, others are modifications of existing approaches. The speakers will present recent advances in this area.

Organizer: Thomas O'Brien
National Energy Technology Laboratory

10:30-10:55 CFD Simulations of Reactive, Bubbling Fluidized Beds
Thomas O'Brien, National Energy Technology Laboratory; and Madhava Syamlal, Fluent, Inc.

11:00-11:25 Agent-Based Model for Bubbling Fluidized Beds
John Halow, National Energy Technology Laboratory; and Stuart Daw and *Sreekanth Pannala*, Oak Ridge National Laboratory

11:30-11:55 Detailed Chemical Calculations in Fluidized Beds
Francine Battaglia and *Rodney O. Fox*, Iowa State University

12:00-12:25 Discrete Element Simulation of the Flow of Granular Material
Jayathi Murthy, Purdue University; and Dhanunjay Boyalakuntla, Carnegie Mellon University

Wednesday, February 12

MS53 (For Part IV, see MS 41) (For Part VI, see MS 65)

Uncertainty Quantification V

10:30 AM-12:30 PM

Mission Ballroom B

The vision of computational experiments predicting the outcomes of physical tests is already a driving force and an accepted model for the future of scientific computing. The emerging field of Uncertainty Quantification addresses issues that are paramount to the validation of model-based predictions and their use as surrogates or supplements to physical tests.

This mini-symposium reviews current research in various aspects of Uncertainty Quantification. These include modeling issues, numerical algorithms, result interpretation, and applications.

Organizer: Steven F. Wojtkiewicz
Sandia National Laboratories

Organizer: Roger Ghanem
Johns Hopkins University

10:30-10:55 Adaptive Solution of Nonlinear Stochastic Problems
Andreas Keese and *Hermann G. Matthies*, Technical University Braunschweig, Germany

11:00-11:25 Wiener-Hermite Expansions for the Problem of Three Interacting Shear Waves
Robert Rubinstein, NASA Langley Research Center

11:30-11:55 Uncertainty Quantification in Electrochemical Microchannel Flow
Bert Debusschere and *Habib N. Najm*, Sandia National Laboratories; Omar M. Knio, Roger Ghanem, and Alain Matta, Johns Hopkins University; and Olivier Le Maitre, Universite d'Evry Val d'Essone, Evry, France

12:00-12:25 Random Oscillators and Polynomial Chaos
George E. Karniadakis and *Didier Lucor*, Brown University

Wednesday, February 12

MS54

Computational Modeling of Functionally Graded Materials

10:30 AM-12:30 PM

Mission Ballroom C

Functionally graded materials (FGMs) are an important area of materials science research, with potentially many important applications, e.g., super-heat resistance materials for thermal barrier coatings and furnace liners, electromagnetic sensors, and graded refractive index materials for optical applications. In a typical FGM, the material properties vary smoothly in one dimension, providing a smooth transition between different materials (e.g., a metal and a ceramic). Computational analysis can be an effective method for designing specific FGM systems, and for understanding FGM behavior. This minisymposium will address recent developments in the mathematical and computational analysis of these non-homogeneous materials.

Organizer: Leonard Gray
Oak Ridge National Laboratory

Organizer: John Berger
Colorado School of Mines

10:30-10:55 Singular Integration of FGM Green's Functions
Leonard Gray, Oak Ridge National Laboratory

11:00-11:25 Crack Tip Fields in FGMs
John Berger, Colorado School of Mines

11:30-11:55 Green's Function for an Exponentially Graded Three-dimensional Elastic Solid
Paul Martin, Colorado School of Mines

12:00-12:25 Title Not Available at Time of Publication
Glaucio Paulino, University of Illinois

Wednesday, February 12

MS55 (For Part II, see MS 67)

Scientific Computing with Radial Basis Functions

10:30 AM-12:30 PM

Island Ballroom A

In this minisymposium, we try to focus on the recent meshless methods using radial basis functions developed in the past decade.

Meshless methods overcome a big shortcoming of traditional numerical methods in that no mesh is needed in the modeling. So it can solve many problems with complicated geometry and is very easy to parallelize. Such techniques have been applied to many areas.

It would be very beneficial for experts in this area to show their results to more general audiences in scientific computations.

The speakers include people from both theoretical areas and engineering community. They will discuss open issues in these areas.

Organizer: Edward J. Kansa
Lawrence Livermore National Laboratory

Organizer: Jichun Li
University of Nevada, Las Vegas

10:30-10:55 A Volumetric RBF Formulation for Time Dependent PDEs
Edward J. Kansa, Lawrence Livermore National Laboratory

11:00-11:25 Collocation Discretizations of the Transport Equation with Radial Basis Functions
Joseph Ward, Texas A&M University

11:30-11:55 Discontinuous Approximations in Meshfree and Radial Basis Function Methods
Ted Belytschko, Northwestern University

12:00-12:25 Quantum Hydrodynamics with Adaptive Grids and Radial Basis Functions
Robert E. Wyatt, University of Texas, Austin

Wednesday, February 12

MS56 (For Part II, see MS 80)

Mimetic Discretization of Continuun Mechanics

10:30 AM-12:30 PM

Island Ballroom B

Problems in continuum mechanics are commonly described by initial boundary value problems for a system of partial differential equations. Such problems can be discretized using finite differences, finite elements, spectral or many related techniques. Mimetic methods follow a different route: they are not used to discretize particular systems of equations, but rather to discretize the continuumn theory. Vector calculus provides a powerful invariant (coordinate free) description of continuum mechanics as does the theory of differential forms. In the vector calculus case, the operators, gradient, curl and divergence play a central role and the equations of continuum mechanics can be written in term of these operators along with the time derivative. The mimetic methods for vector calculus provide discretization of the gradient, curl and divergence, and then these discretizations are used to approximate the partial differential equations that appear in continuum mechanical problems. In this session we will discuss the theoretical aspects of the methods and present some applications.

Organizer: Jose Castillo
San Diego State University

Organizer: Stanly Steinberg
University of New Mexico

10:30-10:55 High Order Mimetic Differential Operators
Jose E. Castillo, San Diego State University

11:00-11:25 A Mimetic Finite Difference Approach for Source and Sink Steady State Problems
Juan M. Guevara-Jordan, Universidad Central de Venezuela, Venezuela

11:30-11:55 Mimetic Finite Difference Method for the Steady Diffusion Equation with Rough Coefficients
Sergio Rojas, Universidad de Oriente, Venezuela

12:00-12:25 Convergence Rates for Mimetic Operators
Mark Yasuda, San Diego State University

Wednesday, February 12

MS57 (For Part I, see MS 33)

A Toolkit Approach to Parallel Application Development

10:30 AM-12:30 PM

Garden Room A

Implementing parallel applications can be complicated and time consuming. Fortunately, software toolkits are available to simplify application development. These toolkits (often available as open-source software) provide services such as partitioning, solvers, optimization, mesh management and visualization. Their designs place minimal requirements on developers, making them easy to use in applications. Compared to large-scale frameworks for parallel applications, the toolkit approach enables greater flexibility, customization and experimentation. The mini-symposium speakers have developed software following this toolkit philosophy. They represent many areas of scientific computing. They will describe their software's design and capabilities, and discuss its use in applications.

Organizer: Karen D. Devine
Sandia National Laboratories

Organizer: Michael Heroux
Sandia National Laboratories

10:30-10:55 Using Trilinos Solver Packages: An Overview
Michael A. Heroux, Sandia National Laboratories

11:00-11:25 SUNDIALS: Suite of Nonlinear, Differential, and Algebraic Equations Solvers
Carol S. Woodward and *Radu Serban*, Lawrence Livermore National Laboratory

11:30-11:55 TAO: Toolkit for Advanced Optimization
Lois Curfman McInnes, Jorge More', Jason Sarich, and *Steve Benson*, Argonne National Laboratory

12:00-12:25 The Visualization ToolKit
Jim Ahrens, Los Alamos National Laboratory; and Berk Geveci and *Charles Law*, Kitware Incorporated

Wednesday, February 12

MS58

Sensitivity Analysis and Applications in Computational Science and Engineering

10:30 AM-12:30 PM

Garden Room C

The range of problems encountered in scientific and engineering research is broad, yet the various fields share many computational issues and objectives. In terms of sensitivity analysis, researchers are typically interested in calculating the sensitivity of simulation with respect to initial conditions or model parameters. In this minisymposium, we discuss various sensitivity analysis techniques and how they are used to carry out such tasks as design optimization, model evaluation, and parameter estimation studies.

Organizer: Steven L. Lee
Lawrence Livermore National Laboratory

10:30-10:55 Sensitivity Analysis for Scientific Simulations: Software and Applications
Steven L. Lee, Lawrence Livermore National Laboratory

11:00-11:25 Continuous Sensitivity Analysis for the Design of Control Systems
Jeffrey Borggaard, Virginia Polytechnic Institute & State University

11:30-11:55 Aero-structural Optimization of Aircraft Configurations Using Coupled Adjoint Sensitivity Analysis
Joaquim Martins, Stanford University

12:00-12:25 Adjoint Sensitivity and Optimal Control for Flow with Discontinuities
Ionel Michael Navon, Florida State University

Wednesday, February 12

MS59

Problem Solving Environments for Simulation and Modeling

10:30 AM-12:30 PM

Garden Room D

This minisymposium focuses on the development and application of problem solving environments (PSE's) for simulation and modeling of systems described using combinations of partial differential equations and/or differential algebraic equations. Contributions to this minisymposium include a range of applications associated with modeling of natural systems, including linear and nonlinear PDE's governing flow in porous media, geochemical and mass transfer reactions, and mechanics. Issues associated with the development of PSE's for complex systms is also a focus, including notions of efficiency for the model developer and efficiency of the resultant simulation model.

Organizer: Casey Miller
University of North Carolina, Chapel Hill

Organizer: Jan Prins
University of North Carolina

10:30-10:55 A PSE for Modeling Transport Phenomena in Porous Medium Systems
Harvey E. Jeffries, Jan Prins, Joseph Kanney, and David Sassen, University of North Carolina; and Matthew W. Farthing and *Casey Miller*, University of North Carolina, Chapel Hill

11:00-11:25 Challenges in Software Development for Multi-Physics Simulation
Hans P. Langtangen, University of Oslo, Norway

11:30-11:55 Mathematical and Computational Modeling of Multiphysics Couplings
Mary F. Wheeler, University of Texas, Austin

12:00-12:25 A GIS-Based Tool for Performing Automated Groundwater Flow and Transport Calculations
Marc Witkowski and *Bruce Robinson*, Los Alamos National Laboratory

Wednesday, February 12

MS60

CAD to Mesh

10:30 AM-12:30 PM

Garden Room F

A major bottle neck for computational simulations in complex 3D geometries is to set up the computational mesh. The problem set-up process consists of all the steps needed to take a geometry description from a computer-aided-design (CAD) program and convert it into a 3D volumetric mesh that can be used to perform the analysis.

This mini-symposium will discuss the state of the art and current directions in unstructured, Cartesian, Overset, and hybrid grid generation techniques and should be of interest to engineers, computational scientists, and applied mathematicians involved in mesh-based simulations in complex geometries.

Organizer: Anders Petersson
Lawrence Livermore National Laboratory

10:30-10:55 Rapsodi: Geometry Preparation and Grid Generation
Anders Petersson, Lawrence Livermore National Laboratory

11:00-11:25 A Geometry-Based Automated Simulation Toolkit
Mark Beall, Simmetrix, Inc.

11:30-11:55 Automatic Generation of Simulation Models from Design-Based Feature Models
Mark S. Shephard, Rensselaer Polytechnic Institute; and Mark W. Beall, Simmetrix, Inc.

12:00-12:25 Cad Interfaces: Why Simple Wrappers Aren't Enough
Tim Tautges, Sandia National Laboratories

Lunch Break

12:30 PM-2:00 PM

Attendees on Own

• *Cash and carry lunch for SIAM Meeting attendees is available in the Koi Pond area of the gardens.*

Wednesday, February 12

IP9

Combinatorial Scientific Computing: The Role of Discrete Algorithms in Computational Science and Engineering

2:00 PM-2:45 PM

Room: Regency Ballroom

Chair: Isabelle Charpentier, Institut d'Informatique et Mathematiques Appliquees, France

Although scientific computing is generally viewed as the province of differential equations and numerical analysis, combinatorial techniques have long played a crucial role. For example, graph theory is essential to the study of molecular structures and material science. Many problems in linear algebra involve discrete algorithms. And the parallelization of scientific computations leads to numerous combinatorial problems. I will review some of these many successes, and offer suggestions for new areas in which work is needed at this exciting intersection of disciplines.

Bruce Hendrickson
Sandia National Laboratories

Coffee Break

2:45 PM-3:15 PM

Regency Annex

Wednesday, February 12

MS61 (For Part I, see MS 37)

Computational Cell Biology

3:15 PM-5:15 PM

Room: Regency Ballroom A

This mini-symposium concentrates on the relatively new and emerging discipline of computational cell biology, where quantitative computer models are used to simulate various aspects of the structure and function of eucaryotic and procaryotic cells. Several levels of complexity exist in generating these "virtual" cell models that progress from simulating well mixed, time-dependent, reaction kinetics to fully 3-D, spatially resolved, time-dependent, reaction/diffusion/advection models. The speakers will cover computational cell biology models, codes and environments for simulating intra- and extra-cellular processes. Specific subjects to be covered include models, algorithms, data management, code development, parallel computing, and biologist/code interfaces relevant to computational cell biology.

Organizer: Petri Fast
Lawrence Livermore National Laboratory

Organizer: Steven J. Plimpton
Sandia National Laboratories

Organizer: Harold E. Trease
Pacific Northwest National Laboratory

3:15-3:40 Studying the Alpha Pathway in Yeast with Moleculizer
Larry Lok, The Molecular Sciences Institute

3:45-4:10 The Impact of Spatial Realism on Microphysiological Models
Thomas M. Bartol, The Salk Institute; and *Joel Stiles*, Pittsburgh Supercomputing Center

4:15-4:40 Mesh Generation and Modeling of Biological Systems Using Cubit
Jason Shepherd, Sandia National Laboratories

4:45-5:10 Application of Continuum, Unstructured Finite Element Numerical Methods to

Spatial Models of Intracellular Calcium Dynamics
Shawn Means, Sandia National Laboratories

Wednesday, February 12

MS62

Computational Hemodynamics

3:15 PM-5:15 PM

Regency Ballroom B

Application of computational fluid dynamics methods to biomedical and bioengineering problems presents a number of unique challenges. Blood exhibits complex behavior, and presents us with a distinct set of criteria for "desirable" flow characteristics. Hemodynamics simulations involve deforming domains, and fluid interaction with the vessel walls, leading to additional complexity.

The minisymposium will address the following topics: analysis of shear-stress levels and blood cell damage, prediction of stagnation patterns and clotting, modeling of interaction between fluid and the deformable vessel walls, and role of simulation in surgery planning and design of biomedical devices.

Organizer: Marek Behr
Rice University

3:15-3:40 Challenges in Realistic Modeling of Hemodynamics from Medical Images
Peter Yim, Peter Choyke, and Robert Lutz, National Institutes of Health; James Burgess, Inova Fairfax Hospital; Rainald Lohner, Marcelo Castro, Orlando Soto, and *Juan R. Cebral*, George Mason University; and Noam Alperin, University of Illinois, Chicago

3:45-4:10 The Use of Numerical Methods for the Development and Optimization of Cardiovascular Artificial Organs
Leonid Goubergrits, Humboldt University at Berlin, Germany

4:15-4:40 Microstructural Simulation of Blood Flow on Parallel Computers
Judy Hill, Carnegie Mellon University

4:45-5:10 Flow Prediction for Complex Centrifugal Blood Pumps
Dhruv Arora and *Marek Behr*, Rice University

Wednesday, February 12

MS63

High Order and Conservative Semi-Lagrangian Methods

3:15 PM-5:15 PM

Regency Ballroom C

Semi-Lagrangian methods have gained considerable popularity in the past 20 years. Interest in this method was limited mainly to the meteorology community but it has branched out into many other fields including computational fluid dynamics. The emergence of this approach is due to its ability to increase the maximum time-step allowed without suffering instabilities or inaccuracies.

Although since its inception the semi-Lagrangian method has proved quite powerful, some complaints of the method have been in regards to its lack of conservation and its low order accuracy (cubic or less). In this minisymposium, we present the current trends in constructing conservative and high-order accurate semi-Lagrangian methods and their possible applications. The applications presented here include: numerical weather prediction, climate modeling, transport modeling, and turbulence simulations.

Organizer: Francis X. Giraldo
Naval Research Laboratory

Organizer: Joern Behrens
Munich University of Technology, Germany

3:15-3:40 Spectral Element Semi-Lagrangian Methods for Numerical Weather Prediction
Francis X. Giraldo, Naval Research Laboratory

3:45-4:10 Achieving Conservation Properties for Adaptive Semi-Lagrangian Advection Schemes
Joern Behrens, Munich University of Technology, Germany

4:15-4:40 Semi-Lagrangian Method for Turbulence Simulation
George E. Karniadakis, Suchan Dong, and *Dongbin Xiu*, Brown University

4:45-5:10 Efficient Conservative Semi-Lagrangian Schemes over the Sphere
Ramachandran Nair, National Center for Atmospheric Research

Wednesday, February 12

MS64

Understanding the Dynamics of the Gulf of California: A Workbench for the GC

3:15 PM-5:15 PM

Mission Ballroom A

The purpose of this minisymposium is to contribute to the understanding of the dynamics at the entrance to the Gulf of California. Specifically, we will focus on how bottom topography affects the currents and spatial distribution of physical properties at that region. We will be presenting some three dimensional numerical experiments on the dynamics at the entrance to the Gulf of California. The simulations were obtained with a full three dimensional curvilinear model, developed by the author, which is able to use adapted grids.

Organizer: Carlos R. Torres
San Diego State University

Organizer: Jose Castillo
San Diego State University

3:15-3:40 Upper-ocean Circulation Patterns in the Northern Gulf of California Expressed in ERS-2 Synthetic Aperture Radar Imagery
Asdrubal Martínez-Díaz-de, Universidad Autónoma de Baja California, Mexico

3:45-4:10 The Seasonal Variation of Geostrophic Velocity and Heat Flux at the Entrance to the Gulf of California, Mexico
Curt Collins, Naval Postgraduate School; and Ruben Castro, Reginaldo Durazo, and *Affonso D. S. Mascarenhas*, Universidad Autónoma de Baja California, Mexico

4:15-4:40 Stratified Flow Over Three-dimensional Submarine Topography
José E. Castillo and *Carlos R. Torres*, San Diego State University

4:45-5:10 Three-dimensional Visualization of the Density Field at the Entrance to the Gulf of California
Carlos R. Torres, Jose Castillo, and *Aaron Lindsau*, San Diego State University

Wednesday, February 12

MS65 (For Part V, see MS 53)

Uncertainty Quantification VI

3:15 PM-5:15 PM

Mission Ballroom B

The vision of computational experiments predicting the outcomes of physical tests is already a driving force and an accepted model for the future of scientific computing. The emerging field of Uncertainty Quantification addresses issues that are paramount to the validation of model-based predictions and their use as surrogates or supplements to physical tests.

This mini-symposium reviews current research in various aspects of Uncertainty Quantification. These include modeling issues, numerical algorithms, result interpretation, and applications.

Organizer: Steven F. Wojtkiewicz
Sandia National Laboratories

Organizer: Roger Ghanem
Johns Hopkins University

3:15-3:40 Strategies for Visualizing 2D Distribution Data
Alex Pang, University of California, Santa Cruz

3:45-4:10 Surrogate-based Optimization Under Uncertainty: Status and Directions
Timothy Trucano, Steven F. Wojtkiewicz, Anthony A. Giunta, and *Michael S. Eldred*, Sandia National Laboratories

4:15-4:40 Non-intrusive Main Effects and Sensitivity Calculations for Uncertainty Quantification
Monica Martinez-Canales, Sandia National Laboratories; and Juan C. Meza, Lawrence Berkeley National Laboratory

4:45-5:10 Nonstationary Excitation Data Condensation for Analytical Probabilistic Dynamic Response Analysis: An application using the 1999 Chi-Chi Earthquake Ground Motion Recordings
Andrew Smyth, Columbia University; and Sami Masri, University of Southern California

Wednesday, February 12

MS66

Automated Multi-Level Substructuring in Structural Dynamics

3:15 PM-5:15 PM

Mission Ballroom C

Dynamic analysis of complex two- and three-dimensional structures frequently involves finite element discretizations with over a million unknowns. In practise, the finite element matrices are projected onto the low frequency eigenspace computed via a partial eigensolution.

An alternative is to compute the needed eigenspace via Automated Multi-Level Substructuring (AMLS) where the structure is recursively divided into thousands of subdomains. Approximations to the eigenvectors are computed from these subdomain eigenvalue problems.

The goal of this minisymposium is to introduce AMLS and its use on large-scale two and three dimensional eigenvalue problems arising in structural dynamics. Analysis and the results of experiments on large-scale structures will demonstrate that AMLS is an extremely effective approach for computational structural dynamics.

Organizer: Richard B. Lehoucq
Sandia National Laboratories

Organizer: Jeffery K. Bennighof
University of Texas

3:15-3:40 Introduction to AMLS
Richard B. Lehoucq, Sandia National Laboratories; and Jeffery K. Bennighof, University of Texas

3:45-4:10 AMLS in Practical Vibration Analysis
Jeffery K. Bennighof, University of Texas

4:15-4:40 Massively Parallel Modal Analysis in Salinas
Kendall Pierson, Sandia National Laboratories

4:45-5:10 Scaling AMLS for 3D problems
Richard B. Lehoucq, Sandia National Laboratories; and *Ulrich L. Hetmaniuk*, University of Colorado, Boulder

Wednesday, February 12

MS67 (For Part I, see MS 55)

Scientific Computing with Radial Basis Functions

3:15 PM-5:15 PM

Island Ballroom A

In this minisymposium, we try to focus on the recent meshless methods using radial basis functions developed in the past decade.

Meshless methods overcome a big shortcoming of traditional numerical methods in that no mesh is needed in the modeling. So it can solve many problems with complicated geometry and is very easy to parallelize. Such techniques have been applied to many areas.

It would be very beneficial for experts in this area to show their results to more general audiences in scientific computations.

Speakers include people from both theoretical areas and the engineering community. They will discuss open issues in these areas.

Organizer: Edward J. Kansa
Lawrence Livermore National Laboratory

Organizer: Jichun Li
University of Nevada, Las Vegas

3:15-3:40 Domain Decomposition with Radial Basis Meshless Methods
Jichun Li, University of Nevada, Las Vegas

3:45-4:10 Radial Basis Functions for Solving PDEs
Xin Li, University of Nevada, Las Vegas

4:15-4:40 Numerical Techniques for Large Scale RBF Computations with Applications to Image Reconstruction and Geophysics
Rick Beatson, University of Canterbury, New Zealand

Wednesday, February 12

MS68

Modeling and Computational Approaches in Electromagnetic Applications

3:15 PM-5:15 PM

Island Ballroom B

Electromagnetic problems are encountered frequently in industrial applications. A thorough understanding of such problems relies on both viable physical models as well as fast and efficient computational methods. The speakers in this session address issues that arise in the modeling and computation of electromagnetic systems. The first talk deals with a model for pressure-dependent electric polarization for use in electromagnetic interrogation techniques. The second gives a theoretical and computational perspective on electromagnetic wave propagation in nonlinear materials. The third focuses on a finite difference time domain technique which is used to model the interaction of an electromagnetic wave with bi-anisotropic media. Finally, the last talk concerns the implementation of reduced order Proper Orthogonal Decomposition techniques in conjunction with eddy current based nondestructive evaluation. Numerical results are presented in each lecture.

Organizer: Michele L. Joyner
State University of West Georgia

Organizer: Julie K. Raye
Virginia Commonwealth University

3:15-3:40 A Pressure-Dependent Polarization Model for Use in Electromagnetic Interrogation
Julie K. Raye, Virginia Commonwealth University

3:45-4:10 Maxwell-systems with Nonlinear Polarization
Gabriella Pinter, University of Wisconsin, Milwaukee; and H.T. Banks, North Carolina State University

4:15-4:40 A Novel Finite Difference Time Domain (FDTD) Technique to Model Bi-anisotropic Media and Its Subclasses
Alkim Akyurtlu, University of Massachusetts, Lowell; and Douglas Werner, Pennsylvania State University

4:45-5:10 Real Time Computational Algorithms for Electromagnetic Interrogation of Structures
Michele L. Joyner, State University of West Georgia

Wednesday, February 12

MS69

Numerical Algorithm and PDE Applications of the Grid

3:15 PM-5:15 PM

Garden Room A

Most effort in grid computing has been devoted to developing the software environment for the application of the grid in a friendly environment Application of the grid is however almost exclusively devoted to large-scale computations with embarrassing parallelism. It is on the other hand yet unclear whether the grid will ever be of use for traditional PDE applications that today are run on traditional supercomputers. The goal of this mini-symposium is to present several attempts to make numerically efficient use the grid for applications such as medical applications, fluid dynamics, or combustion problems. The main emphasis is on an appropriate integration of methods and the design of new algorithms that are highly tolerant to low bandwidth and high latency as in wide area networks. Future research will have to deal with the development of robust and fault tolerant algorithms.

Organizer: Marc Garbey
University of Houston

3:15-3:40 Algorithm for PDE Applications on the Grid
Marc Garbey, University of Houston

3:45-4:10 Metacomputing Application in a Grid Environment
Matthias S. Mueller, Rainer Keller, Edgar Gabriel, Matthias Hess, and *Peggy Lindner*, High Performance Computing Center Stuttgart, Germany; and Michael Resch, University of Stuttgart, Germany

4:15-4:40 Scalable Domain Decomposition Methods on the GRID
Damien Tromeur-Dervout, Universite Lyon, France

4:45-5:10 Teraflop Computational Materials Science
Yang Wang, Pittsburgh Supercomputing Center

Wednesday, February 12

MS70

Computational Methods for Large Scale Inverse Problems

3:15 PM-5:15 PM

Garden Room C

Many applications in diverse areas such as geophysical exploration and medical imaging involve the reconstruction of parameter functions from noisy observations on solutions of models consisting of PDEs or integral equations.

Numerical approaches for the solution of such problems involve a combination of methods and fields such as numerical optimization techniques, sparse and iterative linear algebra, multi-level methods and robust statistics.

This minisymposium will explore such computational methods for the solution of large scale problems.

Organizer: Eldad Haber
Emory University

3:15-3:40 An All at Once Method for Time Domain Maxwell's Equations
Eldad Haber, Emory University

3:45-4:10 Parallel Preconditioned Newton-Krylov Methods for Inverse Wave Propagation
Volkan Akcelik and *Omar Ghattas*, Carnegie Mellon University; and George Biros, Courant Institute of Mathematical Sciences, New York University

4:15-4:40 An Object Oriented Approach to Image Restoration in MATLAB
James G. Nagy, Emory University

4:45-5:10 Computational Methods for Adaptive Optics
Curtis R. Vogel, Montana State University

Wednesday, February 12

MS71

Undergraduate Computational Science and Engineering Education: Status and Trends

3:15 PM-5:15 PM

Garden Room D

Undergraduate courses and programs in computational science and engineering started at large research universities in the 1970s and have now become part of the curriculum at smaller universities and liberal arts colleges. Recently, the first bachelor's degree program in computational science was initiated and the NSF awarded a major grant to train undergraduate faculty in the methods of computational science. This minisymposium will assess the status of undergraduate computational science based on the wealth of experience gained and consider the following questions: (1) What is the intellectual core of computational science? (2) What constitutes an interdisciplinary undergraduate CSE program?

Organizer: Charles D. Swanson
University of Minnesota

3:15-3:40 An Assessment of Undergraduate Computational Science and Engineering Education
Charles D. Swanson, University of Minnesota; and James P. Corones, Krell Institute

3:45-4:10 Elements of Computational Science Education and Degree Programs
Osman Yasar, State University of New York, Brockport; and *Rubin Landau*, Oregon State University

4:15-4:40 Lessons from the National Computational Science Institute: Quantitative Reasoning Across the Curriculum
Robert M. Panoff, The Shodor Education Foundation

4:45-5:10 Internships for Undergraduates in Computational Science
Angela B. Shiflet, Wofford College

Wednesday, February 12

MS72

High-Order Discretizations

3:15 PM-5:15 PM

Garden Room F

High-order discretizations for PDEs have gained increasing attention in recent years.Their theoretical development has reached a high level of sophistication and the range of applications has been broadening, including such diverse areas as global atmospheric modeling, aerodynamics, oceanography, thermal convection and theoretical chemistry. Recent advances include stabilization techniques, high-order time schemes, treatment of singularities, adaptivity, complex geometries, mixed discretization techniques, domain decomposition, and parallelism. The speakers in this minisymposium present an overview of some of these advances in various application areas, including geophysics, biofluids, and aerodynamics.

Organizer: Paul F. Fischer
Argonne National Laboratory

3:15-3:40 Discontinuous Galerkin Methods for Modeling Biot's Consolidation Problem
Mary F. Wheeler, University of Texas, Austin

3:45-4:10 High-order Adaptive Discontinuous Galerkin Methods for Hyperbolic Systems
Mark Shephard, Lilia Krivodonova, Jean-Francois Remacle, and *Joseph E. Flaherty*, Rensselaer Polytechnic Institute

4:15-4:40 Adaptivity and Error Estimation for Inverse Problems Involving PDEs
Wolfgang Bangerth, University of Texas, Austin

4:45-5:10 Robust Spectral Element Methods for Convection-Dominated Flows
Paul F. Fischer, Argonne National Laboratory

Intermission

5:15 PM-5:20 PM

Wednesday, February 12

CP23

Schemes for Complex Flows III

5:20 PM-6:20 PM

Regency Ballroom A

Chair: Fotini Labropulu, University of Regina, Canada

5:20-5:35 Unsteady Flow of a Second Grade Fluid Near a Stagnation Point
Fotini Labropulu, University of Regina, Canada

5:40-5:55 An Exact Solution for Pump-Driven Damped Linearized Isothermal Pressure Waves in Nearly Rigid Rough Oil Pipelines
Guillermo Miranda and *Luis E. Leon*, Universidad Central de Venezuela, Venezuela; and Jose Castillo, San Diego State University

6:00-6:15 Numerical Modelling of the Flow in the Steady Distributed Self-Similar Porous Medium
Olga N. Soboleva, Institute of Computational Mathematics and Mathematical Geophysics; and Gennady A. Kuz'min, Siberian Branch, RAS, Novosibirsk

Wednesday, February 12

CP24

Computational Biology III

5:20 PM-6:20 PM

Regency Ballroom B

Chair: Peter Salamon, San Diego State University

5:20-5:35 Structure-Composition Relationships of Mitochondria Membranes
Arlette Baljon and *Ben Neely*, San Diego State University

5:40-5:55 A Computational Model of Nitric Oxide Transport in the Human Lungs
Steven George and *Satish K. Vutukuru*, University of California, Irvine

6:00-6:15 Genomic Analysis of An Uncultured Marine Viral Community
Bjarne Andresen, University of Copenhagen, Denmark; David Mead, Lucigen Corporation; Mya Breitbart, Joseph Mahaffy, Anca Segall, Forest Rohwer, and *Peter Salamon*, San Diego State University; and Farooq Azam, Scripps Institution of Oceanography

Wednesday, February 12

CP25

Simulation-Based Optimization

5:20 PM-6:20 PM

Regency Ballroom C

Chair: Stefan Koerkel, IWR Heidelberg University, Germany

5:20-5:35 Numerical Methods for Design of Optimal Robust Experiments with Application to Parameter Estimation in Chemistry and Chemical Engineering
Ekaterina Kostina and Georg Bock, IWR - University of Heidelberg, Germany; and Johannes P. Schloeder and *Stefan Koerkel,* IWR Heidelberg University, Germany

5:40-5:55 Selecting the Optimum Quasi-Steady State Species for Reduced Chemical Kinetic Mechanisms
J.-Y. Chen, University of California, Berkeley; Alan Parkinson, Brigham Young University; and Darren Shino, Shane Brunson, David Swensen, Chongguan Yang, and Chris Montgomery, Reaction Engineering International

6:00-6:15 The Surface Hardening of Steel Modeling, Simulation and Optimal Control
Dietmar Hoemberg, Weierstrass Institute for Applied Analysis and Stochastics, Germany

Wednesday, February 12

CP26

Geometric Algorithms

5:20 PM-6:00 PM

Mission Ballroom A

Chair: To Be Determined

5:20-5:35 Towards Efficient Parallel Delaunay Mesh Generation with Guaranteed Quality
Clemens Kadow, Carnegie Mellon University

5:40-5:55 Selection-Based Compression of Simulation Datasets
Scott B. Baden, University of California, San Diego

Wednesday, February 12

CP27

Krylov Methods

5:20 PM-6:00 PM

Mission Ballroom B

Chair: Allison Baker, University of Colorado

5:20-5:35 An Efficient Block Variant of GMRES
Elizabeth Jessup and *Allison Baker,* University of Colorado

5:40-5:55 Exponential Integrators for Differential-Algebraic Equations
Richard B. Lehoucq, Sandia National Laboratories; and *Christopher K. Newman,* Virginia Polytechnic Institute & State University and Sandia National Laboratories

Wednesday, February 12

CP28

Nonlinear and Eigen Solvers

5:20 PM-6:20 PM

Mission Ballroom C

Chair: Russell W. Hooper, Sandia National Laboratories

5:20-5:35 Robust Simulation of Nonlinear Materials Using Nox: An Object-Oriented Nonlinear Solver Library
Russell W. Hooper, Sandia National Laboratories

5:40-5:55 A Tensor-Krylov Method for Solving PDE Problems
Brett W. Bader, University of Colorado, Boulder

6:00-6:15 Eigenvalue Computation by Multiple Explicitly Restarted Arnoldi Method
Seyed Abolfazl Shahzadeh Fazeli and *Nahid Emad*, University of Versailles, France

Wednesday, February 12

CP29

Schemes for Complex Flows IV

5:20 PM-6:20 PM

Island Ballroom A

Chair: Adrian Sandu, Michigan Technological University

5:20-5:35 Modeling the Dynamics and Chemistry of Atmospheric Aerosols
Christian T. Borden and *Adrian Sandu*, Michigan Technological University

5:40-5:55 Finite Difference Approximations in Nonuniform Grids
Enrique Sanmiguel-Rojas, Carlos del Pino, and *Joaquin Ortega-Casanova*, Universidad de Málaga, Spain

6:00-6:15 Mathematical Models and Thermodynamic Limits of Separation Processes
Anatoly Tsirlin, Russian Academy of Sciences, Russia; and Vladimir Kazakov, University of Technology, Sydney, Australia

Wednesday, February 12

CP30

Boundary Integral Equation Methods

5:20 PM-6:20 PM

Island Ballroom B

Chair: Francesco Fedele, University of Vermont

5:20-5:35 Fluorescence Tomography Using the Boundary Element Method
Jeffrey Laible, Margaret J. Eppstein, and *Francesco Fedele*, University of Vermont

5:40-5:55 An Approximation of the Solid Angle for Solving a Poisson-Type Equation
Maria I. Troparevsky, Universidad de Buenos Aires, Argentina; and Diana Rubio, Universidad Nacional de General Sarmiento and Universidad Nacional de General San Martín, Argentina

6:00-6:15 A Fundamental Solution Method for Solving Tracer Flow Equations
Juan M. Guevara-Jordan, Universidad Central de Venezuela, Venezuela

Wednesday, February 12

CP31

Scalable Linear Algebra Methods

5:20 PM-6:20 PM

Garden Room C

Chair: James McCombs, College of Wiliam & Mary

5:20-5:35 Parallel, Multigrain Solvers for Hiding Network Latencies on Mpp's and Networks of Clusters
Andreas Stathopoulos and *James R. McCombs*, College of William & Mary

5:40-5:55 Monte Carlo Linear Algebra Techniques and Their Parallelization
Ashok Srinivasan, Florida State University

6:00-6:15 Block Linear Algebra on the Peer to Peer Xtremweb/yml Platform
Olivier J. Delannoy, University of Versailles, France; and Serge G. Petiton, Universite de Lille, France

Wednesday, February 12

CP32

Discrete Algorithms II

5:20 PM-6:20 PM

Garden Room D

Chair: Minghong Pi, University of Alberta, Canada

5:20-5:35 Load-Balancing in Distributed Retrieval System
Minghong Pi, University of Alberta, Canada

5:40-5:55 A New Method to Obtain Relaxed Problems of Graph Optimization Problems
Sumio Masuda, Tomofumi Nishide, and *Kazuaki Yamaguchi*, Kobe University, Japan

6:00-6:15 Sequential and Parallel Algorithms for the Rectilinear Steiner Tree Problem
Can Ozturan and Nahit Emanet, Bogazici University, Turkey

Wednesday, February 12

CP33

General Topics

5:20 PM-6:00 PM

Garden Room F

Chair: Sachiko Honda, University of Washington

5:20-5:35 Platform Independent Parallel Framework That Uses Network File System For Communication
Bradley Bell, Michael Macaulay, and *Sachiko Hond*a, University of Washington

5:40-5:55 Target Localization Using Computational Geometry
Marcus Graham and *Megan M. Gibson*, Naval Undersea Warfare Center

Intermission

6:20 PM-6:30 PM

SIAM Business Meeting SIAG/CSE

6:30 PM-7:30 PM

Regency A & B

Thursday, February 13

Registration

8:00 AM-2:00 PM

Room: Regency Annex

Closing Remarks

8:15 AM-8:30 AM

Regency Ballroom

David E. Keyes, Old Dominion University and ICASE

Attention Poster Presenters

Posters must be removed by 2:00 PM today. Posters remaining after this time will be discarded. Thank you for your cooperation!

IP10

Arteries and Algorithms: Computational Modelling of the Human Vascular System

8:30 AM-9:15 AM

Regency Ballroom

Chair: John Shadid, Sandia National Laboratories

The association of vascular diseases, such as atherosclerosis, with blood flow properties such as wall shear stress has driven the use of computational methods to model flow in the larger arteries of the human vascular system. The problem presents a range of challenges from the non-Newtonian, pulsatile nature of blood flow, operating at intermediate Reynolds numbers, to the intricate geometric characteristics and distensible properties of the arteries. In this presentation we will discuss the application of spectral/hp element methods to the problem of vascular flow modelling. Starting with a reduced model to simulation the full vascular system we will then consider the complex flow modelling at arterial junctions and outline recent collaborative in-vivo work in arterial bypass grafting.

Spencer Sherwin
Imperial College, London, United Kingdom

IP11

Science Discoveries Using Computational Astrophysics

9:15 AM-10:00 AM

Regency Ballroom

Chair: John Drake, Oak Ridge National Laboratory

This talk will be a broad review of progress and current activities in computational astrophysics and cosmology. I will discuss advances in algorithms and applications afforded by a decade of access to parallel computers of exponentially increasing capabilities. I will highlight several applications where computation has led directly to new paradigms in our understanding of cosmic phenomena.

Michael Norman
University of California, San Diego

Coffee Break

10:00 AM-10:30 AM

Regency Annex

Thursday, February 13

MS73

Applications of MRA Methods to Computational Chemistry and Fluid Dynamics

10:30 AM-12:30 PM

Regency Ballroom A

We present a multiresolution analysis methodology for solving multiscale problems described by differential and integro-differential equations in three and higher dimensions using discontinuous multiwavelets and low separation rank representations. Using this methodology, highly accurate, spatially adaptive, fast and practical algorithms are derived. We review the theoretical and algorithmic aspects of these methods as well as results from applications to computational chemistry and fluid dynamics.

This minisymposium describes effective and practical multiresolution and low separation rank methods and algorithms that produces fast and high precision algorithms for solving PDEs in three and higher dimensions.

Organizer: George Fann
Oak Ridge National Laboratory

Organizer: Gregory Beylkin
University of Colorado, Boulder

Organizer: Robert Harrison
University of Tennessee and Oak Ridge National Laboratory

10:30-10:55 Separated Representations and Multiresolution Algorithms in Multiple Dimensions
Martin Mohlenkamp, Ohio State University; and *Gregory Beylkin*, University of Colorado, Boulder

11:00-11:25 Efficient Representation of the Projector on Divergence Free Functions
George Fann, Oak Ridge National Laboratory; and Gregory Beylkin and Robert Cramer, University of Colorado, Boulder

11:30-11:55 Multiresolution Quantum Chemistry
Robert Harrison, University of Tennessee and Oak Ridge National Laboratory; Takeshi Yanai, Pacific Northwest National Laboratory; Gregory Beylkin, University of Colorado, Boulder; and George Fann, Oak Ridge National Laboratory

12:00-12:25 Adaptive Multiresolution Solvers for a Class of Advection-Diffusion Equations
Aime Fournier, University of Maryland and NCAR; and Gregory Beylkin and *Vani Cheruvu*, University of Colorado, Boulder

Thursday, February 13

MS74 (For Part II, see MS 86)

Quantum Networks for Computation and Control I

10:30 AM-12:30 PM

Regency Ballroom B

Artificial neural networks have been applied to solve engineering problems ranging from computational image processing to control of complex systems---most sinificantly, problems for which there is no apparent path to an algorithmic solution. Quantum computers are expected to outperform classical computers, but only a few quantum algorithms are currently known. This suggests that investigation of quantum `neural' networks might lead to quantum systems which can efficiently solve additional problems. The speakers in this minisymposium will describe several efforts in this direction: quantum perceptrons, quantum networks, and quantum learning. Both analysis and large scale simulations will be represented.

Organizer: David A. Meyer
University of California, San Diego

10:30-10:55 Quantum Perceptrons
Markus Hunziker, University of Georgia

11:00-11:25 Control by Quantum Perceptrons
David A. Meyer, University of California, San Diego

11:30-11:55 Semi-Classical and Quantum Entangled Neural Networks
Fariel Shafee, Princeton University

12:00-12:25 Learning Problems Between Unstructured Search and Majority
Jamie Pommersheim, Pomona College

Thursday, February 13

MS75 (For Part II, see MS 51)

Computational Methods for Simulation of Flows with Dynamic Interfaces III

10:30 AM-12:30 PM

Regency Ballroom C

The minisymposium is cenerted around algorithms for modeling multifluid and flow-solid interactions involving dynamic interfaces. This symposium will focus on the formulation and implementation of the various algorithms used to simulate these challenging problems.

The speakers will cover a wide range of methods and techniques. Methods that scale to large-scale complex 3D problems are of particular interest.

Organizer: Noel J. Walkington
Carnegie Mellon University

Organizer: George Biros
Courant Institute of Mathematical Sciences, New York University

Organizer: Xiaolin Li
State University of New York, Stony Brook

10:30-10:55 Error Distribution Models for Strong Shock Interactions
John W. Grove, Los Alamos National Laboratory

11:00-11:25 Nonlinear Aeroelasticity: Finite Element Formulations and Parallel Solution Algorithms
Soulaimani Azzeddine, Ecole de Technologie Supérieure, France

11:30-11:55 An Embedded Boundary Integral Solver for the Incompressible Navier Stokes with Moving Boundaries
Lexing Ying, Denis Zorin, and *George Biros*, Courant Institute of Mathematical Sciences, New York University

12:00-12:25 A Free Surface Updating Methodology for Marker-Function Based Eulerian Free Surface Capturing Techniques on Unstructured Triangular Meshes
Ahamadi Malidi and *Steven Dufour*, École Polytechnique de Montréal, Canada

Thursday, February 13

MS76

Computational Methods for the Simulation of Heavily-Loaded Gas-Particle Flows

10:30 AM-12:30 PM

Mission Ballroom A

There are many instances of dense particle-fluid flow, ranging from industrial processes to geologic events. These are described by a wide variety of mathematical models. Attempts to simulate these processes quantitatively, by accurate solution of models, have led to the development of a variety of computational methods. Some of these approaches are novel, others are modifications of existing approaches. The speakers will present recent advances in this area.

Organizer: Thomas O'Brien
National Energy Technology Laboratory

10:30-10:55 Discrete Element Simulation of Gas-Particle Flows
Dinesh Gera, Fluent, Inc.

11:00-11:25 Description of Fluidized Beds Using Proper Orthogonal Decomposition
Madhava Syamlal, Fluent, Inc.; Thomas O'Brien, National Energy Technology Laboratory; Paul Cizmas, Texas A&M University; and *Antonio Palacios*, San Diego State University

11:30-11:55 Accurate Numerical Methods for the Solution of Two-Fluid Models
Chris Guenther, Fluent, Inc.

Thursday, February 13

MS77

Fiber-Optic Communication Systems

10:30 AM-12:30 PM

Mission Ballroom B

Fiber-optic communication systems are the basis for modern telephone networks and the internet. Advances in this area continue to occur at a relentless pace. For example, dense wavelength-division multiplexing (DWDM) has made it possible to carry more than 100 signal channels on a single fiber, resulting in transmission systems with bit rates of more than 1 terabits per second. The ever-increasing complexity of such systems has necessitated the use of mathematical modeling and numerical analysis techniques for the design and control of these systems. The talks in this minisymposium cover some recent advances in modeling and simulation of fiber-optic communication systems.

Organizer: Roland W. Freund
Bell Laboratories, Lucent Technologies

Organizer: Lawrence Cowsar
Bell Laboratories, Lucent Technologies

10:30-10:55 Optical Transport Systems: Introduction and Simulation Directions
Tin K. Ho and *Lawrence Cowsar*, Bell Laboratories, Lucent Technologies

11:00-11:25 Estimating the Reliability of Optical Transmission Systems with Importance Sampling
Gino Biondini, Ohio State University; and William Kath, Northwestern University

11:30-11:55 Advances in Modeling High-data-rate Optical Fiber Communication Systems
B.S. Marks, R. Holzloehner, I.T. Lima, Jr., and *Curtis Menyuk*, University of Maryland, Baltimore County

12:00-12:25 Control and Design of Broadband Raman Amplifiers
Tin K. Ho, Leon Vardapetyan, and *Roland W. Freund*, Bell Laboratories, Lucent Technologies

Thursday, February 13

MS78

CS&E Panel: Impact on Solution of Automotive, Aerospace, and Manufacturing Applications

10:30 AM-12:30 PM

Mission Ballroom C

The global competitiveness of each industrial organization is dependent upon how effectively it can continually reduce lead time between concept and production of new products. By doing so, the individual company can rapidly respond to utilization of new technologies, shifting customer needs and desires as well as competition from domestic and foreign rivals. The session panelists will address several aspects of CS&E directly related to their specialities, including such topics as computational fluid dynamics, numerical algorithms, parallel and distributed computing, visualization and computer graphics. Feedback from the audience and amongst the panelists will be permitted and encouraged during this session.

Organizer: Myron Ginsberg
HPC Research and Education

10:30-10:35 Opening Remarks
Myron Ginsberg, HPC Research and Education

10:35-10:55 The Impact of Computational Fluid Dynamics on Aerospace and Automotive Design
Dipankar Choudhury, Fluent, Inc.

11:00-11:25 Web-Based Distributed Simulation of Aeronautical Propulsion System
Greg Follen and *Isaac Lopez*, NASA Glenn Research Center

11:30-11:55 Computer Simulation in the Automotive and Aerospace Industry: The Challenge of the Transition to a New Solution
Gregory A. Clifford, IBM Corporation

12:00-12:25 Aspects of Computational Science in Advanced Material Manufacturing
Ram Mohan, University of New Orleans; and Brian Henz and *Dale Shires*, US Army Research Laboratory

Thursday, February 13

MS79

Software for the Numerical Solution of ODEs

10:30 AM-12:30 PM

Island Ballroom A

The field of numerical ODE software is well established. For example, robust computer codes to numerically solve ODEs have been around for more than a quarter of a century. However, to fully exploit the rapid developments in computer hardware (e.g., processors, memory, and architecture) and programming languages (e.g., object orientation and parallelism), there have been corresponding developments in software. In this minimsymposium, we cover a range of topics related to software for the numerical solution of ODEs. Topics include the numerical solution of initial-value problems by implicit-explicit schemes, boundary-value problems, delay differential equations, differential-algebraic equations, and optimal control problems.

Organizer: Paul Muir
St. Mary's University

Organizer: Raymond J. Spiteri
Dalhousie University, Canada

10:30-10:55 The Case for Implicit-Explicit Methods
Raymond J. Spiteri, Dalhousie University, Canada

11:00-11:25 Software Development for Boundary Value Ordinary Differential Equations
Paul Muir, St. Mary's University

11:30-11:55 DDAE: an integrator for ODEs, DAEs and DDEs
Fred Krogh, Math à la Carte, Inc.; and Philip W. Sharp, University of Auckland, New Zealand

12:00-12:25 SOCS: Software for Large, Sparse Optimal Control Problems
John T. Betts, William P. Huffman, and *Joerg M. Gablonsky*, The Boeing Company

Thursday, February 13

MS80 (For Part I, see MS 56)

Mimetic Discretization of Continuun Mechanics

10:30 AM-12:30 PM

Island Ballroom B

Problems in continuum mechanics are commonly described by initial boundary value problems for a system of partial differential equations. Such problems can be discretized using finite differences, finite elements, spectral or many related techniques. Mimetic methods follow a different route: they are not used to discretize particular systems of equations, but rather to discretize the continuum theory. Vector calculus provides a powerful invariant (coordinate free) description of continuum mechanics as does the theory of differential forms. In the vector calculus case, the operators, gradient, curl and divergence play a central role. The equations of continuum mechanics can be written in term of these operators along with the time derivative. The mimetic methods for vector calculus provide discretization of the gradient, curl and divergence, and then these discretizations are used to approximate the partial differential equations that appear in continuum mechanical problems. In this session, we will discuss the theoretical aspects of the methods and present some applications.

Organizer: Jose Castillo
San Diego State University

Organizer: Stanly Steinberg
University of New Mexico

10:30-10:55 Convergence of Mimetic Discretization Methods
Stanly Steinberg, University of New Mexico; and Mikhail Shashkov and James M. Hyman, Los Alamos National Laboratory

11:00-11:25 Discrete Exterior Calculus
Anil Hirani, California Institute of Technology

11:30-11:55 Lattice Subdivisions for Simplicial 3+1 Electrodynamics
Fernando L. Teixeira, Ohio State University

12:00-12:25 Data Structures for CEM via Algebraic Topology
P. Robert Kotiuga, Boston University

Thursday, February 13

MS81

Locality in Scientific Applications

10:30 AM-12:30 PM

Garden Room A

The current drive toward increased locality can be seen as a response to the development of cache-based architectures. This symposium will explore the current state of the art in improving the locality for scientific applications as well as current obstacles. We will discuss how the drive for greater locality effects the user and what such improvements mean for the applications. A variety of different approaches will be explored: techniques for hand tuning, the use of library based approaches, and compile-time automation to support improved locality within applications. The approaches range from the use of specialized data structures to the use of high level abstractions (hiding many details of the specialized data structures to the use of high level abstractions.

Organizer: Daniel J. Quinlan
Lawrence Livermore National Laboratory

Organizer: Ulrich J. Ruede
University of Erlangen-Nuremberg, Germany

10:30-10:55 Locality-optimized Iterative Algorithms
Ulrich J. Ruede, University of Erlangen-Nuremberg, Germany; and Markus Kowarschik, University of Erlangen, Germany

11:00-11:25 Automated Introduction of User-Defined Locality Optimizations
Markus Schordan and *Daniel J. Quinlan*, Lawrence Livermore National Laboratory

11:30-11:55 Cache Aware Multigrid Algorithms and Their Implementations
Gundolf Haase, Johannes Kepler Universität, Linz; Jonathan Hu, Sandia National Laboratories; and Danny Thorn and *Craig Douglas*, University of Kentucky

12:00-12:25 Interactions of Load Balancing and Locality
F. David Sacerdoti and *Scott B. Baden*, University of California, San Diego

Thursday, February 13

MS82

Automatic Differentiation and Sensitivity Analysis for Differential Equations

10:30 AM-12:30 PM

Garden Room C

Automatic differentiation and sensitivity analysis techniques play an important role in the solution, optimization, and characterization of systems governed by differential equations. The speakers are experts in the field. They describe several tools and techniques and their application to problems in computational science.

Organizer: Paul D. Hovland
Argonne National Laboratory

10:30-10:55 Automatic Differentiation of Industrial CFD Codes: A Case Study with FLUENT
Arno Rasch, Aachen University of Technology, Germany

11:00-11:25 Application of Differentiation-enabled Fortran 95 Compiler Technology
Jan Riehme, Dresden University of Technology, Germany; Barry F. Smith, Paul D. Hovland, and *Uwe Naumann*, Argonne National Laboratory; and Malcolm Cohen, NAG, Ltd., United Kingdom

11:30-11:55 Sensitivity Calculations for Elliptic Interface Problems
Lisa G. Stanley, Montana State University

12:00-12:25 Computing Periodic Orbits in Constrained Multi-body Systems Using Automatic Differentiation and Taylor Series Integration
Eric Phipps, Sandia National Laboratories; and John Guckenheimer, Cornell University

Thursday, February 13

MS83

Developing Usable, Flexible, and Extensible Multiphysics Modeling Software: FEMLAB

10:30 AM-12:30 PM

Garden Room D

Computing hardware, computational algorithms, and user interfaces have seen major advances over the last 25 years. So much so that resources required for advanced scientific computing are now readily available to researchers, engineers, educators, and students. Harnessing these resources, however, remains a challenge. There are clear engineering needs for effective deployment of robust, flexible, and open schemes in usable and intuitive packages for research and teaching. This series of talks will focus on the development of FEMLAB, a partial-differential-equation-(PDE-) based modeling environment for multiphysics. Issues that will be addressed include graphical interfaces, numerical algorithms, symbolic equation specification, and multiphysics coupling.

Organizer: David G. Kan
COMSOL, Inc.

10:30-10:55 Organization and Development of a General PDE Modeling Environment: Challenges and Issues
David G. Kan and *Lars Langemyr*, COMSOL, Inc.

11:00-11:25 Using FEMLAB as a Platform for Studying Time Integration Methods
David Ropp, Sandia National Laboratories

11:30-11:55 Implementing DASPK 2.0 in FEMLAB
Shengtai Li, Los Alamos National Laboratory; and Linda R. Petzold, University of California, Santa Barbara

12:00-12:25 Effective Graphical User Interfaces for Mathematical Modeling in Engineering and Science
Tomas Normark, COMSOL AB; and Magnus Marklund, COMSOL, Inc.

Thursday, February 13

MS84

Modern Hyperbolic Methods for Semiconductor Device Modeling and Astrophysical Jets

10:30 AM-12:30 PM

Garden Room F

Electron flow in classical and quantum semiconductor devices and gas dynamical flows in supersonic astrophysical jets can be modeled by compressible fluid dynamics with source terms. Simulations of the nonlinear conservation laws of gas dynamics for a 2D MESFET and for supersonic jets with radiative cooling using three modern finite-difference hyperbolic methods will be presented and contrasted: the Tadmor central scheme, the WENO-LF method, and CLAWPACK (which employs a second-order Godunov method). A mathematical analysis of the hydrodynamic model for semiconductor devices coupled to Maxwell's equations will also be given.

Organizer: Carl L. Gardner
Arizona State University

10:30-10:55 Overview of Semiconductor Device Modeling and Astrophysical Jets
Carl L. Gardner, Arizona State University

11:00-11:25 Simulation of a 2D MESFET Using the Tadmor Central Scheme
Anne Gelb, Arizona State University

11:30-11:55 Well-posedness for the Initial Value Problem for the Maxwell-Hydrodynamic System
Joseph W. Jerome, Northwestern University

12:00-12:25 WENO Simulation of High Mach Number Astrophysical Jets
ChiWang Shu, Brown University

Lunch

12:30 PM-2:00 PM

Attendees on Own

• *Cash and carry lunch for SIAM Meeting attendees is available in the Koi Pond area of the gardens.*

Thursday, February 13

MS85

Modelling and Analysis of Distributed Parameter Systems via Cellular Automata

2:00 PM-4:30 PM

Room: Regency Ballroom A

The speakers in this minisymposium will present a new approach to modelling and analysis of distributed parameter systems via cellular automata. An application to an ecological system will illustrate the approach. The speakers will discuss: (i) Modelling spatio-temporal systems via CA (ii) Regional controllability and spreadability via CA (iii) Coupling a system of ODE and CA (iv) LUCAS : An original tool for modelling vegetation dynamics based on CA and ODE.

Organizer: A El Jai
University of Perpignan, France

2:00-2:25 Cellular Automata Model for a Continuous Mechanics Problem
A El Jai and *M. Abdellaoui*, University of Perpignan, France

2:30-2:55 Regional Analysis Via Cellular Automata Models
Ammor N., Faculty of Sciences, Morocco; and *S. El Yacoubi*, University of Perpignan, France

3:00-3:25 Coupling ODE and CA for Spatio-Temporal Systems
S. Aassine and *M.C. Simon*, University of Perpignan, France

3:30-3:55 Modelling Vegetation Dynamics with Cellular Automata
P. Jacewicz, Technical University of Zielona Gora, Poland; and A. El Jai, University of Perpignan, France

4:00-4:25 Analysis and Control of Distributed Parameter Systems Via Cellular Automata Application to Spreadability
S. El Yacoubi and *A. El Jai*, University of Perpignan, France

Thursday, February 13

MS86 (For Part I, see MS 74)

Quantum Networks for Computation and Control II

2:00 PM-4:00 PM

Regency Ballroom B

Artificial neural networks have been applied to solve engineering problems ranging from computational image processing to control of complex systems---most sinificantly, problems for which there is no apparent path to an algorithmic solution. Quantum computers are expected to outperform classical computers, but only a few quantum algorithms are currently known. This suggests that investigation of quantum `neural' networks might lead to quantum systems which can efficiently solve additional problems. The speakers in this minisymposium will describe several efforts in this direction: quantum perceptrons, quantum networks, and quantum learning. Both analysis and large scale simulations will be represented.

Organizer: David A. Meyer
University of California, San Diego

2:00-2:25 On Quantum Learning of Small DNF Functions
Jeff Jackson, Duqesne University

2:30-2:55 Quantum Versus Classical Learning
Rocco A. Servedio, Columbia University

3:00-3:25 Computation of Entanglement by a Quantum Neural Network
Elizabeth Behrman, Wichita State University

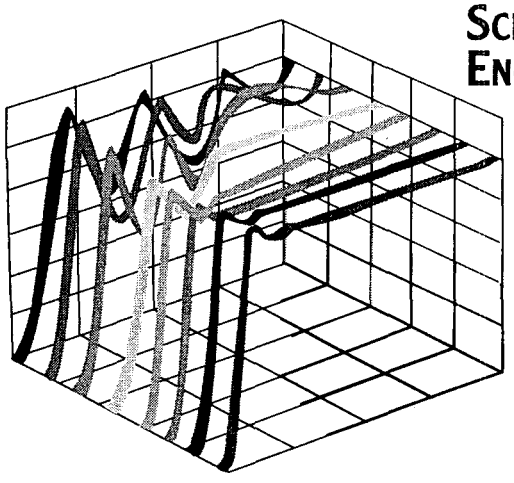
3:30-3:55 Quantum Neurons with Gate Output
Alexander Ezhov, Troitsk Innovation and Fusion Research Institute, Russia

Conference Adjourns

4:30 PM

Abstracts

SIAM Conference on COMPUTATIONAL SCIENCE AND ENGINEERING



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CP1
Using Optimization in Biological Research

Researchers in the biological and biomedical sciences seek answers to many important questions that cannot be addressed solely by traditional microbiology techniques. However, using tools of the mathematical and computational sciences, significant progress can be made in these areas. Furthermore, the incorporation of computational methods (such as optimization) in traditional biological investigations may prove beneficial. We investigate ways that asynchronous parallel pattern search can contribute to the understanding of molecular structures.

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CP1
Nondifferentiable Optimization Methods for Protein Docking

Key problems in protein docking and folding involve determining the global minimizers of potential energy surfaces. The protein docking program Docking Mesh Evaluator (DoME) defines these surfaces using adaptive mesh solutions to the Poisson-Boltzmann equation. DoME computes the global minimizer via the global optimization algorithm CGU using local minima to produce a convex underestimator energy landscape. Since these surfaces arise from finite element solutions, they are naturally nondifferentiable along the edges of the simplices of the mesh. We investigate various techniques for generating local minima over these types of surfaces and how such minima are used in defining the global minimizer.

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CP1
Scalable Parallel Branch-and-Bound for Protein Structure Prediction

Determining the native 3D structure of a protein from its amino-acid residue sequence is one of the foremost problems in computational biology [Samudrala:1999]. Branch-and-bound (B&B) is an exact optimization method that has been used in important protein structure prediction methods like NMR, multiple sequence alignment, and protein threading [Xu:2002], but with little or no parallelization. We present a scalable, parallel B&B algorithm to significantly speedup protein structure prediction.

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CP2
The Accuracy and Efficiency of Shock Capturing Methods for Shocks: High-Resolution Godunov Methods, Weighted Eno Schemes and Neo-Godunov Methods

We describe a quantitative study comparing a fifth-order WENO and a second-order Godunovs method on complex one-dimensional flows with relevance to turbulent flows. An analysis is conducted to find where the two methods are essentially equal in solution accuracy. We then describe modifications of Godunov's method that achieve greater solution accuracy and overall efficiency relative to both methods discussed above. We discuss the implications of our findings for large-scale simulations of fluid instabilities.

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CP2
A Numerical Method for the Coupling Radiation-Hydrodynamics

The coupled radiation and hydrodynamic models play an important role in the simulation of astrophysical or inertial confinement fusion phenomena, or again in the simulation of hydrocarbon flames which produce soot. The main problem of the coupling of hydrodynamics and radiative transfer is that there are both the hydrodynamic and the radiative flow signals in the system with for each one a very different characteristic time: the radiation signals propagate much faster than flow ones. Generally, the time scale of hydrodynamic is the characteristic one and then radiations have to be implicitly treated. The macroscopic radiative M1 model with mean absorption coefficients is here chosen to describe the radiative flow signal. This model is hyperbolic, has a flux limited by the light speed, and dissipates entropy locally. The main goal of this work is to show how to couple hydrodynamic and radiation using a simple factored operator method without doing major modifications of an existing hydrodynamic code. This method, a kind of splitting, will be validated by two test cases: The first one, a one-dimensional radiative shock in an opaque medium, validates our splitting method by computing a solution which is similar to the explicit solution of the problem. Finally, the second test case validates our splitting method for the 2D problem of free convection of air in an oven.

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CP2
A High-Resolution Constrained Transport Method for Magnetohydrodynamic Flows

The magnetohydrodynamic (MHD) equations are impor-

tant in astrophysical fluid dynamics. Numerical methods for MHD must produce solutions that remain accurate near shocks and that satisfy a divergence-free constraint on the magnetic field. We present in this work a high-resolution finite volume method for solving the MHD equations. A discrete divergence-free condition is satisfied by directly solving a magnetic potential equation. A limiting procedure developed specifically for this equation is used to produce a non-oscillatory update.

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CP3

Parallel Solution of the Poisson-Boltzmann Equation for Evaluating Nanoscale Biomolecular Electrostatic Properties

Elucidation of the electrostatic properties of biomolecules has become a standard practice in molecular biophysics. Foremost among the models used to evaluate the electrostatic potential is the Poisson-Boltzmann equation, a nonlinear elliptic partial differential equation. However, existing solution methods have limited the scope of accurate calculations to relatively small biomolecular systems. New numerical techniques will be presented which enable the parallel solution of the Poisson-Boltzmann equation for supramolecular structures orders of magnitude larger in size than those accessible with traditional methods. As a demonstration of this methodology, electrostatic potentials have been calculated for large microtubule and ribosome structures. The results point to the likely role of electrostatics in a variety of activities of these structures.

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CP3

CompuCell, a Multi Model Framework for Simulation of Morphogenesis

CompuCell is a framework that simulates early development of multicellular organisms. It models the gene regulatory network by a combination of reaction-diffusion PDE and a state automaton. These interact with cellular mechanisms modeled using a stochastic Potts model. We present the simulation of the formation of a chick limb skeletal pattern. Biological experiments are used for input and validation. BioLogo, a domain specific language describes simulations of morphogenesis in CompuCell.

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CP3

A Linearly Scalable Hybrid Monte Carlo for Sampling the Conformational Space of Proteins

We propose a new Hybrid Monte Carlo (HMC) algorithm that uses a shadow Hamiltonian (SH) as approximation to the Hamiltonian. The new algorithm, called SHMC, scales as $O(N)$ instead of HMC's $O(N^{5/4})$. Sampling of a small protein using HMC and time step of 2 fs has an acceptance rate of 5% whereas SHMC's is 93%. We show that SHMC correctly samples the conformational space of the protein using a novel sampling metric.

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CP3

Automatic Empirical Optimization of Fast Electrostatics Algorithms

We show empirically that Multigrid summation, an $O(N)$ algorithm for fast evaluation of electrostatic forces recently proposed, is faster than Particle Mesh Ewald for moderate accuracy when $N >= 10000$. The guidelines on choosing the parameters for both methods based on desired system size and accuracy are embedded in MDSimAid and ProtoMol, a suite of programs that automatically determine the optimal fast electrostatic algorithm and parameters for the simulation of a given molecular system.

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CP4

How Close Can We Approach Singular Points in Nonlinear Eigenvalue Problems

We study multigrid methods in the context of continuation methods for semilinear elliptic eigenvalue problems, where the Lanczos method and its variant MINRES are used as the relaxation schemes for the V-cycle, W-cycle and full multigrid V-cycle schemes, respectively. Since the GMRES method is a generalization of the MINRES algorithm, the results of Brown and Walker [5] can be exploited to solve nearly singular symmetric linear systems that occur in continuation problems. We give some error bounds for the MINRES algorithm which are more accurate than those given by Chang and Chien [7]. Some multigrid-continuation algorithms are proposed for curve-tracking in nonlinear elliptic eigenvalue problems. Our numerical results show the algorithms we propose are efficient and robust, which can be easily implemented. Finally, some concluding remarks are given.

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CP4

Scalability of P_1 Nonconforming Multigrid

We study the scalability of a P_1 nonconforming multigrid implementation in the PETSc library framework, with attention to both the convergence rate and the computational performance, as the problem is refined in 2D and 3D fixed-memory-per-processor scalings. P_1 nonconforming models have been shown useful in a variety of nonlinear elliptic problems, especially where conventional models may lose positivity. We consider several P_1 nonconforming multigrid methods, standard multigrid and Galerkin multigrid, and several intergrid transfer operators: standard, simple, covolume-based and P_1 conforming-based intergrid transfer operators. In this paper, we show that CG or GMRES preconditioned with standard P_1 multigrid and covolume-based intergrid transfer operators have good scability, through summarizing existing and new theory, and through numerical experiments.

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CP4

Multi-Level Preconditioners for Adaptive *hp* Finite Element Simulations

We report here on the development of efficient solution methods for adaptive *hp* finite element approximations of three dimensional elastostatics problems. We introduce a grid based hierarchy of the unknowns and develop simple and efficient preconditioners that impose no restrictions on the partitioning or requirements of constructing explicit coarse grids.

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CP5

On Consistent Initial Value Assignment for Electronic Circuit Cad Simulation Tools

Systems of differential algebraic equations (DAEs) arise quite naturally in electronic circuits simulation. Inclusion of more realistic models for circuit elements such as MOSFET transistor results in DAEs with higher order index. Moreover exact formulations of electronic circuits that take the second order effects and transmission line delays into account will result in systems of partial differential algebraic equations (PDAE). In high frequency integrated circuits for today's communications devices, these effects are highly significant. Consistent initial conditions are very difficult to obtain for an index > 1 DAE. Inconsistent initial conditions lead to wild zigzagging of the solution. Numerical jet geometry and numeric-symbolic methods for completion of differential systems are newly born methods that are used to find the constraints of the input differential algebraic system. Apart from the problem of circuit simulation, over and under-determined (non-square) systems of DAE arise in applications such as constrained multi body mechanics and control systems. They are becoming increasingly important in applications as more realistic models naturally lead to such constrained systems. Symbolic algorithms have been developed which use a finite number of exact differentiations and eliminations to reduce over and under-determined systems of polynomially non-linear differential equations to involutive form. The output involutive form enables the identification of consistent initial values, and eases the application of exact or numerical integration methods. However such differential-elimination algorithms, which usually incorporate Groebner bases, have poor complexity and are unsuited for application to systems with approximate coefficients. An underlying principle of the new numeric-symbolic approach is strong emphasis on geometry, in particular jet space geometry, the geometry of differential systems. In comparison to the symbolic differentiation-elimination approaches, where symbolic or algebraic manipulations of the equations figure heavily, new method focuses on the solutions of the system regarded as algebraic equations. A major principle of our approach is to replace what is usually a symbolic-preprocessing step with a variation of Newton's method, to locate points on the hidden constraints. This is quite natural since ultimately variants of Newton's method are used in solving the differential system. The new class of methods presented here can be compared to using an iterative method to solve systems (in our case Newton's method), instead of exact elimination (e.g. Gaussian Elimination, or its non-linear cousin Groebner Bases). The systems of polynomial equations involved in most physical phenomena are usually not square and generally have positive dimensional components (submanifolds) of solutions. Our treatment of such systems, using homotopy methods, is made possible by recent theoretical progress made by Sommese et al. in the developing area of numerical algebraic geometry. The new techniques rely on embedding the given systems in square polynomial systems, by the inclusion of extra (slack) variables and random linear equations if necessary. The key idea behind these methods is to reduce to the zero dimensional case (where there are only finitely many solutions), by slicing the solutions with a random linear space of the appropriate dimension. Enough points are located to interpolate the smooth components of a differential system by lowest degree polynomials. In this paper the physical problem in electronic circuit simulation is presented. Also the application and usefulness of the new numeric-symbolic algorithms to find hidden constraints in circuit differential system is examined.

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CP5

Novel Algorithms for Inductance Extraction

With VLSI circuit components getting faster and smaller, the parasitic resistance, inductance and capacitance of the on-chip interconnect has become the primary source of signal delay. At higher frequency, the inductive effects dominate this delay, making accurate inductance extraction an important issue in the VLSI industry. This paper presents a novel preconditioned iterative algorithm called the *solenoidal basis method* for solving large-scale dense linear system arising in inductance extraction. A reduced system, obtained by restricting current to a discrete solenoidal subspace, is solved by preconditioned GMRES method. Near-optimal preconditioners for these systems lead to significant improvement over existing techniques on several

benchmark problems.

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CP5

Preconditioning Techniques for Large Dense Matrices From Electromagnetic Wave Scattering Simulations

We investigate preconditioned iterative solutions of large dense complex valued matrices arising from discretizing the integral equation of electromagnetic scattering. The main purpose of this study is to evaluate the efficiency of preconditioning techniques based on incomplete LU (ILU) factorization and sparse approximate inverse for solving this type of dense matrices. We solve the electromagnetic wave equations using the BiCG method with the preconditioners in the context of a multilevel fast multipole algorithm (MLFMA). The novelty of this work is that the preconditioners are constructed using the near part block diagonal submatrix generated from the MLFMA. Experimental results show that the ILU and sparse approximate inverse preconditioners reduce the number of BiCG iterations substantially. We also discuss the advantages and disadvantages of the two classes of preconditioning techniques in this particular application.

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CP6

Parallel Performance of An Adaptive-Mesh Reactive Hydrodynamics Simulation Code

The FLASH code is a freely-available parallel adaptive-mesh reactive hydrodynamics simulation code developed at the ASCI FLASH center at the University of Chicago, and uses the PARAMESH meshing package. Adaptive mesh codes present difficult parallel efficiency problems. We examine our code's parallel performance on a number of different archictectures, and attempt to quantitatively model this performance in simple cases.

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CP6

Benchmarking Applications with Irregular, Dynamically Changing Memory Access

The goal of this work is to develop an unstructured adaptive (UA) mesh benchmark that models scientific applications featuring irregular and dynamically changing memory access patterns. UA supplements the NAS Parallel Benchmarks (NPBs) and solves a stylized 3D heat transfer problem using a Spectral Element Method (SEM). The high order of SEMs increases the computation-to-communication ratio, allowing us to concentrate on memory access performance. The Cartesian mesh is adapted isotropically to track a moving heat source. The parallel implementation employs space filling curves for dynamic load balancing.

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CP7

New Adjoint-Based Methods for Targeted Observations in Atmospheric Modeling

The problem of the optimal design of an adaptive observations system is presented in the context of four-dimensional variational (4D-Var) data assimilation. The temporal dimension of the 4D-Var scheme is fully taken into account by considering multiple targeting instants in the assimilation window. In particular, it is shown that the interaction between routine and targeted observations taken at distinct instants in time plays a significant role in the efficiency of the adaptive methods. The adjoint method is used to develop new adaptive strategies using analysis sensitivity and leading singular vectors. Second order adjoint modeling is used to extend the sensitivity to observation technique to the 4D-Var data assimilation. Potential benefits to the forecast error reduction are presented in a comparative analysis for a two-dimensional shallow water model.

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CP7
Solving inverse acoustic scattering problems using shape sensitivity analysis

A new efficient method for the solution of inverse acoustic scattering problems is proposed. The method is based on the calculation of the domain derivative of a cost functional that measures the difference between a trial solution and measured far-field scattering data. An adjoint-based method is proposed to efficiently calculate the domain derivative. This method is particularly efficient since the cost to compute the derivative is independent of the number of parameters used to describe the shape of the scatterer. Numerical examples showing the efficacy of this approach to solve inverse scattering problems with full and limited aperture data will be presented. Sandia is a multiprogram laboratory operated by Sandia Corporation, a Lockheed Martin Company, for the United States Department of Energy under contract DE-AC04-94-AL85000.

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CP7
Light Aircraft Noise for the Estimation of Ocean Depth in Shallow Water

A propeller-driven aircraft produces low frequency sounds (100 - 1000 Hz) which can penetrate into the ocean waveguide. Analysis of such a source demonstrates that it has the potential to be used for Matched Field Processing inversions of array data (either vertical or horizontal arrays). Such data may be appropriate for the estimation of geoacoustic parameters such as ocean depths in shallow water. While the S/N is low except for near array passes (within 300 m ranges), i.e., this method demands close source-array range processing, array design and flight patterns may offer sufficient coverage to allow for successful, rapid, and environmentally benign inversions of some ocean parameters. This presentation will offer computations of idealized scenarios estimating ocean depth for a variety of arrays and scenarios using sources simulating low flying aircraft.

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CP8
A New Implementation of the Space Filling Curve Load-Balancing Algorithm

A new implementation of the Space Filling Curve (SFC) load-balancing method will be presented. The new method avoids the parallel sorting of objects performed by past SFC load-balancing implementations by using an adaptive binning approach. The new SFC load-b alancing algorithm was implemented inside the Zoltan library (www.cs.sandia.gov/Zoltan/). Results will be presented comparing th e new SFC algorithm to other load-balancing algorithms in Zoltan. Theory showing that the SFC partitioning algorithm is incremental in nature under certain conditions will also be presented.

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CP8
Through-Vertex Paths in 2D and 3D Simplicial Grids

Space-filling curves and self-avoiding paths through the elements of a grid have been shown to be useful for partitioning the grid into subregions for load balancing in a parallel computation. However little is known about when a continuous path, and hence connected partitions, exists in a general grid. We prove that one can always find a connected path through a triangle or tetrahedron grid such that the path goes from element to element through vertices.

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CP8
A Comprehensive Evaluation of Parallel Algorithms for the Linear Assignment Problem

Large linear assignment problems (LAPs) are computation intensive and many NP-hard problems require solving numerous LAPs. Therefore, many parallel algorithms have been proposed for it [Bertsekas:89-93, Burkard:98-99, Clausen:95, Kennington:89-91, Pekny:91, Phillips:88, Story:92, Toth:99, Wein:90]. In this paper, we present for the first time a comprehensive performance analysis of the most competitive parallel algorithms for LAP, namely, those based on the auction and shortest augmenting path approaches, by using them to solve large LAP instances on an IBM SP2.

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CP9
Coupled Continuum and Molecular Simulation of Dilute Polymer Solutions in Turbulent Flow

Small concentrations of polymers significantly modify the turbulent flow of a liquid. The basic mechanism is the extension of a polymer molecule by the shear forces in a

turbulent flow. In this work a coupled simulation of continuum scales and the microscopic scales is carried out. Molecular dynamics is used to model the extension of the polymer molecules. An adaptive mesh refinement solver of the Navier-Stokes equations is used to capture the continuum turbulent flow. The principal question studied in this work is the extent of the microscopic sampling needed to obtain the correct, instantaneous constitutive laws for the dilute polymer solution.

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CP9

Loosely Coupled Multiscale Modeling of Growth of Carbon Nanotubes

The growth of Carbon Nanotube (CNT) is one of the most complicated multi-scale phenomena spanning several orders of space- and time-scales. Two forms of growth mechanisms are observed in chemical vapor deposition method - root growth and tip growth. In root growth the CNT grows on the support catalyst and in the tip-growth a small catalyst particle is detached from the support and CNT is formed between the particle and the support. In both mechanisms, the carbon containing gas dissociates at one end of the catalyst particle and forms a carbide layer in the catalyst, carbon diffuses through the catalyst particle, carbon ejects on the other side of the particle forming the CNT. Because of the length and time-scales involved all the tools available (DFT, MD and Continuum heat and mass transfer simulations) are used to understand the rate limiting steps in the growth of CNT. This study will help in giving better insight into how the growth process depends on the conditions and act as a stepping stone to future rigorous multiscale approaches.

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CP9

A Simulation Software Architecture for Interacting Discrete and Continuous Phases of Matter

We present an attempt to resolve several issues encountered in using object-oriented programmig (OOP) in scientific simulation. A software architecture for simulating mass, momentum, and energy transfer between discrete matter and fluid continua is discussed. The class structure is specified using the Unified Modeling Language and implemented using recently developed techniques for OOP in Fortran 90 (Decyk et al., ACM Fortran Forum, 16:1). Research and pedogogical issues will be discussed, emphasizing performance and effective design communication.

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CP10

A Nested Iterative Scheme for Indefinite Linear Systems in Particulate Flows

In this paper, we present a nested iterative scheme for solving saddle-point problems and related indefinite linear systems of equations that arise in particulate flows. The proposed algorithm may be considered as a variant of the well-known Uzawa scheme, and is designed so as to be suitable for implementation on parallel computational platforms. We relate the rates of convergence of the outer and inner iterations, and prove that the convergence rate of the proposed scheme is independent of the size of the problem. Several preconditioners for these indefinite systems are considered, and extensive comparisons with Krylov subspace methods are conducted.

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CP10

Variations on dristributed Schur Complement techniques in pARMS

Parallel Algebraic Recursive Multilevel Solver (pARMS) is a library for the parallel solution of distributed sparse linear systems, which implements standard Schwarz approaches alongside with more complex Schur complement methods. The pARMS framework is designed to be flexible to allow the development of various preconditioning techniques as well as direct solution codes in a single framework. The talk will discuss a few variants of two-level Schur Complement preconditioners. These methods differ in the way in which the Schur complement system is constructed and solved. In particular, this system may include internal interface and interdomain interface nodes if the pARMS framework is used. We study the effect of the Schur Complement system expansion with the internal interface nodes.

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CP10

Inexact Krylov Subspace Methods

We provide a general framework for the understanding of Inexact Krylov subspace methods for the solution of symmetric and nonsymmetric linear systems of equations. In these methods, the matrix-vector product at each step is not performed exactly. This framework allows us to explain the empirical results reported in a series of CERFACS technical reports by Bouras, Frayssé and Giraud in 2000, where the exactness of the matrix-vector product is allowed to deteriorate as the Krylov subspace method progresses. Furthermore, our analysis produces computable criteria to bound the inexactness of the matrix–vector multiplication in such a way as to maintain the convergence of the Krylov subspace method. The theory developed is applied to several problems including the solution of Schur complement systems, linear systems which depend on a parameter, and

eigenvalue problems. Numerical experiments for some of these scientific applications are reported, where the computable criteria are successfully applied.

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CP11

Recursive Use of Domain Decomposition Methods for Solving Linear Systems of Equations

Domain decomposition methods such as FETI-DP (Dual-Primal Finite Element Tearing and Interconnecting) have demonstrated near optimal scalability when applied to large-scale systems of equations running on thousands of processors. It is shown how the recursive application of FETI-DP can improve the overall performance and scalability of the algorithm. Numerical studies of Poisson, 2D elasticity, and 3D elasticity are presented to support this claim.

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CP11

Parallel Preconditioning Using Blocked Incomplete Cholesky Factorization and Selective Inversion.

We report on the performance of an incomplete Cholesky parallel preconditioner for sparse linear system solution using Conjugate Gradients (CG). Our incomplete factorization can serve a range of preconditioning needs through flexible combinations of different drop-threshold heuristics. We describe our implementation which uses variable block sizes with a left-looking supernodal factorization to improve cache-performance and reduce inter-processor communication. We also discuss latency-tolerant distributed triangular solution using "selective inversion" to apply such a preconditioner at each CG iteration. We provide extensive empirical results and analysis for model sparse matrices.

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CP11

Massively Parallel Large-Scale Pool Fire Simulations

In order to produce accurate large scale fire simulations, massively parallel processing is needed to solve the complex linear equations. Implementing PETSc and HYPRE into a fire simulation tool provides suites of parallel linear solvers and preconditioners. Comparisons between various solvers and preconditioners and scalability performance are obtained from different supercomputer platforms at the national laboratories. These tests are performed on SGI, IBM SP and Linux machines up to 1,000 processors.

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CP12

Stability Conditions for Numerical Methods Applied to Stiff Systems of Reaction Diffusion Equations

The electrical activity in the heart can be modeled by a stiff system of partial differential equations. The ion transportation models vary in complexity and the more recent models can have more than 50 state variables. The models tend to become increasingly complex. Our aim is to analyze the stability of numerical methods for these models, based on analytical and numerical investigations. We present recent results and discuss their implications.

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CP12

Cycling Behavior in Coupled Cell Systems

A generic pattern of collective behavior of symmetric networks of coupled identical cells is cycling behavior involving steady-states (fixed points), periodic solutions (orbits), and even chaotic attractors. In this presentation, we use computer simulations to demonstrate the existence of cycling behavior in near-identical coupled cell systems and generalize its existence in systems with large number of cells.

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CP12

Numerical Methods for Electrophysiology Models of Cardiac Cells

Electro-chemical reactions and ionic concentration in cardiac cells are usually modeled by systems of ODEs. Several systems have been proposed in the literature, and the complexity of solving these systems usually comes from strong

nonlinearities and stiffness of the systems. In this talk we present some numerical methods for solving such systems. Our algorithms are based on standard methods like Runge-Kutta, but the special structure of the systems is exploited.

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CP13

A Newton-Krylov Based Solver for Finite Rate Chemistery CFD Modeling

To follow per email 09/20.

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CP13

Modeling Continua with Implicit Evolution Equations

A dispersive extension of shallow water magnetohydrodynamics to finite layer depths, analogous to the Green–Naghdi equations, contains mixed spatiotemporal derivatives. Spatial discretization yields implicit systems of ordinary differential equations that are readily integrated using differential-algebraic system solvers. Solutions are compared with those computed using the three dimensional equations for $O(1)$ layer depths. The same techniques are applied to Chen, Rao, and Spiegel's [*Phys. Lett. A* **271** 87] macroscopic equations for rarefied gases.

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CP13

Removal of Spurious Modes with a Chebyshev Collocation Method

Stokes problem is in the base of many fluid dynamics problems. In this work special boundary conditions are posed in a Stokes problem in a square. They are obtained by the continuity equation or/and the normal component of momentum equations at the boundaries. We prove how these boundary conditions allow to reduce the space of spurious modes in a Chebyshev collocation method.

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CP14

Eigen Mode Computation for High Dimensional Problems of Microwave and Laser Structures

Using a finite-volume approach for Maxwell's equations an eigenvalue problem can be derived, whose solutions correspond to the propagation constants of the modes. The modes of smallest attenuation are located in a longsome region bounded by two parabolas, and are found solving a sequence of eigenvalue problems of modified matrices applying the Arnoldi iteration with shift-and-invert technique. To reduce the execution times a coarse and a fine grid, and two levels of parallelization are used.

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CP14

Accurate and Unconditionally Stable Algorithms That Solve the Time Evolution of Electromagnetic, Elastodynamic and Acoustic Wavefields

We present two new numerical algorithms that solve the time-dependent hyperbolic first order partial differential equations governing electromagnetic, elastodynamic and acoustic phenomena. The first algorithm is unconditionally stable, and conserves the total energy density regardless of the time step used, the second algorithm provides a numerically exact answer, based on the Chebyshev polynomial expansion. In case of the Maxwell equations, results are presented, ref. [Kole et al., Phys.Rev.E64 p.066705-1 (2001)].

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CP14

Fast High-Order FEM Solutions for Dielectric Waveguides

This paper presents a formulation for the analysis of dielectric waveguides. The formulation results in a well-conditioned matrix, which makes solving the system equation with an iterative solver reliable. High-order hierarchal vector bases are constructed to provide maximum mutual orthogonality in both vector space and the range space of curl operator. These new bases yield optimal rates of convergence when the resultant matrix is solved using with the multilevel preconditioned conjugate gradient method.

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CP15
Multigrid Algorithms for Solving Constrained Linear Systems

Optimal linear solvers are becoming necessary as the cost of linear system solves becomes prohibitive in implicit finite element analysis. Unstructured multigrid methods provide this optimality. Many finite element applications have constraints, enforced with Lagrange multipliers. We are not aware of any unstructured multigrid algorithms that are designed for such systems. This talk will present a framework for designing multilevel algorithms for constrained linear systems as well as applications to contact problems in solid mechanics.

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CP15
Parallel Finite Element Computation of Contact-Impact Problems with Large Deformations

In this talk, we will present a framework for parallel explicit dynamics simulation of contact and impact problems involving shells and solids. For contact enforcement, we introduce a new algorithm, which exactly satisfies the kinematic impenetrability constraints and conserves linear and angular momenta. Contact detection is performed in parallel with orthogonal range queries based on a sparse bucket data structure. Several applications, such as crumpling of shells and high velocity impact of solids, will be presented.

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CP15
Numerical Solution of Saddle Point Problems Arising from Linear Elasticity with Intersecting Slide Constraints

Incorporating slide surface constraints in implicit structural finite element analyses using Lagrange multipliers gives rise to an indefinite linear system of equations which is difficult to solve by iterative methods. Algebraic elimination has been shown to be effective in improving the solution process by restoring positive definiteness to the matrix. This paper extends these techniques to applications with intersecting slide surfaces. We present a graph-theoretic algorithm and compare its performance with Uzawa and block preconditioned Krylov methods.

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CP16
Parameter Sensitivity Analysis of Stochastic Simulation Codes

The computation of parameter sensitivities for stochastic simulation codes is complicated by the simulation noise. Finite difference expressions for the parameter sensitivities are derived that optimally take the stochastic fluctuations into account. The new expressions give much high accuracy than past expressions. The approach is applied to a Kinetic Monte Carlo simulation of copper electrodeposition from a sulfate bath onto a flat copper substrate in the presence of a three-additive system.

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CP16
Discrete Adjoints for Stiff Systems

Comprehensive chemistry-transport models (CTMs) are used to study the fate of pollutants in the atmosphere. A "best estimate" of the chemical state of the atmosphere can be obtained by assimilating the measurements into the model predictions. Building the tangent linear model and its adjoint is very challenging due to the presence of stiff chemical terms. In this talk we discuss some theoretical aspects of discrete adjoints for stiff ODEs. Software tools that automatically generate the adjoint models for chemical kinetic systems and numerical results will also be presented.

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CP17
Smoothing and the Discrete Wavelet Transform: The PDE Connection

We describe a method of associating an evolutionary PDE to any discrete wavelet transform by a semi-discrete approximation procedure. One step in the marching algorithm of the discretized version of the PDE associated to the discrete wavelet transform coincides to one smoothing step in the discrete wavelet transform. Applications include design of recipes for the correct treatment of boundaries, wavelet transforms for curvilinear grids, and a version of multiscale transform for irregular grids.

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CP17
Wavelet Collocation for Ode Boundary Value Problems

We present a collocation method for second order ODE boundary value problems based on integrated B-spline wavelets. We show how to choose a basis for the integrated B-spline wavelets constructed to satisfy the bound-

ary conditions. In addition, we present numerical results for a number of well-known difficult linear boundary value problems and we discuss the condition of the collocation matrix.

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CP18
Simulation for Mesoscopic Models

One means of mathematically describing multiscale phenomena is through mesoscopic models, which are typically stochastic partial differential equations (SPDEs). In this talk, mesoscopic models for surface processes will be introduced. Then, new spectral-based computational schemes for SPDEs will be introduced and validated through the use of exactly solvable benchmark problems. Finally, a variety of mesoscopic simulation results will be given.

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CP18
Adaptive Solution of Nonlinear Stochastic Problems

For systems modeled by stochastic partial differential equations (SPDEs), often only functionals of the solution are of interest. This offers the possibility of adaptation by a goal-oriented approach. We solve nonlinear SPDEs by spectral stochastic finite elements and use the solution of a dual problem for adapting the stochastic discretisation with respect to the error of a functional. This way the results have high accuracy with little effort, as demonstrated by examples and efficiency indices.

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CP19
Solving Differential-Difference Equations and Their Application to Crystalline Growth

We describe a general purpose code for boundary value differential-difference equations where the difference terms may contain both advances and delays. The code is an extension of the COLMOD, COLNEW, and COLSYS family. The application of interest in this talk is interface motion and solidification in materials with an underlying lattice or lattice complex structure in the solid.

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CP19
Effects of Electrostatic Forces on the Phase Distribution in Droplet Suspension. Three-Dimensional Numerical Simulations

If an electric field is applied to a drop in another fluid, the electrostatic stresses lead to a prolate or oblate deformation depending on the dielectric properties of both fluids. When a suspension of drops is introduced in a channel flow and an electric field is applied, the interaction between the drops and between the drops and the walls lead to different droplets distribution in the channel. A numerical study of the physical mechanisms governing this interaction and the resulting droplets distribution is presented.

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CP19
Coalescence of Unequal Particles by Surface Diffusion

We study the coalescence of a cluster of small particles by surface diffusion. With the proposed joining conditions at the triple junctions, we compute the development of grain boundaries as well as the surface evolution. The surface movement is governed by a fourth order nonlinear parabolic-like partial differential equation system, which is solved by the method of lines with finite volume discretization in space. A comparison to the experimental result on the coalescence of two particles is made. The evolution of crystal surfaces with anisotropic surface free energies is explored.

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CP20
Adaptive Treecode Algorithms for Particle Simulations

In this talk I will present some recently developed treecode algorithms for particle simulations. The algorithms rely on Taylor approximation in Cartesian coordinates and use recurrence relations to compute the necessary Taylor coefficients. A number of adaptive techniques are employed to gain efficiency. These include variable order expansions, nonuniform rectangular clusters, a optimized runtime choice between Taylor approximation and direct summation, and tree traversal look ahead.

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CP20
Targeted Langevin Stabilization of Molecular Dynamics

We introduce the B-spline Mollified Impulse (MOLLY) and the Targeted MOLLY (TM). TM uses targeted Langevin coupling to stabilize B-spline MOLLY. Analysis shows that TM samples the canonical ensemble. Results show that TM is stable when the outer time step is 16 fs for flexible waters. Self-diffusion coefficient is correctly estimated, and a six-fold speedup is obtained as compared to leapfrog with step size of 1 fs. TM also correctly recovers the radial distribution functions.

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CP20
Computational Techniques for Efficient Carbon Nanotube Simulation

Molecular dynamics simulation of Carbon nanotubes, typically using Brenner's potential, is of considerable interest due to the variety of its applications to nanotechnology. Several studies have suggested (relatively simple) techniques to improve the speed. These studies include parallelization in message-passing and shared-memory paradigms. We will discuss the effectiveness of more sophisticated techniques, including those from graph theory and computational geometry.

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CP21
A High-Level Approach to the Synthesis of High-Performance Codes for Quantim Chemistry

We present an approach to the synthesis of high-performance parallel programs for a class of problems encountered in quantum chemistry and physics which are expressed as a set of tensor contractions. The synthesis system transforms a high-level specification of the problem into high-performance parallel code tailored to the characteristics of the target architecture. We will explain the components of the synthesis system and their operation.

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CP21
A Framework for Check-Pointed Fault-Tolerant Out-of-Core Linear Algebra

ScaLAPACK is considered by many as a widely-accepted standard to perform parallel linear algebra computations. We present a framework that uses ScaLAPACK as a set of base set of computational operations. The framework uses sequences of these operations to perform numerical linear algebra transformation such as LU factorization. We show how the framework can be used to easily incorporate checkpointing and fault-tolerance into LU. A number of scientific codes rely on long-term computations. Possibility of staging such computations is one of the important applications of our framework.

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CP21

The Architecture of a Problem-Solving Environment for Computational Biology and Bioinformatics

Computational Cell Environment (CCE) is a problem-solving environment with the goal of providing data management and analysis through all aspects of biological study including sequence characterization, gene/protein expression, intra-cellular networks, extra-cellular networks, tissue, organs, and community interaction. CCE provides uniform and integrated access to distributed heterogeneous biological data sources, and applications through a multi-tiered architecture using WebDAV. The WebDAV protocol is implemented through a Jakarta/Slide implementation that coordinates data management, content management, versioning, and security.

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CP22

A Scalable One-Level Schwarz Algorithm for the Unsteady Nonlinear Radiation Diffusion Problem

We consider scalable parallel numerical methods for solving the nonlinear radiation diffusion equation. In addition to the nonlinear terms in the governing equation, the commonly used flux-limiting form of the diffusion coefficient introduces extra degree of nonlinearity to the system. Several successful attempts have been made recently using multilevel methods combined with some variant of Newton-type method. The main advantage of multilevel methods is their optimal convergence rate which is independent of the mesh size and the number of processors, and therefore the methods are suitable for machines with many processors. A disadvantage of multilevel methods is that sometimes creating high quality coarse meshes can be difficult especially in the case of unstructured grid. In the talk we present a one-level Newton-Krylov-Schwarz method and show numerically that the method is scalable with respect to the mesh size and the number of processors for the unsteady radiation diffusion equation. The method is very easy to implement on massively parallel computers because there is no need to have any coarse grids to achieve the optimal convergence rate.

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CP22

Alternating Explicit Implicit Domain Decomposition for Parabolic Equations

Explicit-implicit domain decomposition (EIDD) is a class of globally non-iterative, non-overlapping domain decomposition methods for the numerical solution of parabolic problems on parallel computers, which are highly efficient both computationally and communicationally for each time step compared with other domain decomposition methods. However, most of the existing EIDD methods has some level of instability. There are two types of EIDD methods which exhibit unconditional stability-like convergence in numerical experiments, but no proven explanation was given for the observed good stability. In this talk, we present an EIDD method which is algorithmically simple, efficient for each time step, and unconditionally von Neumann stable in the sense that the spectral radius of the amplification matrix is bounded by one without any restriction on the ratio of time step size to the spatial mesh size. Numerical experiments with machine size from 1 to 128 processors indicate excellent speedup and scalability and excellent numerical stability.

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CP23

Unsteady Flow of a Second Grade Fluid Near a Stagnation Point

The two-dimensional stagnation-point flow is an interesting problem in the history of fluid dynamics and has received considerable attention. This work considers the unsteady two-dimensional flow of an incompressible viscoelastic second grade fluid impinging on an infinite flat plate. We assume that the plate is making harmonic oscillations in its own plane. Series methods are employed to evaluate the solution for small and large frequencies of the oscillations.

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CP23

An Exact Solution for Pump-Driven Damped Linearized Isothermal Pressure Waves in Nearly Rigid Rough Oil Pipelines

For Laminar isothermal flow the standard pipeline equations are linearized considering small perturbations about the exact steady state solutions. Linear charactersitics for the driving pump at the injection end of a rough and nearly rigid oil pipeline, a linear state equation for the oil transported, and a linear expansion equation for the pipeline are assumed. Under this assumptions an exact solution is worked out. The pressure and velocity waves caused by time-harmonic perturbations of the injection pressure show dispersion and exponential decay. This solution has been used for testing non-standard numerical methods developed for compressible oil flow in elastic pipelines.

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CP23

Numerical Modelling of the Flow in the Steady Distributed Self-Similar Porous Medium

We consider a 3-D fluid flow through porous medium with parameters having pulsations from an extreme wide range of scales. The scaling properties of different characteristics of media (porosity, permeability) are assumed. Recently we considered the scaling log-normal theory (Kuz'min & Soboleva, J. Appl. Mech.Tech. Phys., Vol. 43, No. 4, 2002.) The log-normal theory violates the conditions of the Carleman's theorem and other troubles arise in the limit of the infinitely long cascades. For these reasons, we consider the more general theory supposing the steady distribution for permeability. The parameters of the distribution were taken to be similar to the experimentally observed ones. The flow field is found by the direct numerical computation. The simple statistical characteristics of the flow are presented.

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CP24

Structure-Composition Relationships of Mitochondria Membranes

The recoil-regrowth Monte Carlo algorithm has been used to study how lipid composition is related to sponteneous curvature of biological membranes. In particular we will discuss to what extent the strong curvature recently observed in several parts of mitochondria membranes is due to lipid composition. Analytical theory predicts that sponteneous curvature varies with type and concentration of phospholipids. These calculations have several limitations though, which can be handled by our MC calculations.

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CP24

Genomic Analysis of An Uncultured Marine Viral Community

The talk describes the mathematical techniques for estimating diversity and richness from the observed number of contigs in a shotgun sequencing sample. The sample is a mixture of all the viral genomes contained in a certain 200 liters of seawater. Several independent mathematical models based on the observed contigs predict that the most abundant viral genome comprises 4% of the total population, which is estimated to contain between 262 and 6,500 genotypes.

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CP24

A Computational Model of Nitric Oxide Transport in the Human Lungs

Nitric Oxide (NO) in the exhaled breath is an important physiological signal, which can be measured experimentally. Recent theoretical models describing NO exchange in the human lungs have facilitated the interpretation of experimental data. However, these models do not consider parallel inhomogeneity or axial dispersion in the airways. We propose a new computational framework that considers these transport mechanisms, and demonstrate the impact on the estimation of flow-independent exchange parameters from experimental exhalation profiles.

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CP25

The Surface Hardening of Steel Modeling, Simulation and Optimal Control

In most structural components in mechanical engineering, there are surface parts, which are particularly stressed. The aim of surface hardening is to increase the hardness of the corresponding boundary layers by rapid heating and subsequent quenching. This heat treatment leads to a change in the microstructure, which produces the desired hardening effect. In the talk I will present a mathematical model for laser and electron beam hardening. Main parts are a system of ODEs to describe the occuring phase transitions, coupled to a nonlinear heat equation and a model for the laser or electron beam radiation absorption in the workpiece. To maintain the surface quality, it is important to prevent melting. To this end the problem of surface hardening is formulated in terms of an optimal control problem. As usual the complete control problem with PDE constraints is too big to be treated numerically. Therefore I will discuss possibilities of model reduction and conclude the talk with some numerical simulations of laser

and electron beam surface hardening.

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CP25

Numerical Methods for Design of Optimal Robust Experiments with Application to Parameter Estimation in Chemistry and Chemical Engineering

Optimization of dynamic experiments to maximize accuracy of parameter estimation results subject to cost and other inequality-constraints leads to very complex optimal control problems. First, the objective function already depends on a generalized inverse of the Jacobian of the underlying estimation problem. Second, optimization results depend on the assumed parameter values which are only known to lie in a confidence region. Hence, robust optimal experiments are required. New efficient methods and numerical results are presented.

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CP25

Selecting the Optimum Quasi-Steady State Species for Reduced Chemical Kinetic Mechanisms

The automated creation of reduced chemical kinetic mechanisms to serve as submodels in computational fluid dynamics simulations of reacting flows using quasi-steady state (QSS) assumptions is a promising approach to improving the realism of these simulations. Optimizing the choice of species assumed in QSS using genetic and gradient-like algorithms increases the accuracy of the reduced mechanisms over those created using a kinetic criterion to select the species for QSS.

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CP26

Selection-Based Compression of Simulation Datasets

Feature extraction can play an important role in data compression and its significance is often neglected. We advocate a compression strategy that employs knowledge about the application to store only those data corresponding to "interesting" physical structures. Using this approach we have realized up to an order of magnitude in compression in DNS of turbulent flows. Unlike multi-resolution methods employed in visualization, our approach enables the user to control both storage and access costs.

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CP26

Towards Efficient Parallel Delaunay Mesh Generation with Guaranteed Quality

Quality mesh generation of complex domains is required for finite element calculations. Many problems require frequent remeshing as the solution evolves; i.e. problems involving dynamic interfaces. This calls for fast, efficient and robust quality mesh generators. We present an incremental algorithm based upon the ideas of Bowyer/Watson and Ruppert to solve the meshing problem. Further we discuss a careful parallel implementation extending the projection-based optimal parallel Delaunay triangulation algorithm by Blelloch, Miller et al. This is joint work with N. Walkington, G. Miller, G. Blelloch, and O. Ghattas.

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CP27

An Efficient Block Variant of GMRES

We present an alternative to the standard GMRES algorithm for solving a single right-hand side linear system based on solving the block linear system $AX = B$, where multiple starting vectors and right-hand sides are chosen so as to accelerate convergence. Efficiency is gained by reusing the matrix A in block operations with X and B. The cost of the extra matrix-vector operations is reduced via innovative programming techniques. We discuss the new algorithm and present numerical results.

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CP27

Exponential Integrators for Differential-Algebraic Equations

Exponential integrators utilize the exponential of the Jacobian, which can be approximated efficiently by Krylov subspace methods. These methods also provide a stable time integration with a time step that exceeds the CFL restriction. Typically exponential integrators are used for ordinary differential equations. Our goal is to apply these methods to large systems of differential-algebraic equations and reduce the required computational resources inherent in conventional methods. Results will be presented for the Stokes equation.

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CP28

A Tensor-Krylov Method for Solving PDE Problems

This talk will present an iterative, Krylov-subspace based approach to solving large-scale systems of nonlinear equations using tensor methods. The proposed tensor-Krylov method bases each iteration on a linear model augmented with a limited second-order term and employs a linesearch globalization scheme that imitates a trust region method. Numerical comparisons with Newton-GMRES on fully coupled Navier-Stokes problems with heat and mass transport are presented.

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CP28

Eigenvalue Computation by Multiple Explicitly Restarted Arnoldi Method

The Multiple Explicitly Restarted Arnoldi Method (MERAM) is a technique based upon a multiple use of Explicitly Restarted Arnoldi method to accelerate its convergence. MERAM allows to update the restarting vector of an ERAM by taking the interesting eigen-information obtained by the other ones into account. This paper presents results achieved by MERAM. These results show that we can obtain a good acceleration of the convergence compared to ERAM and IRAM (Implicitly Restarted Arnoldi Method).

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CP28

Robust Simulation of Nonlinear Materials Using Nox: An Object-Oriented Nonlinear Solver Library

This talk addresses the performance of a variety of nonlinear solution methods applied to solid mechanics problems involving material and geometric nonlinearities. Performance in terms of cost and robustness for variants of Newton-based, trust region and tensor methods along with various linesearches is readily assessed via object-oriented interfacing to NOX. Results will be presented for finite strain and plastic material finite element simulations performed on massively parallel platforms with discussion focusing on optimizing performance metrics.

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CP29

Finite Difference Approximations in Nonuniform Grids

New expressions for the finite difference approximations of any derivative with discrete points are given with the characteristic that the points do not need to be equidistant. The approximations given here have the following advantages: the position of the points do not have to be given by an analytic function (stretching function) so they can be put at arbitrary locations (one can select the exact positions of the points); the order of the truncation error of the approximation is a function of the local separation between points; and the nonuniform grid can be adapted to any arbitrary geometry. The accuracy and efficiency of these approximations have been checked in different fluid dynamics problems of interest.

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CP29

Modeling the Dynamics and Chemistry of Atmospheric Aerosols

Aerosols are small particles suspended in the atmosphere; recent developments demonstrated their significant impacts on global climate and chemistry, and human health. To accurately study the effects of aerosols models must resolve both their size distribution and their chemical composition. In this paper we focus on the numerical solution of coupled dynamics and chemistry equations that govern the evolution of multiple component aerosols. These high resolution methods are to be used in comprehensive three dimensional simulations.

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CP29

Mathematical Models and Thermodynamic Limits of Separation Processes

This paper studies thermodynamic limits of separation processes. It is shown that mechanical and thermal driven separation have different limiting behavior. Productivity of former is increasing function of spent energy. Productivity of latter decreases if the amount of used energy is higher than some threshold. New results for distillation are presented include ideal operating line with minimal amount of heat spent per unit of objective flow and the corresponding profile of heat supply/ removal.

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CP30

Fluorescence Tomography Using the Boundary Element Method

Frequency domain fluorescence tomography requires repeated forward solution of a pair of coupled elliptic partial differential equations. The classical boundary element method (BEM) requires an internal finite element mesh to model the internally distributed source for the fluorescence emission equation. We propose two BEM approaches that preclude the need for internal meshing. One approach directly decouples the two equations. The other directly generates the fundamental solution. The methods are compared and potential applications discussed.

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CP30

A Fundamental Solution Method for Solving Tracer Flow Equations

A new approach of the Fundamental Solution Method for solving tracer flow equations is presented. It combines a modified version of the Image's Method and the Singular Value Decomposition algorithm to obtain semianalytical expressions for the reservoir pressure and velocity fields. The tracer concentration is determined by solving a convection-diffusion equation on a streamline-potential coordinate system using the time flight concept. This strategy reduces the multidimensional concentration equation into a sequence of one dimensional problems which are efficiently solved. The new technique is validated by comparison against analytical solutions and applications to reservoirs engineering problems in two dimensions. These studies show that the main advantages of the new method are the reduction of CPU times in comparison with the boundary element methods, its lack of numerical diffusion in the solute concentration and the freedom of selecting time step sizes without stability restrictions.

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CP30

An Approximation of the Solid Angle for Solving a Poisson-Type Equation

The value of the solid angle subtended by a surface E at a point r appears frequently when solving a Poisson-type equation by BEM. Under some conditions it becomes an improper integral that cannot be calculated accurately by usual methods. We present an approximation of the value of the solid angle based on geometric properties and study its error. As an example, an application to the solution of the Forward Problem in EEG is presented.

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CP31

Block Linear Algebra on the Peer to Peer Xtremweb/yml Platform

Peer to peer global computing is well designed for coarse grain numerical algorithms, particulary block based methods. *XtremWeb* is a peer to peer experimental platform and *YML* is a langage we designed to controle such a platform. *YML* is component based and provide facilities for component definition and coordination. We presente an asynchronuous block Gauss-Jordan implementation for this platform. We discuss results obtain for very large dense matrices. As conclusion, we analyse iterative method behaviour on such system.

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CP31

Parallel, Multigrain Solvers for Hiding Network Latencies on Mpp's and Networks of Clusters

Large network latencies in networks of clusters can impede the performance of iterative solvers not constructed specifically for these environments. To hide latencies, we have developed a multigrain technique that can be applied to block iterative methods that use an inner iterative method to correct the approximation of the outer method. This is accomplished by assigning smaller subgroups of processors to precondition each vector in the block concurrently. Our experiments on an IBM SP and a network of clusters show a fourfold improvement in runtime over fine-grain implementations.

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CP31

Monte Carlo Linear Algebra Techniques and their parallelization

Monte Carlo techniques for solving linear systems are based on estimating the result of some simple stationary iteration. This results in slow convergence, and has therefore limited the application of Monte Carlo. We discuss a new technique that improves the rate of convergence. We also discuss parallelization of Monte Carlo linear algebra techniques, mention inadequacy of the "embarrassingly parallel" approach, and suggest alternatives.

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CP32
Sequential and Parallel Algorithms for the Rectilinear Steiner Tree Problem

We present branch-and-cut algorithms for solving Rectilinear Steiner Tree Problem. A new *cutsec* constraint is introduced in addition to *sec* constraint that is widely used in Travelling Salesman Problem. We show that both of these constraints can be found by solving maximum flow problem on the same network. Our implementation performs faster than GEOSteiner software by Winter, Zachariasen, and Warme in most SteinerLib tests. Moreover, our MPI-based parallel program shows good speedups on a Beowulf cluster.

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CP32
Load-Balancing in Distributed Retrieval System

Limitations on the bandwidth to a server makes the retrieval of a large-size high-resolution image, even compressed, very time-consuming. To speed up this process we have replaced the retrieval process from a single server with the retrieval from multiple servers, i.e., simultaneously retrieving different part of an image from multiple server sites. Specifically, in a related work we have implemented a block-based distributed retrieval strategy for Wavelet compressed images. In the paper, we model block-based distributed retrieval as a combinatorial optimization problem, and prove this problem is NP-Complete. We propose a heuristic algorithm to solve the optimization problem. Experimental results are given to show that the heuristic algorithm performs reasonably well in the initial tests performed.

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CP32
A New Method to Obtain Relaxed Problems of Graph Optimization Problems

Lagrangean relaxation is known to be one of the efficient methods for some optimization problems. But it is not efficient for maximum clique problem, maximum independent set problem, or some other graph optimization problems. We propose a method to add some redundant inequalities derived from some perfect subgraphs or supergraphs of the original graph before applying Lagrangean relaxation. We show by some experiments that our method work efficiently.

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CP33
Target Localization Using Computational Geometry

A visual method of target localization, using cone angle measurements from a line array, is developed under a minimum of statistical and target motion assumptions. Each geometric measurement is represented by the volume of target locations that could have produced it. These volumes are discritized, decomposed into convex subsets, expanded to account for target motion over time, and intersected to find the volume that supports multiple measurements. The method is extensible to arbitrary measurement types.

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CP33
Platform Independent Parallel Framework That Uses Network File System For Communication

We use the Microsoft network file system as our means of parallel execution of the subproblems by a collection of personal computers. We report on a pharmaceutical example for which the wall clock time required to run the distributed and parallized version is approximately the wall clock time required to run the same single machine version divided by the number of machines that participate.

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MS1
Median Partitioning for Diversity Selection, Compound Classification, and Virtual Screening

The Median Partitioning (MP) method does not depend on pair-wise molecular comparisons and has been developed to select diverse sets of molecules from very large compound pools. In subsequent MP steps, a population of molecules is divided into subpopulations above and below the median value of a particular property descriptor to produce defined partitions. In addition to diversity selection, MP has also been adapted for classification of bioactive compounds and virtual screening.

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MS1

The Poisson-Boltzmann Equation: How to use Greek Symbols with Chemists and get Away with it

Use of Poisson-Boltzmann (PB) theory in macromolecular chemistry has been hampered by the perception that Partial Differential Equations are somehow hard to understand. In fact, the PB equation allows for a remarkably simple interpretation that not only demystifies the mathematics but also allows deep physical insight into the nature of solvation effects in aqueous environment. Examples will be given, including: dielectric focussing and shielding, simple approximations to desolvation energies, analysis of sources of numerical error and stability, improvement in computational speed and implementation of numerical derivatives. It also allows for an appreciation of the limitations of methods that attempt short-cuts in order to mimic the physics properly described by PB.

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MS1

Wavelet Transforms in Protein Structure Determination

Potential applications of wavelet transforms for protein structure determination and analysis and for the study of interactions of small molecules with macromolecules will be described. The goal of these applications is to facilitate high-throughput protein structure determination and structure-based drug design. The problems at hand can best be described as related to pattern recognition and noise filtering. Technical aspects of the choice of wavelets will be discussed.

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MS1

Scoring Methods in Virtual Ligand Screening

In virtual drug discovery efforts, 3-D small molecule models are "docked" into a model of the protein target, and the docking is scored according to a variety of possible criteria: an approximate calculation of the free energy of binding, a prediction of the root-mean-square deviation of the ligand pose based on known complex structures, or a prediction of the biological activity of the compound based on known activities. This talk will cover efforts to improve scoring functions in all these directions.

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MS2

Computational Modeling of MEMS and BioMEMS

Microelectromechanical Systems (MEMS) are miniaturized sensors, actuators, devices and systems. MEMS are geometrically very complicated and typically involve several energy domains. For example, simulation of electrostatic MEMS requires coupled analysis of mechanical, electrostatic and fluidic energy domains. In this talk, we will present several meshless techniques for analysis of MEMS. First, we will present a finite cloud method [1] for analysis of partial differential equations in interior domains. Finite cloud method employs a fixed kernel technique to compute interpolation functions given a scattered set of points and a collocation technique to discretize the governing partial differential equations. Finite cloud method is a true meshless technique and we use it for analysis of micromechanical structures. Electrostatic analysis is performed by solving the potential equation in an exterior domain. A classical approach to solve partial differential equations in an exterior domain is to use a boundary-integral method. In this talk we will present a boundary cloud method for exterior electrostatic analysis. A boundary cloud method [2] is a combined scattered point/boundary integral approach for analysis of exterior problems. A key difficulty when combining scattered point techniques with boundary integral methods is the computation of interpolation functions. Classical approaches such as moving least-squares cannot be used to compute interpolation functions as they give rise to singular coefficient matrices. We will present a generalized least-squares approach to compute Hermite-type interpolation functions given a scattered set of points on the surface of an object. Boundary integral methods give rise to dense linear systems. We will present a fast algorithm combined with the boundary integral method for rapid analysis of exterior electrostatic problems. The final energy domain that needs to be considered when analyzing electrostatic MEMS is fluidics. An issue with gas flows in microscale geometries is the breakdown of continuum theories e.g. Stokes or Navier-Stokes equations. When the Knudsen number gets larger, rarefaction effects, such as velocity slip and temperature jump, become important. Since rarefaction effects cannot be captured by classical continuum theories, we have developed Direct Simulation Monte Carlo (DSMC) [3] techniques for analysis of gas transport in microscale geometries. However, the continuum theories breakdown only in small regions of the device. An attractive approach is to employ DSMC in the regions where continuum theories breakdown and to treat the rest of the device by continuum theories. We will describe a multiscale approach [4] combining meshless continuum theories with molecular techniques and we will show results on the application of the multiscale technique for microfluidic devices. References: 1) N. R. Aluru and G. Li. Finite Cloud Method: A true meshless technique based on a fixed reproducing kernel approximation. International Journal for Numerical Methods in Engineering, Vol. 50, No. 10, 2373-2410, 2001. 2) G. Li and N. R. Aluru, "Boundary cloud method: a combined scattered point/boundary integral approach for boundary-only analysis", Computer Methods in Applied Mechanics and Engineering, Vol. 191, No. 21-22, pp. 2337-2370, 15 March 2002. 3) O. Aktas, N. R. Aluru and U. Ravaioli, "Application of a parallel DSMC technique to predict flow characteristics in microfluidic filters", Journal of Microelectromechanical Systems, Vol. 10, No. 4, pp. 538-549, December 2001. 4) Atkas and N. R. Aluru, "A combined continuum/DSMC technique for multiscale analysis of microfluidic filters", Journal of Computational Physics, Vol. 178, No. 2, pp. 342-372, 20 May 2002.

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MS2

Unified Computational Models for Microfluidics-Specific Applications

Microfluidics applications encompass a plethora of physical phenomena, which makes their modeling a rather daunting task. A multitude of driving forces (pressure gradi-

ents, electric field, surface tension, etc.) are utilized in various combinations to achieve best results. Also rigorously utilized are the electro-chemical properties of the resident fluid and analytes, which are manifested in the well known electrokinetic effects. Accurate analysis of these electrokinetic phenomena can only be performed when the chemical interaction of the analytes, which may be acid, base or an ampholyte (e.g. proteins), with the system are taken into consideration. Often neglected are the special kinds of boundary phenomena that are inherent in these applications. Reduction-Oxidation (Redox) reactions at the electrodes, an example being electrolysis of water, special adsorbtion-desorption kinetics which are often the performance determiner in hybridization chips, are a few examples of the need to evolve special computational tools to accurately model them and incorporate them with the rest of the system. Phenomena and applications mentioned above, and many more, constitute the bulk of contemporary microfluidic applications. Furthermore, these diverse phenomena are interrelated. Majority of the contemporary work in this regard have treated these diverse phenomena separately making their utility for real life applications limited. In this work we propose to develop a unified computational framework for such applications. Among the many challenges would be accurate development of a generalized chemical stoichiometry for multivalent weak analytes and its coupling with local transport phenomena, treatment of broad spectrum of temporal and spatial scales, and development of high-order boundary conditions for special boundary phenomena. Novel domain decomposition based multi-block finite volume scheme is developed, which apart from rendering high accuracy for complex geometries, is also amenable to parallelization on parallel computer architectures.

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MS2

Two-Beam Optical Trap System for Detecting Index of Refraction and Size of Colloids and Live Cells

Two-beam or counterpropagating beam traps were the first optical traps to capture and move micron-sized particles (Ashkin 1970), and since then they have been applied to various applications. Recently, fiber optic two-beam trap and OCAM system have been developed to sort biological cells using image processing technique. However, image processing may not be adequate and sensitive enough for generic applications. Here we propose a photodetection based counterpropagating beam trap system consists of an optical trap generation, detection, and a visualization components for detection of particle index or size including colloids and live cells. Compared to previous studies, we use two-beams with different power levels, at a ratio of 0.5 or less. Consecutively changing power ratio can move the trap position; however, such effect has only been simulated quantitatively for fiber optic traps. The beams used have a divergence angle intermediate between a single beam trap (1.2 numerical aperture or higher) and a fiber optic two-beam trap (5m to 25m beam waist). This allows a longer working distance than a single beam trap, which has difficulty trapping objects beyond 30m in depth from a thin cover slip due to spherical aberration. On the contrary, with our two-beam trap system particles can be trapped and manipulated within 200m wide microfluidic channels. Next, by measuring the forward scattered light from a particle in a counterpropagating trap, we compare index of refraction and size of different particles and live cells. And a model for the forward scattered light that is integrated with the ray optics analysis of optical force is also developed. In this model, forward scattered rays by the particle are summed and used as a detected power signal for differentiating size and index of different particles. To our knowledge, this is the first theoretical approach is used to calculate detected power scattered from an optical trap. Finally, particles varying from 5-20 m in diameter and varying in index from 1.34 to 1.59 are detected using our system and these results are confirmed with our model. Combining fine index of refraction specificity and size differentiation with high throughput we believe that this counter-propagating two-beam trap can be useful for many applications involving high throughput arrays such as cell arrays and various lab-on-a-chip applications.

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MS2

Design and Analysis of Microcantilevers for Biosensing Applications

Microcantilevers can be used as very sensitive biochemical sensors in ambient and aqueous environments. A biochemical reaction over a cantilever surface can be monitored as a bending of the cantilever due to change in the surface stress. In addition, the change in mass upon binding can be detected as a change in the resonant frequency of the cantilever. In this paper, we have analyzed the deflection of microcantilevers utilized in biosensing chips. First, the primary deflection due to the chemical reaction between the analyte molecules and the receptor coating, which produces surface stresses on the receptor side is analyzed. Bi-material effects on the microcantilever, which influence the deflection, are established analytically. Oscillating flow conditions, which are the main source of turbulence in cantilever based biosensing chips, are found to produce substantial deflections in the microcantilever at relatively large frequency of turbulence. On the other hand, bi-material effects are discovered to be significant at relatively low frequency of turbulence. In the absence of any bi-material effects, turbulence increases the deflection due to chemical reactions and it also increases the noise effects due to the increased dynamical effects of the flow on the microcantilever. We present experimental results of resonant frequency change by using the biotin-avidin reaction in commerically available cantilevers. Finally, several different microcantilever assemblies are proposed, that will give capability for increased deflection due to chemical reactions while decreasing those deflections due to dynamical flow effects, resulting in lowered noise factors during detection.

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MS3

Deforming filaments in a Viscous Flow using Overset Grids

We consider the interaction of viscous flow with deforming time-dependent physical boundaries. Curvature of the wall, and momentum imparted by a moving boundary, causes significant departures from the classical boundary layer flow. To simulate such flows, we have developed a

moving overset grid method where a thin, body-fitted grid follows the motion of a time-dependent boundary, while most of the domain is discretized with a fixed Cartesian mesh. We present numerical studies of flow past deforming filaments.

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MS3

How an Elastic Body Reduces its Drag

Recent studies of biological structures have quantified dramatic decreases in fluid drag as they deform in high-Reynolds-number flows. We study the simplified case of a glass fiber wetted into a 2-D soap-film flow and identify a transition to large deformations that greatly reduce drag. This behavior is captured by a simple model which shows a similar transition, and a reduced $U^{4/3}$ drag law, as results of an emerging self-similarity of shape.

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MS3

Direct Simulations of Suspensions of Long Slender Filaments

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MS3

Applying the Free-Lagrange, Moving Adaptive Mesh Method to Solving Time and Space Dependent Systems Biology Problems

This presentations concentrates on the use of moving, adaptive mesh technology to capture the time-dependent movement of complex geometrical boundaries and structures associated with systems biology by using a numerical integration technique called the Free-Lagrange Method (FLM). The FLM is based on time-dependent, multi-dimensional, unstructured, hybrid meshes that can be dynamically optimized, adapted, refined, and reconnected. Coupled sets of PDEs (representing hydrodynamics, structural mechanics, and reaction/diffusion equations) are solved in time and space using these meshes for computing derivatives and fluxes. The types of systems biology that can be captured using these techniques include everything for computational cell biology to complex organ level simulations, where the evolving, time-dependent geometrical descriptions of surface/volume relationships of the system are explicitly taken into account.

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MS4

Self-Consistent Models of Earthquake Ruptures in the Los Angeles Area

We are simulating dynamic ruptures in the Los Angeles area using models of dynamic friction on faults. We are trying to determine which features must be included in the friction models in order to create stresses on faults that are compatible with a broad range of geologic, seismological, and geodetic observations. In doing so we enforce self-consistent behavior, that is, the model generates realistic ruptures at various locations and times directly from the evolution of the stress field.

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MS4

A Dynamic-Stochastic Model for the Earthquake Rupture Process

Lacking sufficient ground motion data recorded very close to large earthquakes, predictions of the severity ground motions from future earthquakes depends on our ability to develop realistic earthquake source models. We use dynamic source models developed using a Boundary Integral Method to simulate earthquake rupture by specifying the fracture energy and stress drop as spatial random fields in a way that is consistent with past earthquakes. We find that spatial and temporal variations in slip determined from dynamic rupture models differ significantly from those assumed in kinematic source models and have a strong influence on near-source ground motion.

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MS4

Octree-based Finite Element Ground Motion Modeling in Large Basins

This work reports on the development of a parallel numerical octree-based finite element methodology for simulating earthquake-induced ground motion in large, highly heterogeneous, basins. We use an out-of-core octree-based

mesh generator developed by Tu and OHallaron (2002), which allows us to generate meshes of essentially arbitrary resolution, and an efficient portable mesh solver to model the elastic wave propagation problem on distributed memory parallel supercomputers. We report on parallel performance on the Cray T3E and the TCS at the Pittsburgh Supercomputing Center. The results indicate that, despite the highly irregular structure of the problem, excellent performance and scalability are achieved.

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MS4
Large-Scale Parallel 3-D Simulation of Seismic Wave Propagation using the Earth Simulator

With the recent development of high-performance parallel computer, the Earth Simulator (5120CPU, 40Tflops), it is now possible to perform realistic 3-D simulationsof seismic wave propagation over a regional scale. At the same time, a dense strong motion network of K-NET and KiK-net allows direct visualization of seismic wave propagation during large earthquakes. We have been able to demonstrate the agreement between the observation and computer simulation of regional wavefields for the 2000 Tottori-ken Seibu earthquake. The improvements in the prediction of strong ground motions for future earthquake scenarios will depend on maintaining a close link between the available dense observations and comparable computer simulations.

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MS5
Quantification and Management of Uncertainty in the Aerothermal Design of Aircraft Engines

In this presentation, we will discuss the impact of uncertainty in the aerothermal design of aircraft engines. Various applications will be considered including compressor airfoil design, multi-stage compressor design, and turbine blade durability. For the compressor design studies, we consider how geometric variability due to manufacturing and wear impacts the aerothermal performance, and present robust design strategies which minimize the impact of this variability. In the turbine durability study, we investigate the uncertainty in turbine blade life due to variability arising in the cooling air supply system. We propose an adjoint-based methodology to help identify components in the air supply system which could lead to uncertainty in blade life.

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MS5
PDV Arithmetic in Uncertainty Computation

To deal with uncertainties in numerical computation, we design PDV significance arithmetic for computer simulations that uses an unspecified point in an interval with probability distribution as the basic data type, called Probability Distribution Variable (PDV). The correctness and effectiveness of PDV significance arithmetic are studied. Correlations or dependencies among PDVs are well handled in the arithmetic so that good approximations of the results are guaranteed. For application, we verify the effectiveness of the PDV significance arithmetic rules by extending FORTRAN to account for the creation and propagation of uncertainties in a computer program due to uncertainties in the data.

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MS5
Representing Geometric Uncertainty via Hermite Polynomial Chaos

This paper provides details on the application of the Hermite Polynomial Chaos (PC) method for representing geometric uncertainty. Results have been obtained for Laplace's equation in two dimensions in which the location of one of the boundaries is uncertain. Detailed comparisons between Polynomial Chaos and Monte Carlo simulations are made including precision and convergence studies of the statistics of the distributions as well as pointwise comparisons of histograms within the domain.

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MS5
Distribution-Free Uncertainty Quantification

One of the primary factors that hinders the practical application of probabilistic methods to the uncertainty analysis of computational models is the arbitrary selection of probability models used to represent uncertain aspects of the computational model. This problem is exacerbated in the case of uncertainty analyses requiring high degrees of resolution. For instance, a probabilistic risk analysis of a nuclear reactor often requires estimates of extremely small probabilities. The choice of uncertainty model greatly influences the tail behavior of the response which is exactly the region pertinent to the analysis. The influence of the choice of uncertainty model is also pronounced when faced with a scarcity of experimental data. In this presentation, methods of distribution-free uncertainty quantification will be discussed and applied to several engineering applications.

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MS6

Simulation of Epitaxial Growth with Strain

This talk will describe a new approach to simulation of epitaxial growth with strain. An island dynamics model with a level set numerical method is used for the growth; a lattice statics model is used for the strain. The model is partly atomistic in order to properly treat atomistic scale variation of the strain field at a step, but partly continuum in order to reduce its computational complexity. Computational and analytic results, as well as comparison to previous methods, will be presented.

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MS6

The Fine Structure of Dislocation Pile-Ups near Grain Boundaries and Resulting Macroscopic Scaling Relations

We formulate the problem of single-crystal plasticity as a nonconvex minimization problem. The functional which delivers the displacement field of the crystal accounts for elasticity, crystallographic slip, latent hardening and the self-energy of the dislocations. This latter term introduces a length scale into the variational problem, which would otherwise lack lower semicontinuity and not attain its infimum. We present a branching construction which delivers the optimum scaling for the energy of a grain forced to undergo affine boundary conditions around its boundary. The dislocation structures corresponding to the branching construction, and the attendant scaling relations between macroscopic flow stress, deformation and grain size are compared with experiment.

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MS6

Level Set Computations of Faceted Polycrystalline Thin Films

In this talk I will discuss the numerical computation of faceted polycrystals using level set methods. I will review level set methods and the construction of the Wulff shape and the solution of an inverse Wulff shape problem. I will then describe how one connects these ideas and extends them to polycrystals. I will demonstrate the application of this method to the computation of diamond thin films using the van der Drift model and discuss the evolution of surface microstructure and development of fiber texture.

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MS6

Structures of Local Minimizers of a One-Dimensional Higher Order Variational Problem

We present results on the structures of local minimizers of a one-dimensional variational problem. The energy functional under investigation is motivated by the study of coherent solid-solid phase transformations and the competition between the effects from the regularization and formation of small scale structures. We can prove the periodicity of all local minimizers with low enough energy. This is due to some intricate interactions between the boundaries of different phases.

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MS7

An Overview of Some Fast Algorithms for Elliptic PDEs

We will present some fast and accurate algorithms for solving elliptic equations in regular domains developed by the author and his colleagues in recent past. These almost spectrally accurate algorithms are analysis-based, easy to implement on serial as well as parallel computers, and have low computational complexity. Combined with techniques for boundary and distributed control, these algorithms have been extended to solve problems in irregular geometries on serial and parallel computers. Purpose of this talk is to present these algorithms, and highlight their advantages as well as mention current difficulties. Numerical results based on computations using these algorithms will be presented.

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MS7

An Efficient Cell-Centered Finite Volume Solver For Navier Stokes Equations On Vector Parallel Processors

In this study, MIMD parallel computation of coupled nonlinear partial differential equations governing the mass and momentum conservation of a 3D viscous incompressible unsteady flow on distributed memory based vector parallel processing system (VPP700) under UXP/VPPF90 has been discussed. The parallel numerical implementation is based on a time accurate cell centered Finite Volume Method in conjunction with Roes flux difference splitting of non-linear terms and pseudo-compressibility technique. Data flow graphs necessary for combined parallelization and vectorization have been generated to provide a logical basis for parallel code development. The performance of the parallel implementation measured in terms of speedup and efficiency factors is found to be good. The parallel code is tested on test problems of practical significance.

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MS7

Sub-Stepping and Semi-Lagrangian Formulations of the Spectral/HP Element Navier-Stokes Equations

To alleviate the CFL timestep restrictions using spectral/hp element methods both sub-stepping and semi-Lagrangian approaches have been adopted. In general terms both these techniques are related by considering a characteristic treatment of the advection terms, however a notable distinction arises in their implementation. We will compare accuracy and cost for internal and external flows of the two approaches within the context of a high order splitting formulation to the Navier-Stokes equations.

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MS7

An Efficient and Exponentially Accurate Parallel h-p Spectral Element Method for Elliptic Problems on Polygonal Domains - The Mixed Boundary Conditions

The convergence achieved by the current formulations of spectral methods to solve elliptic boundary value problems on polygons can at most be algebraic. Conformal mapping of the form of $z = \xi^{\alpha}$, can be used to enhance the convergence, however, exponential convergence can't be fully restored. A new parallel h-p spectral element method is presented which solves these class of problems to exponential accuracy and which is asymptotically faster than conventional FEM. The computational algorithm is devised for distributed memory parallel computers. We choose spectral element functions non-conforming everywhere except at the vertices of the elements on which they are defined. A least-square collocation approach is used to discretize the equation. The resulting normal equations, which is a symmetric and positive definite system, are solved by a preconditioned conjugate gradient method. These computations can be efficiently carried out at element level, without having to compute and store any mass and stiffness matrices, and is readily parallelizable. The load issues are discussed and the communication involved is shown to be small. Acknowledgement: The financial support from the CSIR, India (Project no. 9/92(123)/95-EMR-I) and ARDB, India (Project No. 95255) is gratefully acknowledged. First author is also thankful to the Faculty of Mathematical Sciences, University of Twente, The Netherlands, for the financial support and computational resources.

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MS8

Radio Frequency Field Interactions in Magnetized Plasmas

Magnetized plasmas support a wide range of electromagnetic waves whose characteristics depend on the wave frequency relative to, e.g., plasma frequencies and cyclotron frequencies. Computational solutions for wave fields is a demanding problem because of multiple wavelength scales and complex wave topology in 2- and 3-D systems. High resolution solutions have been obtained for many problems through use of large parallel computers and collaboration with computational scientists on algorithms that effectively use these resources.

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MS8

3D Extended MHD Calculations of Magnetically Confined Plasma

We discuss the status of the SciDAC Center for Extended Magnetohydrodynamic Modeling (CEMM). This center is focused on using advanced computing methods to evaluate the stability of fusion confinement configurations. A combination of the very wide range in temporal and spatial scales, extreme anisotropy, the importance of geometric detail, and the requirement of causality (which makes it impossible to parallelize over time) makes this problem one of the most challenging in computational physics.

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MS8

Micro-turbulence and its Impact on Plasma Confinement

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MS8

The National Fusion Collaboratory

Magnetic fusion confinement research is performed by over one thousand scientists who are distributed across the majority of the United States. The National Fusion Collaboratory Project is funded by the USDOE SciDAC Initiative to develop a persistent collaboration infrastructure to transform fusion research and accelerate scientific understanding and innovation so as to revolutionize the design of a fusion energy source. Specifically, this project is creating and deploying collaborative software tools throughout the national magnetic fusion research community. These tools are designed to enable more efficient utilization of existing experimental facilities and more effective integration of experiment, theory, and modeling. The computer science research necessary to create the Collaboratory is centered on three activities: security, remote and distributed computing, and scientific visualization. Results from the project and lessons learned will be presented.

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MS9
How to use Hybrid MPI-OpenMP on IBM SP Systems

Computational experiences with hybrid message passing and multithreading techniques on SMP clusters generally show poorer performance than pure message passing approaches. This paper attempts to understand the performance of hybrid MPI and OpenMP programs by decomposing and describing performance using four parameters: multithreading efficiency, relative cache efficiency, network interface efficiency, and message passing scaled efficiency. These parameters are used to assess a sparse matrix-vector product kernel, which is typical of many parallel scientific computations, running on an IBM SP computer. Tests with various problem sizes using up to 216 nodes (864 processors) reveal, for example, the benefit of using a hybrid implementation compared to an MPI implementation when the computation uses small messages and is not network bandwidth limited. Otherwise, the MPI implementation generally shows superior performance.

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MS9
An Overview of Some Design Issues for High-end Supercomputers

The design and implementation of a supercomputer architecture involves many decisions that involve cost-performance trade-offs, or favor some target applications over others. In this presentation we discuss some of the key design parameters and how they affect application performance. As part of this discussion, we highlight important issues that characterize the differences between the supercomputer architectures of today, connecting choice of these parameter values to application performance.

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MS9
Cray X1: Extreme Performance for the Most Demanding Applications

The Cray X1 is an extreme performance, high efficiency, MPP supercomputer designed to address both the high-end vector and MPP markets. It combines the best of the Cray parallel vector processor (PVP) systems with the highly-scalable microprocessor-based cache-oriented architecture used in the Cray T3E system. The Cray X1 system is a highly scalable system with a Single System Image OS. It is designed to excel at capability class commercial and user-developed applications. The X1 architecture is targeted at communication intensive applications with very high memory bandwidth requirements. The Cray X1 architecture complements commodity-based systems, which are more suitable for applications that demand little from the memory and interconnection network.

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MS9
Solid Earth Simulation Using GeoFEM Platform on the *Earth Simulator*

An efficient parallel iterative method for unstructured grids for SMP cluster architectures such as the *Earth Simulator* using GeoFEM platform is developed. The method is based on a 3-level hybrid parallel programming model, including message passing for inter-SMP node communication, loop directives by OpenMP for intra-SMP node parallelization and vectorization for each processing element (PE) with PDJDS/CM-RCM reordering. Examples of large-scale solid earth simulation on the Earth Simulator with 640 SMP nodes (5120 Vector Processors) will be presented.

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MS10
A Reduced Sqp Method for the Shape Optimization of Turbine and Compressor Blades

The shape optimization of blades is a crucial step within the design cycle of a whole turbomachine. The talk presents the results of a joint project between academia and industry leading to an efficient solution for this problem to be used in the daily work of concerned engineers. We describe the special properties of the optimization problem which minimizes loss of pressure subject to a PDE constraint which models the flow between two blades, and subject to additional geometry constraint. A solution method is developed which is a parallel, multiple setpoint, reduced Sequential Quadratic Programming method that takes the special structures due to the discretized flow equations as well as the multiple setpoint optimization into account. Convergence properties are discussed and numerical results are presented.

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MS10
Order-Reduction in a Wavelet Basis for a Problem of Data Assimilation In oceanology

Key problems of a variational data assimilation process in geosciences (meteorology or oceanology) are the design of the functional to minimize and the choice the space of control where the minimization is performed. In this presentation we will show the interests of wavelet basis (regularization and adaptivity properties) ´ı as a reduced space of control for the identification of initial condition in geoscience problems. Numerical results will be presented using an oceanological model.

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MS10

Application of Advanced Large-Scale Minimization Algorithms for Inverse Problems and Data Assimilation.

A large-scale minimization algorithm using the hybrid enriched method (proposed by Morales and Nocedal 2002) was first tested against L-BFGS and HF-TN for an optimal control problem in 2-D involving data assimilation and control of initial conditions in a limited area model of the nonlinear shallow water equations. In terms of the number of iterations the hybrid method for the above For particular choices of length of L-BFGS and HF-TN cycles the new algorithm performed better than the pure L-BFGS but lagged behind pure HF-TN. We then compared the performance of the hybrid algorithm with that of several robust large-scale minimization algorithms for the minimization of the cost functional in the solution of inverse problems related to parameter estimation applied to the parabolized 2-D Navier-Stokes equations. The minimization methods compared consisted of quasi-Newton (BFGS), a limited memory quasi-Newton (L-BFGS),the Hessian free Newton method and the new hybrid algorithm . The hybrid method emerged as a serious competitor to both the Hessian-free Newton method and to the L-BFGS.

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MS10

Managing Pod Models for Optimal Control Problems

Reduced order models gain increased popularity among various application areas, e.g. industrial food processing. We review some of the most recent approaches in food engineering where Proper Orthogonal Decomposition (POD) models are used. We present an optimization based approach to solve the optimal control problem in an efficient way using these low order models.

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MS11

A Computational Science Case Study: Classification of Hybrids using Genetic Markers and maximum-likelihood estimates

A self-contained undergraduate level "case study" in computational science/biology will be presented. This application brings together tools and techniques from genetics, statistics, numerical methods, and both symbolic and numeric computing into a single unified course project. The project involves the classification of individuals that may be the result of hybridization between genetically divergent parents. Data consisting of inherited genetic markers allow the evaluation of alternative model parameters by maximum-likelihood. In their implementation of the classification model students use Maple for visualization and prototyping, and the GNU Scientific Library and C++ for computation of model parameters.

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MS11

Scientific Visualization in Undergraduate Computational Science Education

Because of the importance of scientific visualization to computational science, an undergraduate CSE student should understand the basic capabilities and processes of computer graphics, a visual approach to scientific problem solving, and visualization applications in the sciences. This talk presents how, using STELLA, Mathematica, and C with OpenGL and online materials developed by the authors (http://www.cs.csustan.edu/ rsc/NSF and http://www.wofford.edu/ecs), an undergraduate computational science program can give students the background they need to have this understanding.

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MS11

Building Assessment into the Development of Undergraduate Computational Science Curricula

University faculty develop curricula in their specialty as a natural part of their professional obligations. They also undergo evaluation of their teaching, service and research on a regular basis to ensure promotion and recognition among their peers. But it is not always the case that when starting the process of developing a curricula, a faculty member considers how to assess the students' attitudes towards the topic, how these attitudes might change during the course and what the impact of the semester-long learning experience has been for the student. We present how the on-line analysis tool, the Sociology Workbench (SWB), was used with surveys, based on the SALG (Student Assessment of Learning Gains) from the LEAD Center at the University of Wisconsin, in developing a curriculum on High Performance Computing for computational science. Along with the SWB, the Automatic Survey Creation Process (ASCP) was used to easily prepare and administer surveys to students. Both the curricula and its assessment tools will be

shared in this presentation.

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MS11

A Computational Science Curriculum For A Liberal Arts Environment

Computational science, defined as the intersection of mathematics, computing, and science, can be naturally integrated into existing undergraduate math and science curricula. Funded by grants from NSF (DUE - CCLI)Battelle and the W.M. Keck Foundation, Capital University is designing a comprehensive undergraduate program in Computational Science. In addition, a cadre of faculty from eight institutions have established the Keck Undergraduate Computational Science Education Consortium (KUCSE) with a goal to develop on-line educational materials in an array of computational subdisciplines. The primary goal of the Computational Science program is to present mathematics within the context of science problems, and also to demonstrate how computing technology (symbolic, numeric, parallel, graphical/visualization) can be used to solve problems from various scientific disciplines. The presentation will address the efforts of the KUCSE consortium, the overall structure of the computational science curriculum and will outline the content of various courses.

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MS12

MESQUITE: The Mesh Quality Improvement Toolkit

Mesh quality is critically important to achieving accurate, efficient numerical solutions to PDE-based applications. Unfortunately, there has been no freely-available, comprehensive software package designed specifically for the mesh quality improvement problem. To rectify this situation, we have created MESQUITE, the Mesh Quality Improvement Toolkit. MESQUITE works with a large number of element topologies, uses state-of-the-art mesh quality improvement algorithms, and achieves wide tool applicability through the use of the TSTT-defined common mesh interfaces. In this talk, we describe the design goals for MESQUITE, the underlying mesh optimization algorithms, and its use in a variety of application problems to improve element shape. We also discuss our future plans for extending the toolkit to new improvement goals such as those using a posteriori solution errors.

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MS12

Mesh Untangling

The issue of untangling structured and unstructured meshes is addressed in this work, using both new and existing methods. Two of these methods are based on geometrical analysis of the problem (feasible set, simplex method), the others use numerical optimization of an appropriate objective function. Best results were achieved with suitable combination of both types of techniques. All methods have been developed primarily in two dimensions, but preliminary work in 3D has also yielded good results.

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MS12

Toward a Theory of Preconditioners for Mesh Quality Improvement

In theory, a good way to automate improvement of mesh quality is to numerically optimize an 'L-infinity' objective function which maximizes the minimum of some element quality metric. Unfortunately, algorithms to do so can be slow compared to simple Laplace smoothing which, although fast, does not guarantee improved quality. A compromise is to first apply Laplacian smoothing for one or two passes over the initial mesh before initiating numerical optimization of an L-infinity objective function. This hybrid technique can give both good quality and relative efficiency. We move in this investigation toward a theory of mesh 'preconditioners' that would explain the observed behavior and suggest improvements to the existing hybrid algorithm.

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MS12

What Is a Good Linear Finite Element? Interpolation, Conditioning, Anisotropy, and Quality Measures

I present new bounds on interpolation errors over linear triangular and tetrahedral elements, including bounds for cases where the function being interpolated has anisotropic curvature. I also discuss the relationship between element shape and stiffness matrix conditioning, for isotropic and anisotropic PDEs. From these relationships I develop element quality measures suitable for use in numerical or combinatorial optimization of meshes, to help reduce the interpolation error or condition number. Some surprising conclusions about anisotropy (and the large angle condition) follow from these results.

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MS13

A Computational Framework for the Efficient Simulation of Stochastic Chemical Kinetics (Part II)

See abstract under "A Computational Framework for the Efficient Simulation of Stochastic Chemical Kinetics (Part I)."

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MS13

Stochastic Chemical Kinetics

The time evolution of a well-stirred chemically reacting system is traditionally modeled by a set of coupled ode's called the reaction rate equations (RRE). The resulting picture of continuous deterministic evolution is, however, valid only for infinitely large systems. That condition is adequately approximated by most "macroscopic" chemical systems. But in the microscopic systems formed by living cells, the small numbers of some reactant molecules can result in dynamical behavior that is noticeably discrete rather than continuous, and noticeably stochastic rather than deterministic. In that case, a more accurate mathematical modeling is obtained using the machinery of Markov process theory, specifically, the chemical master equation (CME) and the stochastic simulation algorithm (SSA). This talk will discuss recent efforts to establish an analytical connection between the CME and the RRE, and to approximate the SSA by speedier simulation strategies.

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MS13

Meaningful Noise in Biological Systems

Cellular processes are inherently stochastic due to the underlying molecular reactions. In most practical studies, this is merely a nuisance that has to be taken into account by appropriate statistical analysis of data. In some instances, however, noise is believed to trigger distinct patterns. In hematopoiesis, for example, the decision between different differentiation pathways (red blood cells, white blood cells, platelets) appears to be stochastic; there is sufficient spacing between transcription events that the stochastic choice between transcribing gene A or gene B first can dictate the faith of the cell. Conversely, noise can also help stabilize non-linear systems relying on few regulatory molecules as illustrated for stochastic focusing. Finally, noise may render proposed models of pattern formation meaningless, necessitating careful evaluation of such models robustness to noise.

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MS13

A Computational Framework for the Efficient Simulation of Stochastic Chemical Kinetics (Part I)

In microscopic systems formed by living cells, the small numbers of reactant molecules can result in dynamical behavior that is discrete and stochastic rather than continuous and deterministic. These two talks will introduce a new class of discrete stochastic methods based on Poisson processes which more accurately reflect the underlying cellular models. The stochastic simulation algorithm (SSA) due to Gillespie has become a fundamental tool for simulating individual molecular reactions in the modeling of cellular behavior and regulation. However, this method can be computationally quite demanding. Gillespie has recently proposed an approximation to the SSA called tau-leaping which offers a great potential for speeding up the computation in many situations of practical interest. In these talks we will introduce a new class of numerical methods - which we call Poisson Runge-Kutta methods - which generalize and extend the tau-leaping idea, along with a theoretical framework for their analysis. A general formulation and order theory for this class of Poisson Runge-Kutta methods will be given, and high order methods will be constructed. Attention will be given to such issues as stiffness and efficient implementation. Numerical simulations will be presented to illustrate the performance of the new methods.

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MS14

Numerical Modeling of Small-Scale Heat Recircu-

lating Burners

Since hydrocarbon fuels have 100 times higher energy per unit mass than lithium-ion batteries, nanoscale/microscale fuel-to-electricity conversion devices could potentially replace batteries in portable electronics. CFD is a necessary design and analysis tool because such small devices cannot be properly instrumented with existing laboratory techniques. We have modeled the effects of heat recirculation, heat losses, heat transfer along walls, and catalytic versus gas-phase reaction in small-scale combustion devices. Implications for optimal thermal/chemical system design are discussed.

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MS14

Modeling of Transport Phenomena in Carbon Nanotube Synthesis

This study is aiming at to find optimal conditions of formation of carbon nanotubes, to propose needed computational tools, and to discuss fluid physics features crucial for this technology. The needed computational tools include continous (steady, time-averaged and stochastic) fluid mechanics, higher-Kn number Burnett flow equations, and molecular dynamics simulations for solid material-laser interaction. Considered processes of production of nano-tubes are laser ablation (LA), chemical vapor deposition (CVD), and decomposition of high-pressure carbon oxide (HiPco). The practical choice of the process is a trade-off between product quality and quantity. All processes are controlled by metal catalyst particles, which initialize synthesis of carbon nanotubes from feedstock gas. In the HiPco process, the catalyst particles enter the HiPco reactor at room temperature and are heated up to 1000C in the reactor. To avoid formation of Fe clusters, which do not act as good catalysts, the catalyst particles should be heated as quickly as possible. Straightforward measures such as increasing hot gas consumption, increase the angle between hot and cold incident jets, and splitting the cold jet are not sufficient to achieve fast heating because of the behavior of particle trajectories. The poor performance of the original reactor configuration is explained in terms of features of particle trajectories. Classification of trajectories has been proposed and applied to optimization of HiPco process. Validity of turbulence models for high-incidence jets will be discussed. In the laser vaporization process, the feedstock plume loaded with catalyst particles expands explosively into the background gas. The relative strength of different mixing mechanisms and validity of self-similar solution for plume expansion will be obtained. Lagrangian approach to obtain temperature profile for catalyst particles will be discussed. Use of TVD-based algorithms for multi-species explosion-type laser-ablated plume will be discussed. Finally, the interaction of a feedstock gas with growing carbon nanotubes in CVD will be considered. The low-Re flow passes through the forest of nanotubes interacting with catalyst particles located at the basis of nanotubes. The flow features seem more predictable than those for LA and HiPco process. However, the sub-micron diameter of nanotubes leads to higher Knudsen number and the micro-fluid model is introduced as a departure from continuous mechanics towards molecular-level dynamics of formation of nano-tubes. This model desribes mass transfer and growth of a single nanotube growth and should be used as a compliment to macro-fluid continuous mechanics equations.

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MS14

Modified Characteristic Scheme for Quantum Hydrodynamic Simulation of Nanoscale Heterostructures

The characteristic scheme [1] developed in the computational aerodynamics is adapted to accommodate quantum hydrodynamic simulation of nanoscale semiconductor devices. A mass freezing technique is proposed, together with the characteristic scheme, to handle the large mass gradient or discontinuity and to remove the instability caused by the discontinuity. The modified characteristic scheme has been successfully applied to quantum hydrodynamic simulation of heterojunction devices with band-gap and effective-mass discontinuities. Acknowledge - This work was supported by SRC under Grant No. 2000-RJ-873G and by NSF under Grant No. DMR-0121146. 1. A. Jameson, Int'l J. computational dynamics, Vol. 4, 1995, pp. 171-218

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MS14

Modeling of Active Propulsion in Capillaries

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MS15

Recent Progress on MILES for High-Re Flows

In MILES, the Subgrid Scale (SGS) flow physics is pro-

vided by intrinsic, non-linear, high-frequency filters built into the discretization using. Detailed properties of the implicit subgrid model are related to the flux limiter, which in turn depends on the specifics of the numerical scheme; we illustrate how the latter properties can directly affect their potential in the MILES framework. Major unresolved issues are discussed in this context.

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MS15

From Numerical Analysis to Implicit Subgrid Turbulence Models

Basic techniques in the numerical analysis of PDEs can provide the form of implicit subgrid models. The technique is the derivation of the modified. As turbulence is an intrinsically nonlinear phenomenon, it is the nonlinear truncation errors that provide an unambiguous connection between explicit and implicit forms of modeling. These nonlinear terms are a consequence of the PDE's form and nonlinear differencing. With this analysis available, the parallels with standard turbulence modeling will be discussed.

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MS15

Treatment of Small Scale Vortices as Solitary Waves: a New Approach to LES.

A new approach to LES is presented, based on Vorticity Confinement: A simple, nonlinear "confinement" term is added to the discretized Euler pde's which vanishes at large scales, but which produces a stable, overall negative diffusion at smaller scales. The result is an implicit model for the smallest scale vortices, which can propagate indefinitely on the lattice as nonlinear solitary waves with no numerical spreading, with a diameter 2 grid cells. Comparisons with experiment for 3-D turbulent wakes will be presented.

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MS15

On the Transition between DNS and LES Simulations of Turbulence

The distinction between Direct Numerical Simulation (DNS) and Large Eddy Simulation (LES) is one of resolution (rather than of flow regime). We study a particular turbulent flow and physical viscosity, using the nonoscillatory finite volume scheme MPDATA. We employ a sequence of resolutions encompassing fully resolved DNS at one extreme and LES at the other. We demonstrate the consistency of our results, i.e., that all LES results represent appropriate grid integrals of the DNS run.

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MS16

Numerical and Scale-Model Simulation of Earthquake Rupture

Scale-model earthquake experiments provide detailed recordings of seismic motion unavailable for natural earthquakes and thereby offer an opportunity to test numerical earthquake simulation methods. Among the advantages realized from the use of experimental data are optimal sensor locations, precise knowledge of bulk and surface properties of the medium, detailed knowledge of the initial stress state, and experimental repeatability. We perform numerical simulations that closely mimic the experimental observations and provide new insights into earthquake ground motion excitation.

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MS16

Large-Scale Source and Material Inversion for Earthquake Ground Motion Modeling

We consider a regularized output least squares formulation of the inverse problem of estimating the source and/or material parameters for an earthquake ground motion model, given surface observations of the response. A Galerkin finite element method is used to discretize the resulting optimality system; specifically, state, adjoint, and inversion parameters are all approximated on the same finite element mesh. The advantage of this grid-based approximation is that no *a priori* knowledge of the structure of the source or material field is assumed in their parameterization. The disadvantage is the extremely large number of inversion parameters that ensues. We show that appropriate optimization solvers can be constructed that are insensitive to the large number of parameters.

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MS16

Fully Non-Linear Inversion of Dynamic Earthquake Rupture Parameters

Conventional inversion methods matching recorded and synthetic accelerograms are limited to estimates of the movements on the fault, although the radiated waves are highly sensitive to variation of dynamic stress and frictional parameters on the fault. We have developed a new non-linear inversion method to estimate such dynamic rupture parameters using high-performance computing, which will allow routinely generation of more physically correct models for large earthquakes, an important step towards earthquake prediction.

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MS16

Seismic Methods for Imaging Basin Properties

Predicting the severity of earthquake shaking in a basin is dependent on two factors: accurate modeling of realistic wave propagation in the basin model, and accurate estimation of the basin's physical properties, such as the attenuation, density and velocity distributions. In this talk I overview the major seismic methods for estimating basin properties. They can be organized with respect to scale length, and mathematically unified by recognizing that they are special cases of the Generalized Radon transform.

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MS17

Iterative solvers for Wave Propagation in Random Media

This paper deals with numerical simulations of wave propagation in heterogeneous random elastic media. Methods to this problem are first based on model reduction both with respect to the physical dimension to account for unbounded media and with respect to the random dimension of the problem accounting for homogeneous and non-homogeneous random fields. The method to solution of the stochastic problem is based on Monte Carlo Simulations. For each of these simulations, iteratives solvers are used together with global (for all similations) and local (dedicated to each simulation) preconditionners built using a Polynomial Chaos expansion. At last, numerical examples in the field of earthquake engineering and comments on the relationship of the proposed approach with theoritical approaches to waves in random media are given.

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MS17

Dynamic Systems Subjected to a Class of Equivalent Inputs

Consider a collection of stochastic processes Y(t), t¿0, that are equivalent in the sense that they have (1) the same second moment properties or (2) the same second moment properties and marginal distribution. Let X(t), t¿0, be the state of a linear or nonlinear dynamic system subjected to a member of the collection of equivalent processes Y(t). If the dynamic system is linear, then the second moment properties of X(t) are independent of the particular version of the input. However, higher order moments and other properties of X(t) depend on properties of Y(t) beyond its first two moments. If the dynamic system is nonlinear, even the second moment properties of X(t) depend on higher order statistics of the input. Frequently in applications the available information on the input is limited to the first two moments or the first two moments and the marginal distribution so that the input can be viewed as a member of one of the two classes of stochastic processes Y(t). The paper examines the sensitivity of the probability law, sample properties, and other features of the state X(t) to the particular version of the input. Numerical results are presented for diffusion, translation, and filtered Poisson input processes that are equal in the second moment or higher order sense.

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MS17
Equation-Free Multiscale Computation

We present and discuss a framework for computer-aided multiscale analysis, which enables models at a "fine" (microscopic/stochastic) level of description to perform modeling tasks at a "coarse" (macroscopic, systems) level. These macroscopic modeling tasks, yielding information over *long* time and *large* space scales, are accomplished through appropriately initialized calls to the microscopic simulator for only *short* times and *small* spatial domains. Traditional modeling approaches first involve the derivation of macroscopic evolution equations (balances closed through constitutive relations). An arsenal of analytical and numerical techniques for the efficient solution of such evolution equations (usually Partial Differential Equations, PDEs) is then brought to bear on the problem. Our equation-free (EF) approach, introduced in [?], when successful, can bypass the derivation of the macroscopic evolution equations *when these equations conceptually exist but are not available in closed form.* We discuss how the mathematics-assisted development of a computational superstructure may enable alternative descriptions of the problem physics (*e.g.* Lattice Boltzmann (LB), kinetic Monte Carlo (KMC) or Molecular Dynamics (MD) microscopic simulators, executed over relatively short time and space scales) to perform systems level tasks (integration over relatively large time and space scales, "coarse" bifurcation analysis, optimization, and control) directly. In effect, the procedure constitutes a systems identification based, "closure on demand" computational toolkit, bridging microscopic/stochastic simulation with traditional continuum scientific computation and numerical analysis. We illustrate these "numerical enabling technology" ideas through examples from chemical kinetics (LB, KMC), rheology (Brownian Dynamics), homogenization and the computation of "coarsely self-similar" solutions, and discuss various features, limitations and potential extensions of the approach. The work involves collaborations with several colleagues that will be mentioned during the talk.

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MS17
Variable Reduction in Mechanical Models of a Heat Bath

I will review recent developments in variable reduction in mechanical systems that mimic the motion of a particle immersed in a heat bath. In the limit where the number of particles in the heat bath tends to infinity the motion of the "distinguished" particle can be (weakly) approximated by a stochastic equation of Langevin type. Long time ergodic properties are analyzed, as well as numerical aspects such as the use of "large" time steps, where high frequencies are underresolved.

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MS18
Evolution of Deformation-Induced Microstructures

Deformation of metals leads to special microstructures composed of dislocation-rich boundaries separating nearly dislocation-free regions. A significant part of these boundaries are called geometrically necessary boundaries (GNBs). These GNBs form a characteristic layered pattern with a characteristic spacing. Experimentally the evolution of these special microstructures follows a general pattern. It is observed that the average spacing between boundaries decreases monotonically with increasing strain for tension, compression, torsion and rolling. It has also been found for many different metals that the probability distributions of GNB spacings collapse into a single function when scaled by their average spacings. We have extended the previous experimental observations by generating bit maps of boundary tracings in a given area. These maps allow for a statistical measurement of all boundary spacings in that area, thereby obtaining a more precise definition for the tails of the scaling distribution. The technique led to the refinement of the scaling properties for the GNBs. This information is also used to give insight into the boundary creation process during deformation. This insight will form the basis for formulating the evolution of the spacing probability distributions. This work was supported by the Office of Basic Energy Sciences, the U.S. DOE under contract no. DE-AC04-94AL85000.

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MS18
Quasiconvexity and Multiscale Methods in the Modelling of Soft Elasticity of Nematic Elastomers

Nematic elastomers are polymeric materials which combine the elastic properties of rubbers with the optical properties of nematic liquid crystals. Their mechanical behavior is extremely complex, as a consequence of the symmetry-breaking phase transition which transforms the isotropic high temperature phase into a uniaxial (nematic) phase. Typical equilibrium configurations exhibit fine-scale oscillations of the state variables, which can be interpreted as energy-minimizing phase mixtures. Starting from the microscopic free-energy proposed in the physics literature, energy minimizing configurations are computed through a hybrid analytic-computational procedure articulated in three steps. First, the microscopic free-energy is coarse-grained by computing the energetically optimal microstructures associated with a given macroscopic deformation gradient (quasiconvexification). In this way, small scale oscillations of the state variables are correctly accounted for in the energetics, but averaged out in the kinematics. Second, the macroscopic fields of interest (stresses, strains, etc.) are computed with the finite element method. Third, the fine scale oscillations are reconstructed from the computed macroscopic deformation gradients by 'inverting' the

quasiconvexification procedure followed in the first step. The comparison of numerical results with experimental evidence sheds new light on the physics of nematic elastomers.

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MS18

The Application of Quasiconvex Relaxation in Shape Memory Alloys

Shape memory alloys and other materials that admit phase transformations under mechanical/electrical/thermal loadings are very attractive for designing novel engineering systems. One impediment, however, to effective design with such materials is the lack of a general purpose (constitutive) model suitable for use in solving boundary value problems using analysis software such as FEA programs. Recently, however, development of such models for macroscale modeling has been moving toward a common generalized thermodynamic framework. Several promising models utilizing single martensitic variants and some with multiple variants have appeared recently. In this work we develop a model using some new results in quasi-convexity theory in a general multivariant framework for single crystals that is based upon lattice correspondence variants. Evolutionary aspects of the model are generated from dissipation hypothesis or from full relaxation methods. These new results are based upon some surprisingly simple energy bounds which we are able to show are quite tight under certain common circumstances. The presentation will provide an introduction to generalized notions of convexity and their exploitation in model development. Example computations will be shown and correlated to detailed experimental results on single crystals in tension and tension-torsion for the cases of 7 and 13 variant systems.

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MS18

Homogenization and Microstructure Development in Non-Convex Standard Dissipative Solids

The lecture provides an overview about recent developments in the formulation and numerical implementation of incremental minimization principles for inelastic solids. Consistent with the broad class of standard dissipative materials we outline a distinct incremental variational formulation of the local constitutive response where an incremental stress potential is obtained from a local minimization problem with respect to the internal variables. The existence of this stress potential allows the formulation of IBVPs for standard dissipative solids as a sequence of incremental minimization problems. The stability of these incremental problems is controlled by weak convexity properties of the incremental stress potential. Microstructure developments due to phase decompositions in incrementally non-convex dissipative solids can be resolved by relaxation methods based on convexification analyses. The relaxed problems provide a well-posed overall response of the instable dissipative solid as close as possible to the original problem. We outline the basic set up of relaxation analyses for dissipative standard materials in terms of incremental minimization problems for exact and approximated quasi- and rank-one convexifications and discuss details of their algorithmic implementations. The methods are applied to a set of representative model problems in non-convex plasticity and damage mechanics.

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MS19

Scalable Solution of CFD Problems on Unstructured Meshes

Unstructured meshes have many advantages in the solution of computational fluid dynamics problems, particularly for handling complex geometries and computational features. However, building applications that use unstructured meshes can be difficult from the standpoints of both correctness and performance, even on single processors. For parallel machines, the problem is so daunting that some view unstructured problems as intrinsically non-scalable. High performance, scalable unstructured mesh codes are possible, but they require careful attention to memory issues. With such attention, scalable performances of over 220 GFlops on 3000 processors has been achieved. The key to achieving such performance is to simultaneously exploit both the mathematics of the problem and the organization of parallel computer. Many problems have natural hierarchies; algorithms can take advantage of these. In addition, these hierarchies provide a natural way to structure memory use for performance. Domain decomposition methods are an example of algorithms that provide a good match to real architectures. These memory hierarchies can also guide the organization of the data structures to aggregate data transfers, both within and between processors, to make efficient use of memory systems. In addition, numerical libraries can provide tools to aid in the construction of scalable solvers by providing operations that support aggregate and hierarchical operations. This talk will discuss the operations provided by the PETSc library that simplify the construction of scalable solvers for unstructured problems.

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MS19

Scalable Parallel Direct Solution of General Sparse Systems of Linear Equations

We present symbolic and numerical factorization algorithms that have enabled the development of a scalable parallel direct solver for unsymmetric sparse systems of linear equations with partial pivoting. The symbolic algorithms are cabable of inexpensively computing

a minimal task-dependency graph and near-minimal data-dependency graph for factoring a general sparse matrix. These graphs, computed solely from the nonzero pattern of the sparse matrix, are valid for any amount of pivoting induced by the numerical values during LU factorization.

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MS19

Algorithms for Terascale Computations of PDEs

Though architectural concurrency is easy to achieve (e.g., 8192-fold in ASCI White), algorithmic concurrency to match is less so in scientific codes, due to global domains of influence in implicitly discretized operator equations, implicitness being required for multiscale systems. We review optimal parallel algorithms for PDE simulations in the Newton-Krylov methodology, preconditioned with Schur and Schwarz decompositions, including multilevel generalizations of the latter. We also discuss research in progress on nonlinear Schwarz preconditioning and optimization of PDE-constrained systems, and describe major goals of a five-year, nine-institution project, Terascale Optimal PDE Simulations.

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MS19

New Error Estimators and Adaptive Schemes for Updated Lagrangian Formulations

We will report here on the development of a new class of a posteriori error estimators for large deformation nonlinear problems solved using updated Lagrangian formulations and explicit integration schemes. Our estimators are element residual based and use some approximate techniques for evaluating the residuals to keep the cost of the estimates low. We have also implemented techniques for obtaining estimates of the error in user defined quantities of interest.

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MS20

An Overview of Compatible Discretizations in Electromagnetics

Compatible discretizations inherit and/or mimic fundamental structural properties of the underlying PDE model. In this talk we will present a summary of compatible Finite Element, Finite Volume and Finite Difference discretizations arising in computational electromagnetics. We will used the formalism of differential forms to expose the intrinsic connections that exists between compatible FE, FV and FD schemes. Importance of discrete compatibility will be illustrated by several numerical examples.

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MS20

Higher order covolume techniques for vector field problems

This talk will discuss the covolume approach to solving Maxwell's equations and other vector field equations. Algorithms and error estimates will be covered. Some recent proposals for higher order approximations will be presented.

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MS20

Stability and Conservation Properties of Transient Electromagnetic Simulations Using FIT

The Finite Integration Technique (FIT) is a well-established, general discretization method for electromagnetic fields. Based on a 3D staggered computational grid, Maxwell's equations are transformed into a set of algebraic equations which are the origin of a large variety of different algorithms. We present some basic properties of this approach which are responsible for a class of important stability and conservation properties of FIT. Several time integration schemes for transient fields are discussed.

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MS20

Mimetic Discretizations for Maxwell's Equations and the Equations of Magnetic Diffusion

We have constructed reliable finite difference methods for approximating the solution to Maxwell's equations and the equations of magnetic field diffusion using accurate discrete analogs of differential operators that satisfy the identities and theorems of vector and tensor calculus in discrete form. The numerical approximation does not have spurious modes and mimics many fundamental properties of the underlying physical problem including conservation laws, symmetries in the solution, and the nondivergence of particular vector fields. Numerical examples demonstrate the high-quality of the method when the media is strongly discontinuous and for nonorthogonal, nonsmooth, structured and unstructured computational grids.

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MS21

Components for Scientific Computing: An Introduction

Component environments are emerging as tools to help computational scientists manage the complexity of the software systems they develop. I will present a brief overview of concepts, tools, and technologies relating to the development and use of component-based scientific applications, including how this approach relates to more traditional software development methods, and some of the benefits of the component environment.

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MS21

CCA-Component Based Simulation of Flows on Adaptively Refined Structured Meshes

We present a design and proof-of-concept implementation of a component-based scientific simulation toolkit for hydrodynamics. We employed the Common Component Architecture, a minimalist, low-latency component model as our paradigm for developing a set of high-performance parallel components for simulating flows on structured adaptively refined meshes. We find that the architecture is sufficiently flexible to allow a straight-forward decomposition into reusable components. Two examples, a reactive-diffusive system and shock-hydrodynamics are employed to show reuse as well as test single-processor and scaling performance.

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MS21

Creating Grid-Enabled Applications Through Cactus and GridLab

Cactus (http://www.cactuscode.org) is a component-based framework originally created to satisfy the computational requirements of the Numerical Relativity community. As Cactus branched out to support more applications, the power of the framework model to accelerate software development by hiding the complexities of the underlying supercomputer environment has become apparent. We will discuss the architecture of the Cactus framework as well as new work by the GridLab effort (http://www.gridlab.org) to apply these principles to tame complex Grid computing environments.

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MS21

The BioPSE Software System: Releasing and Supporting An Open Source Problem Solving Environment

The SCIRun problem solving environment is a software architecture designed to facilitate collaborative investigation of large-scale scientific computing applications. The Biomedical Problem Solving Environment (BioPSE) is an open source superset of SCIRun, developed through the Scientific Computing and Imaging (SCI) Institute's NIH-NCRR Center. While other SCI projects have worked to enhance SCIRun's core infrastructure, the NCRR Center has focused on increasing the system's usability through dynamically compiled algorithms, documentation libraries, example datasets, and user support.

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MS22

Shape Optimization of an Acoustic Horn

Shape optimization of an acoustic horn is performed with the goal to minimize the portion of the wave that is reflected. The analysis of the acoustical properties of the horn is performed using a finite element method for the Helmholtz equation. The optimization is performed employing a BFGS Quasi-Newton algorithm, where the gradients are provided by solving the associated adjoint equations. To avoid local solutions to the optimization problem corresponding to irregular shapes of the horn, a filtering technique is used that applies smoothing to the design updates and the gradient. This smoothing technique can be combined with Tikhonov regularization. However, experiments indicate that regularization is redundant for the optimization problems we consider here. However, the use of smoothing is crucial to obtain sensible solutions. The smoothing technique we use is equivalent to choosing a representation of the gradient of the objective function in an inner product involving second derivatives along the design boundary. Optimization is performed for a number of single frequencies as well as for a band of frequencies. For single frequency optimization, the method shows particularly fast convergence with indications of super-linear convergence close to optimum. For optimization on a range of

frequencies, a design was achieved providing a low and even reflection throughout the entire frequency band of interest.

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MS22

Towards a Comprehensive Framework for the Regularization of Adjoint Analysis in Multiscale Pde Systems

Adjoint analysis lies at the heart of model-based control, optimization, and forecasting of PDE systems. Typical applications include the optimization of open-loop control distributions in space and time, shape optimization, state reconstruction and parameter estimation in weather forecasting, the development of subgrid-scale models for large-eddy simulations, and the Riccati-based feedback control of unsteady flows. In high-dimensional discretizations of PDE systems which exhibit multiscale complexity, such as turbulent flows, we have found that it is quite important to regularize the analysis in an appropriate fashion in order to get a meaningful, numerically-tractable result. We have found that there are 4 distinct places in the process of adjoint-based optimization where regularization may be applied, namely:

1. The adding of model terms to the governing equation to account for unresolved, subgrid-scale effects,
2. The definition of the norm used to measure the field in the cost function,
3. The definition of the duality pairing used to define the adjoint operator, and
4. The definition of the inner product used to define the gradient.

The present talk will take a close look at the intricate relationship between these four issues, first in the context of a simple model problem, then in the context of larger systems of interest in fluid mechanics.

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MS22

Linear and Nonlinear Optimal Control in Spatial Boundary Layers

Instabilities in a spatially-developing three-dimensional boundary layers are controlled through blowing and suction at the wall. The performance of the control is tested in direct numerical simulations (DNS) of the incompressible Navier–Stokes equations for Tollmien–Schlichting (TS) waves, optimal transiently-growing streaks in a Blasius boundary layer, and cross flow vortices in a Falkner–Skan–Cooke (FSC) flow. Feed-back optimal control is applied, using a strategy designed to operate locally on a spatially-developing flow. The feed-back operator is constructed from the Orr–Sommerfeld–Squire equations. Assuming the flow to be locally parallel makes it feasible to solve the associated Riccati equations for each wave number pair in the stream- and spanwise directions. The feed-back is applied to a DNS of the flows mentioned above. The method performs surprisingly well, in spite of the limitations with respect to being able to account for strong nonlinear effects. It is demonstrated that TS waves are stabilized and that transient growth is considerably lowered by the controller. Moreover, the controller successfully inhibits growth of steady cross flow vortices in the FSC flow: The linear optimal control is then compared with the control computed from a quasi-Newton optimization algorithm which is applied to solve an off-line optimal control problem. A solver for the adjoint equations has been implemented in the spectral DNS code used. This method adapts naturally, without modification, to nonlinearities such as a strongly varying mean flow. However, it is computationally expensive and storage demanding, needing numerous solves of the Navier–Stokes and associated adjoint equations.

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MS22

Reduced Order Modelling for Optimal Control of Wake Flows Using Pod

We consider the possibility of controlling the wake behind a flat wing with reduced-order modeling. Reduced-order controller is designed based on proper orthogonal decomposition (POD) and Galerkin projection. POD allows one to extract the dominant modes in the observed physical phenomena and to define the smallest possible solution space. This can be exploited in a Galerkin framework to reduce a nonlinear infinite dimensional model to a small finite dimensional model. Detailed finite element simulations are performed, and POD is applied to the resulting data to ex-

tract the most energetic eigenmodes. These global eigenmodes are then used in conjunction with the Galerkin projection to obtain a reduced-order (low-dimensional) model. Reduced-order models are not only attractive for real-time control computation but also crucial for detailed stability and bifurcation analysis. We investigate the design of optimal controller for wake flow behind a flat wing with this model where actuation (suction/blowing) is performed on a small part of the boundary.

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MS23

Combinatorial Preconditioners and Support Theory

Preconditioning large, sparse linear systems is a research area of great importance to many CSE applications. Support Theory is a new mathematical toolkit for bounding eigenvalues and condition numbers. We describe combinatorial preconditioners based on spanning trees of a graph and generalizations based on matroid theory, and then discuss some recent developments. We show that discrete and combinatorial techniques can be valuable tools in applied linear algebra.

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MS23

Modifying a Sparse Cholesky Factorization

Given a sparse matrix AA' and its sparse Cholesky factorization, we develop techniques for obtaining the new factorization after adding a column to A or deleting a column from A. The method relies on an inseparable intertwining of linear algebra and discrete mathematics. With multiple-rank updates, the performance is comparable to a supernodal Cholesky factorization. Updating/downdating the factors is faster than solving a system using the factors; we present a method to update/downdate the forward solve.

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MS23

Fill Reduction Algorithm Using Diagonal Markowitz Scheme with Local Symmetrization

We introduce new fill reduction ordering algorithms for sparse unsymmetric factorization. The symmetric orderings preserve large entries on the diagonal. Unlike the traditional approaches, our ordering algorithms are based solely on the (unsymmetric) structure of A, not on that of $A + A^T$. Their efficient implementations require us to extend the (symmetric) quotient graph model to the bipartite quotient graph. The experimental results show that we can better preserve the sparsity while exploiting asymmetry.

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MS23

Computing a Nice Basis: Matroids and Matchings

The nice basis problem is that of computing a basis for the column space of an underdetermined matrix from among its columns, with the basis required to satisfy some optimality property. A desirable property is that it should be easy to solve multiple linear systems of equations with the chosen basis. This problem arises in constrained nonlinear optimization, modeling slide surface constraints in structural analysis, and in circuit and device simulations. We show that many variants of this problem can be solved exactly using the combinatorial tools of matroids and matchings. The matroid greedy algorithm gives exact solutions to these problems, and matchings enable extremely fast computation of approximate solutions guaranteed to be at least half as good as the optimal solutions. We have also designed and implemented hueristic algorithms for problems that do not fall into the matroid framework. Our preliminary results indicate that many problems have block diagonal bases with small average block size. We will report more extensive computational results on several variants of the basis problem.

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MS24

Spectral Element Methods for the Shallow Water Equations

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MS24

High Resolution Algorithms for Fluid Mixing

We present a combined front tracking and AMR algorithm based on a merger of the front tracking code FronTier and the AMR code Overature. Simulations of the breakup of a diesel jet into spray will be presented, based on this algorithm. Comparison with experimental data from Argonne will be given. Other mixing simulation studies will be presented; tracked and untracked simulations will be contgrasted and compared to experiments for 3D Rayleigh-Taylor unstable flows.

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MS24

Solving Elliptic PDEs on Overlapping Grids with Multigrid

We describe a method for automatically generating the coarse grids and coarse grid equations for the multigrid algorithm when solving boundary value problems on composite overlapping grids. By relaxing the requirements for interpolation between component grids, and allowing the grids to grow larger as they are coarsened, very coarse grids can be generated. A Galerkin averaging procedure is used to generate the coarse grid discretization of the partial differential equation given the discretization on the finest grid. An adaptive smoothing algorithm is used to keep the residuals on the different component grids about the same size, significantly improving the convergence rates. The combination of these ideas results in an easy to use solver that hides the multigrid details from the application. Numerical results in two and three dimensions show that good multigrid convergence rates can be obtained.

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MS24

A Discontinuous Galerkin Method for Radiative Transfer

Pure isotropic scattering in a gray, spherical stellar atmosphere (Milne's problem) is analyzed via a discontinuous Galerkin method. Mesh and polynomial degree adaptivity is used to capture accurately the diffusive and streaming limits, and the transition region as well. By increasing the diameter of the atmosphere by three orders of magnitude an accurate approximation of the evolution of the singularities at the origin and at the outer boundary is obtained. The proposed method outperforms the discrete ordinate method.

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MS25

Enhancing Protein Secondary Structure Prediction by Sequence-to-Structure Alignments

Predicting protein secondary structures from the primary amino acid sequence facilitates greatly computational fold and function recognition. Secondary structure prediction methods have recently reached accuracy of about 80%. However, the existing methods that utilize neural networks and other pattern recognition protocols to capture evolutionary information included in sequence profiles do not account for effects due to "non-local" tertiary contacts. We present a novel method for secondary structure prediction, which combines Elman recurrent and other contextual type neural networks that account for "local" propensities with sequence-to-structure alignments to improve the accuracy of the method.

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MS25

Enumerating and Counting Protein Folds using Distance Information

We present a technique counting and enumerating folded proteins matching distance constraints. While the protein folding problem is computationally NP-hard, distance geometry techniques can efficiently retrieve protein structures when n(n-1)/2 distance constraints are given. In this paper, we rigorously prove that folded structures can be uniquely determined in linear time when only O(n) distance constraints are provided. We apply our result to membrane proteins. These findings drastically reduce the experimental effort required to compile distance information.

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MS58

Continuous Sensitivity Analysis for the Design of Control Systems

Feedback control for systems modeled by partial differential equations can be computationally challenging since standard techniques require solving the Riccati equation. Thus, if the discretization is $O(n)$, the Riccati solution requires finding $O(n^2)$ unknowns. A daunting task for large values of n. In this study, we consider the problem of designing these control systems. For example, we consider determining "optimal" locations for actuators and sensors. To make this problem tractable, we look at the (practical) special case of low dimensional control inputs ($m << n$) and outputs ($p << n$). For this case, we can assess the quality of each feedback control design by solving $(m+p)$ inputs ($m << n$) and outputs ($p << n$). For this case, we can assess the quality of each feedback control design by solving $(m+p)$ Chandrasekhar PDEs, each with an $O(n)$ discretization. To facilitate the use of a gradient-based optimization algorithm for locating the actuators and sensors, we develop continuous sensitivity equations for the Chandrasekhar PDEs. As we shall show, sensitivity information itself gives information about where actuators and sensors should be located, independent of their use in an optimization algorithm.

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MS58

Sensitivity Analysis for Scientific Simulations: Software and Applications

Numerical simulations are used widely in the solution and analysis of large-scale physical systems. We will describe the sensitivity analysis capabilities of our solvers for problems that can be modeled as ordinary differential equations (ODEs). In particular, we discuss the use of sensitivity computations for model evaluation and uncertainty quantification for radiation transport problems.

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MS58

Aero-structural Optimization of Aircraft Configurations Using Coupled Adjoint Sensitivity Analysis

An adjoint method for sensitivity analysis within an aero-structural aircraft design framework is presented. The aero-structural analysis uses high-fidelity models of both the aerodynamics and the structure. The aero-structural sensitivities are computed using a coupled-adjoint approach that is based on previously developed single discipline sensitivity analysis. Alternative strategies for coupled sensitivity analysis are also discussed. The aircraft geometry and a structure of fixed topology are parameterized using a large number of design variables. The aero-structural sensitivities of aerodynamic and structural functions with respect to these design variables are computed and compared with results given by the complex-step derivative approximation. The coupled-adjoint procedure is shown to yield very accurate sensitivities and to be computationally efficient, making high-fidelity aero-structural design feasible for problems with thousands of design variables.

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MS58

Adjoint Sensitivity and Optimal Control for Flow with Discontinuities

Optimal control strategies for the shock tube problem are investigated and aimed at relocating discontinuities at desired locations. The subgradients and gradients of the cost functional, obtained from the adjoint of the discrete forward model, are employed for carrying out nonsmooth/smooth minimization. Discontinuity detection improves results by removing points where shocks occur from the cost functional and its gradient. The control variables are the initial conditions for pressure and density. The numerical solution of optimal control problem matches very well the observations and satisfies the entropy condition characteristic of the true physical solution.

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MS59

Challenges in Software Development for Multi-Physics Simulation

Techniques for faster and more reliable development of multi-physics simulation software are discussed. This includes object-oriented programming and high-level scripting. Particular attention is paid to the interplay between modular software components and methods for verifying the implementations. An integral part of the verification is empirical assessment of the accuracy of the computations, and methods for measuring accuracy and using the results in a scientific approach to debugging are also presented.

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MS59

A PSE for Modeling Transport Phenomena in Porous Medium Systems

Modeling of fluid flow and contaminant transport and re-

actions in multiphase porous medium systems is a class of scientific application characterized by relatively high complexity, a large and evolving set of possible model formulations, and a need for sophisticated algorithms and numerical approximation techniques. This set of circumstances leads to a significant computational science challenge. We report on initial efforts to develop a problem solving environment for this class of problem, focusing on a high-level, mathematical interface, parsing of instances of this interface, and generation of simulation models that link to state-of-the-art and legacy numerical libraries to produce complete simulators. Our examples include models to simulate multispecies, nonlinear, interphase mass transfer and reactions in porous medium systems.

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MS59

A GIS-Based Tool for Performing Automated Groundwater Flow and Transport Calculations

Predictions of contaminant transport in porous media typically involve the interplay of several models, including representation of the contaminant source term, the vadose zone, the underlying aquifer, and a receptor such as a water supply well. All of these models are to some extent uncertain, making the quantification of the overall uncertainty in the prediction just as important as the mean or nominal case. Quantification of uncertainties for such a model is typically performed using a Monte Carlo approach, which is a computationally demanding task requiring automation of the calculation. To address this challenge, a problem solving environment (PSE) has been developed that employs a GIS software system to carry out the calculations and visualize the results. The GIS model serves as an interface to the underlying flow and transport simulations, allowing a hydrogeologic model, a model for the surface infiltration, and the vadose zone flow and transport simulations to be accessed quickly and automatically. Parameters distributions can be queried and values assigned for each realization of the simulation. In this study, we present this PSE, demonstrate its use, and discuss improvements that could further enhance its utility and accessibility.

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MS59

Mathematical and Computational Modeling of Multiphysics Couplings

Multiphysics couplings can happen in different ways. One may have different physical processes (e.g. flow, transport, reactions) occurring within the same physical domain, or one may have different physical regimes (e.g., surface/subsurface environments, fluid/structure interactions) interacting through interfaces. We will discuss both of these types of multiphysics couplings during this presentation. Of particular interest will be the development of interpolation/projection algorithms for projecting physical quantities from one space/time grid to another, and the investigation of mortar and mortar-free methods for coupling multiple physical domains.

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MS60

A Geometry-Based Automated Simulation Toolkit

One of the biggest issues in dealing with CAD data is errors that are introduced by translating that data from one representation to another. A general, automatic solution to this problem does not exist today as evidenced by the large ongoing efforts by CAD companies and others to solve this in the context of CAD to CAD translation. In the context of mesh generation, this translation issue is the source of dirty geometry . By directly interfacing with the CAD kernel it is possible to totally eliminate the dirty geometry problem. Unfortunately this leads to the problem of clean geometry that we don t really like such as small model features that exist to ensure that the CAD model is closed and clean. However this is a much easier problem to solve. By using a unified topology model approach and procedures to eliminate small model features that do not require modifying the underlying CAD model, Simmetrix has developed uniquely robust automatic meshing tools that interface with the majority of CAD kernels on the market.

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MS60

Rapsodi: Geometry Preparation and Grid Generation

We discuss our approach to grid generation on complex geometries and our implementation in the application code **rap**, which is part of the **Overture** library. While some simple geometries can be made from scratch inside **rap**, most complicated geometries must be imported using a neutral file format. This approach removes the reliance on commercial geometry kernels and potentially also reduces the memory requirement of the code. Presently, we work with IGES files for importing the geometry, which often contain errors that must be rectified before any grid

generation can take place. Examples of common error are trimming curves that do not form loops and missing or duplicated surface patches. For this reason, a number of repair methods have been implemented in **rap**, mostly to rectify trimming curve problems, but also for making new surface patches. Another challenge with IGES files is that they usually do not contain topological information. We have therefore implemented an edge matching algorithm (following the ideas of Steinbrenner, et al.) to pair up each surface edge with a neighboring edge. Once the topology is established, the surface can be triangulated. Grid points are first distributed along edge curves, after which each surface patch is triangulated using a Delauney technique in parameter space. Since the grid points coincide along all edges, the union of all sub-triangulations provides a water tight surface triangulation of the entire model. The surface triangulation is used for two purposes. First, to provide good initial guesses when points are projected during the construction of overlapping surface grids. More recently, the triangulation have also been used to cut embedded boundary grids. In the latter case, the surface triangulation must be refined/improved so that the deviation of each edge from the curved surface is less than a prescribed tolerance.

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MS60

Automatic Generation of Simulation Models from Design-Based Feature Models

The effective use of advanced simulation technologies in engineering design requires the ability for design engineers to have the needed simulation models automatically generated from the CAD data they work with. In more advanced design systems, this means going directly from feature-based representations to properly defined geometric discretizations of the domain in terms of meshes of topologically simple entities. This presentation overviews key technical aspects of developing generalized functional interfaces between CAD systems and fully automatic mesh generators.

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MS60

Cad Interfaces: Why Simple Wrappers Aren't Enough

Several efforts to define and implement CAD-neutral geometry APIs vary in the correspondence between the underlying geometric model and that presented to applications. For true portability, the interfaces must present a consistent model no matter what the underlying modeler. This presentation will describe some of the "extra" functionality needed in these interfaces, including filling out the set of topological entities in the model, shared interface detection and representation, and alternative query and modify functionality.

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MS61

Studying the Alpha Pathway in Yeast with Moleculizer

A difficulty common to both stochastic simulation of biochemical reaction networks, as well as most simulation by ordinary differential equations, is the sheer size of reaction networks that are encountered when protein species, along with their modified forms, can associate into complexes. Combinatorics puts generation and maintenance of such reaction networks beyond "hand work" and forces a regime of automatic extrapolation. Moleculizer is a traditional stochastic simulator extended to extrapolate biochemical reaction networks from a specification of the "indivisible" proteins and the kinetics of their pairwise bindings. Reactions are generated when the species that they depend on are created by other reactions, and the network expands as the simulation progresses. Reaction networks generated by Moleculizer for parts of the yeast mating signal transduction pathway involve tens of thousands of species and hundreds of thousands of reactions.

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MS61

Application of Continuum, Unstructured Finite Element Numerical Methods to Spatial Models of Intracellular Calcium Dynamics

Biological cellular systems utilize calcium concentration changes for various signalling mechanisms. These changes can vary over several orders of magnitude, and simulations of these calcium dynamics provides numerically challenging problems with multiple time and spatial scales in addition to these concentration variations. I will present results of application of finite-element methods to several examples of reaction-diffusion, intracellular calcium dynamics models.

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MS61

Mesh Generation and Modeling of Biological Systems Using Cubit

In this talk, we will present techniques and research for modeling and generating meshes on biological systems using the CUBIT Mesh Generation Toolkit. Current and fu-

ture research activities within the CUBIT framework will also be discussed.

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MS61

The Impact of Spatial Realism on Microphysiological Models

Using Monte Carlo algorithms, we have simulated cellular signaling in spatially realistic models, and compared the predicted variance to that of matching stochastic Markov chain simulations (identical time evolution of reaction intermediates). The results can differ dramatically, and depend strongly on the spatial model architecture. Thus, spatially realistic models may be required to correctly predict the variability of complex cellular processes, and to assess their propensity to switch between different operating modes and/or to fail.

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MS62

Flow Prediction for Complex Centrifugal Blood Pumps

The development of implantable ventricular assist devices, in the form of continuous-flow axial and centrifugal pumps, offers hope for many patients waiting for donor hearts. The design challenges can be itemized as high levels of shear, thrombus formation, and loss of pump efficiency. Elevated shear stress levels are particularly evident in mechanical biomedical devices, and are known to cause hemolysis. Computational modeling is now aiding the design of blood pumps being developed at the Baylor College of Medicine. We will report on three-dimensional unsteady simulations of blood flow in a detailed pump model, and discuss blood damage indicators.

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MS62

Challenges in Realistic Modeling of Hemodynamics from Medical Images

In this paper we identify and discuss several of the challenges that still exist for realistic modeling of arterial hemodynamics from medical images. Among these, we consider: importance of non-Newtoinan effects, problems with modeling vessel wall compliance, temporal and spatial resolution requirements, specification of physiologic boundary conditions, and validation of the computational models. Several examples are presented to illustrate various aspects and limitations of the methodology. We include: flows in carotid arteries, renal arteries and the circle of Willis. We conclude that despite several limitations, the methodology is mature enough for clinical applications involving diagnosis and treatment plannig.

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MS62

The Use of Numerical Methods for the Development and Optimization of Cardiovascular Artificial Organs

The use of computational fluid dynamics (CFD) methods is beginning to significantly impact the development and optimization of cardiovascular artificial organs such as cardiac assist devices and heart valve prostheses. Since the flow conditions in the artificial organs are very complex (3-dimensional, transient/pulsatile and partly turbulent) the requirements for numerical simulation are very high as well. The development of cardiovascular artificial organs needs to focus on flow phenomena such as flow separations and stagnant flow. These phenomena are crucial for thrombus generation, which are defined by Virchow's triad - the interaction between blood, flow and wall. Furthermore, shear induced blood damage should be integrally combined with traditional hydrodynamic design parameters. The Biofluidmechanics laboratory, Humboldt University Berlin has

extensively used CFD as the primary tool to analyze and design of various novel heart valves developed for use in ventricular assist devices.

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MS62

Microstructural Simulation of Blood Flow on Parallel Computers

The advent of multi-teraflop computers enables us to contemplate, for the first time, large-scale microstructurally-based simulations of blood flow. Such simulations, which resolve individual cell deformations and their interaction with surrounding plasma, are necessary to better understand blood damage and to develop more rational macroscopic blood models. This talk will summarize our efforts in developing the geometric algorithms and numerical models necessary for simulating complex flows on large parallel systems.

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MS63

Achieving Conservation Properties for Adaptive Semi-Lagrangian Advection Schemes

Semi-Lagrangian advection feature several desired properties, like inherent parallel structure, unconditional stability, high order, etc. However, without substantial modifications, semi-Lagranian schemes are not conservative. To achieve mass, or energy conservation, we propose several strategies for semi-Lagrangian algorithms, suitable for adaptive mesh refinement. These algorithms are differently computationally intense. The most expensive scheme is conservative up to machine precision, while other, less demanding schemes achieve only conservation up to the order of discretization. We demonstrate the effectiveness of several algorithms by simple test cases with converging and diverging wind fields.

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MS63

Spectral Element Semi-Lagrangian Methods for Numerical Weather Prediction

Semi-Lagrangian methods have been quite popular in atmospheric modeling. However, until recently only spectral transform methods had been used in this discipline mainly due to their high-order accuracy. The problem with this approach is that the combination of semi-Lagrangian with spectral transform severely diminished the order of accuracy of the method because only cubic interpolation was used for the former. By combining the spectral element with the semi-Lagrangian method (SESL) we have devised a method which is high-order accurate (to any order imaginable), stable at very large time-steps (due to the Lagrangian formulation), and directly applicable on unstructured fine-scale grids (by virtue of the geometric flexibility of spectral elements). In this talk we show the power of SESL by applying it to the shallow water equations on the sphere and the full 3D atmospheric equations. In addition, we discuss why SESL is ideally suited for modeling transport processes in the atmosphere.

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MS63

Efficient Conservative Semi-Lagrangian Schemes over the Sphere

A computationally efficient mass-conservative semi-Lagrangian advection scheme over the sphere is proposed. The scheme combines a conservative finite-volume based method with an efficient semi-Lagrangian scheme in a dimension-splitting cascade interpolation framework. A regular latitude-longitude grid is used on the sphere, however, for computational purpose, this grid is transformed into an area-preserving orthogonal Cartesian grid. In the regions near the poles where the upstream Lagrangian cells are not well-defined, a globally conservative but locally approximate method is employed. The resulting conservative cascade scheme (CCS) is applicable for the cases where the polar Courant number C_t less than or equal to one. The CCS is further extended for more general application where $C_t > 1$. In such cases, a cell-integrated semi-Lagrangian scheme (CISL) is used on the polar regions where cascade schemes breaks down, and elsewhere on the sphere CCS is used. The scheme (2D) is evaluated using a standard solid-body rotation test and a deformational flow test. Compared to the traditional semi-Lagrangian scheme combined with bicubic-Lagrange interpolation, the present scheme is significantly more accurate and efficient while conserving mass exactly.

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MS63

Semi-Lagrangian Method for Turbulence Simulation

We present a parallel semi-lagrangian method for the channel geometry. Stable schemes of second-order accuracy in time and spectral accuracy in space are adopted. We employ a spectral element expansion in the wall-normal direction and Fourier expansion in the two homegeneous directions. Local interpolation procedures are implemented for computing the departure points, improving a previous implementation which used all the Fourier modes in the homogeneous directions. High parallel efficiency is achieved by overlapping the communications with useful computations. The convergence behavior of the method with re-

spect to the spatial and temporal refinements is investigated. We also present a direct numerical simulation of a turbulent channel flow with this method and compare against timings with the Eulerian approach.

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MS64

The Seasonal Variation of Geostrophic Velocity and Heat Flux at the Entrance to the Gulf of California, Mexico

Geostrophic velocities and heat fluxes were computed from CTD data collected on nine cruises conducted at the entrance to the Gulf of California since 1992. During winter and spring (exception of February '94) most of the baroclinic outflow is found near Baja California, with a mean core 45 km wide extending beyond 700 dbar in depth (1400 in May '98). The baroclinic inflow is found either through the center of the section and/or through the Sinaloa coast. Summer and fall show a rather complex pattern with alternating cores of positive (in) and negative (out) velocities, but with an inflow along Sinaloa in all cruises. The maximum outflow velocities are found in spring (May '98; 0.6-0.7 m/s) with velocities of 0.2 m/s reaching 800 dbar. Inflow and outflow velocities of 0.1 m/s were observed up to 1400 dbar. The mean geostrophic field reveals a cyclonic circulation, the incoming flux along the Sinaloa coast and outgoing along Baja California. Smaller scale, opposite flows are found at the center of this cyclonic circulation associated to the Alarcon Seamount. The EOF geostrophic first mode accounts for 37% of the total variance, exhibiting a strong seasonal signal, with the maximum amplitude in May and the minimum in September. This mode is related to a maximum flow towards the Gulf occurring during May at the center of the section. Also, the first mode amplitude resembles an annual variation with heat being exported through the entrance during winter and spring (except in Feb'94) and imported during summer and fall (except to Nov'97). The main heat outflow occurs near BC during Feb'99, May'92 and 98, Nov'97 and Dec'92, with maximum in spring (May). A seasonal function was fitted to the net heat flux data which explained 97% of the observed variance. The maximum heat gain (38 TW) occurs around May 30 while heat loss (76 TW) in November 16. This considerable amount of heat, added to or subtracted from the Pacific coastal waters, must force some movements at annual and semi-annual scales.

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MS64

Three-dimensional Visualization of the Density Field at the Entrance to the Gulf of California

The density structure around the Seamount Alarcn is numerically simulated with a high-resolution three-dimensional curvilinear ocean model. The flow is assumed to be uniform and linearly stratified. Visualizations are made for the time evolution of the density surfaces for various cases of stratification.

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MS64

Upper-ocean Circulation Patterns in the Northern Gulf of California Expressed in ERS-2 Synthetic Aperture Radar Imagery

ABSTRACT ERS-2 SAR frames were collected over the Northern Gulf of California during the winter 1999. The frames, presented here as a single composite image (100 by 300 km), expresses a meso-scale meander or eddy-like feature of approximately 80km wide located close to the Peninsula of Baja California. The eddy is expressed as bright, concentric bands that curve in an anticyclonic sense. The location and dimensions of the eddy are in very good agreement with the winter circulation of the Northern Gulf of California described by Lavn et al., (1997), from the analysis of direct observations using satellite-tracked drifters and hydrografic surveys. The SAR image also depicts other smaller, cyclonic eddy-like features, located close to the mainland, which we hypothesize are associated to the general circulation induced by the anticyclonic eddy. We conclude that SAR images, together with the reduced number of insitu observations, can provide valuable, and new, information about the meso-scale circulation of the upper ocean in the Gulf of California, even when cloud cover prevents the use of other remote sensors, such as infrared radiometers and visible imaging systems.

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MS64

Stratified Flow Over Three-dimensional Submarine Topography

We present a complete 3-dimensional curvilinear fluid flow model in boundary-fitted grids. The model solves the primitive non-linear Navier-Stokes equations under the Boussinesq approximation. Three-dimensional simulations are made for a stratified flow over a bell-shaped mountain. The results for the velocity and density fields are presented and discussed.

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MS65

Surrogate-based Optimization Under Uncertainty: Status and Directions

In this paper, formulations for optimization under uncertainty employing surrogate models are investigated. A surrogate model may appear at the optimization level, at the uncertainty quantification level, or both, and may involve either data fit or hierarchical surrogates. Of critical interest is the extension of algorithmic techniques for rigorous, provably-convergent surrogate-based optimization to these surrogate-based optimization under uncertainty formulations. Key components to be discussed include the consistency and verification requirements of provable-convergence theory. Whereas a predicted optimum from an approximate optimization cycle can be readily verified for deterministic optimization, the corresponding procedure for optimization under uncertainty involves an adaptive procedure which seeks relative verification through non-overlapping confidence bounds. Preliminary computational results will be presented and alternative approaches will be surveyed.

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MS65

Non-intrusive Main Effects and Sensitivity Calculations for Uncertainty Quantification

Uncertainty quantification (UQ) has received a great deal of attention within the scientific and engineering community due to its potential use in validation of large multi-scale, multi-physics application codes. Two important aspects of this validation process involve experimental design and robust optimal design. In this talk, we will discuss techniques for experimental design that can be used to determine the most important model parameters in a simulation. This information can be used to focus on the subset of parameters that will yield the highest payoff in an experiment. We will also describe non-intrusive techniques for robust optimization that compute the sensitivity of a simulation to model paramters. This information is especially useful in determining robust optima in design problems.

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MS65

Strategies for Visualizing 2D Distribution Data

Visualization methods exist for handling scalar, vector, tensor, or multivariate fields. However, if the data is a distribution, the available options are quite limited. This is particularly true as the dimensionality of the data increases. This talk will present a number of approaches for visualizing 2D fields where the data at each point is a distribution. Distribution data is a rich form of representing uncertainty. These data sets may come about from sensitivity analyses, ensemble forecasts, conditional simulations, etc. It is also possible to have more than one distribution at each location e.g. one distribution for each field variable. In contrast, multivariate visualization techniques typically deal with a scalar value for each variable. Hence, the usual multivariate techniques are not applicable to such data sets.

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MS65

Nonstationary Excitation Data Condensation for Analytical Probabilistic Dynamic Response Analysis: An application using the 1999 Chi-Chi Earthquake Ground Motion Recordings

A method recently developed by the authors for the condensation and compact analytical description of measured nonstationary random processes into a particular form for probabilistic nonstationary dynamic response analysis is presented through a large-scale application. The application data-set is the measured ground-motion excitations from the 1999 Chi-Chi earthquake (Taiwan). The data condensation technique involves Karhunen Loeve spectral decomposition and orthogonal polynomial analytical approximation.

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MS66
AMLS in Practical Vibration Analysis

Automated Multilevel Substructuring (AMLS) has quickly become a standard tool for analyzing vibration throughout much of the international automobile industry. Although the first software implementation has been available for only about one year, the dimensions of finite element discretizations used and the frequency ranges addressed have grown substantially. We describe the industrial application of this method, technical issues that have surfaced and their resolution, and performance issues on various hardware platforms

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MS66
Scaling AMLS for 3D problems

Automated multilevel substructuring (AMLS) recursively subdivides a structure into numerous subdomain and interface eigenvalue problems. For two-dimensional problems, AMLS is efficient and accurate high into the frequency range because the interface problems grow slowly. Unfortunately, for three-dimensional problems, the efficiency of AMLS decreases because the size of the interfaces grow rapidly. My talk will study some modifications of the original method to preserve efficiency for three-dimensional problems.

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MS66
Introduction to AMLS

Our presentation will introduce AMLS as a recently introduced alternative for efficiently computing the eigenspace needed in modal analysis. AMLS first recursively divides the structure into numerous subdomains and interfaces. Then, approximations to the eigenspace are computed by solving eigenvalue problems on subdomain and interface eigenvalue problems produced by the substructuring.

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MS66
AMLS for Large-scale 3D Structural Dynamics

In this talk we will present preliminary results on serial/parallel AMLS(Automated MultiLevel Substructuring) in a massively parallel finite element code, Salinas. Of interest will be the performance of AMLS on 3D meshes, compared with its performance on shell problems. Accuracy at high frequencies will be addressed by comparing AMLS to a Lanzcos-based eigensolver.

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MS67
Numerical Techniques for Large Scale RBF Computations with Applications to Image Reconstruction and Geophysics

The energy minimisation characterisations of polyharmonic splines, and the invertibility of the corresponding interpolation/smoothing matrices under weak conditions on the geometry of the nodes, make radial basis functions an attractive tool for many large data fitting problems. Unfortunately, until recently, obstacles of computational cost and numerical conditioning stood in the way of the use of this tool. In this talk I will outline some of the numerical techniques that have overcome these difficulties.

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MS67
Domain Decomposition with Radial Basis Meshless Methods

Both overlapping and non-overlapping domain decomposition methods (DDMs) with matching and non-matching grids have been developed for the radial basis meshless methods (RBMMs). Numerical examples show that overlapping DDM with RBMMs can achieve much better accuracy with less nodal points compared to finite difference methods and finite element methods. Our results also show that non-matching grid DDM can achieve almost the same accuracy within almost the same iteration steps as the matching grid case, which makes our method very attractive, since it is much easier to generate non-matching grid by just putting blocks of grids together, where each block grid can be generated independently.

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MS67

Radial Basis Functions for Solving PDEs

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MS68

A Novel Finite Difference Time Domain (FDTD) Technique to Model Bi-anisotropic Media and Its Subclasses

This paper presents a novel FDTD (Finite-Difference-Time-Domain) technique for modeling electromagnetic wave interactions with bi-anisotropic media, which represent the most general linear media. The theoretical foundation for this method is based on a wavefield decomposition technique. This technique presents a very powerful tool to analyze electromagnetic wave interaction with novel media and to uncover many potential applications. Validations of this new model are demonstrated for the interaction of an electromagnetic wave propagating transversely through a uniaxial bi-anisotropic half-space.

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MS68

Real Time Computational Algorithms for Electromagnetic Interrogation of Structures

In the field of nondestructive evaluation, new and improved techniques are constantly being sought to facilitate the detection of hidden flaws in structures such as air foils. We use eddy current based nondestructive evaluation techniques and reduced order modeling to explore the feasibility of detecting such subsurface damages in a real-time setting. We implement this methodology using both simulated and experimental data. The methods prove to be robust as well as fast; our findings suggest a *significant* reduction in computational time.

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MS68

Maxwell-systems with Nonlinear Polarization

We consider a model describing the propagation of electromagnetic waves in the terahertz range through a nonlinear medium. The material properties are represented by a nonlinear polarization in the form of a convolution. We present theoretical and numerical results based on a variational framework for the problem.

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MS68

A Pressure-Dependent Polarization Model for Use in Electromagnetic Interrogation

Electromagnetic interrogation techniques have many useful applications, including foliage penetration, identification of underground objects, and noninvasive tumor detection. We consider a technique in which a traveling acoustic wave acts as a virtual interface for an oncoming electromagnetic wave. We suggest that the interaction between the electromagnetic wave and the acoustic wave can be described using a pressure-dependent model for electric polarization. We present both theoretical and computational results.

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MS69

Algorithm for PDE Applications on the Grid

The purpose of this talk is to introduce the problem of designing efficient numerical algorithm for the grid and present some of the mathematical tools that might be used depending on the problem. We will present various techniques to relax communication constraints on solver for PDEs such as a posteriori stabilization of explicit time stepping terms via filtering, or extrapolation methods. Main applications will be in CFD.

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MS69

Metacomputing Application in a Grid Environment

Metacomputing applications have been one of the driving forces in GRID computing many years ago. While the focus of the GRID has changed over time, these applications are still out there looking for the combined performance of distributed supercomputers. The talk will present some of these applications. We will elaborate on the characteristics of the codes and will present some results. Emphasis will be given to the role of optimized algorithms for metacomputing.

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MS69
Scalable Domain Decomposition Methods on the GRID

The purpose of this talk is to introduce the problem of designing efficient numerical algorithm for the grid and present some of the mathematical tools that might be used depending on the problem. We will present various techniques to relax communication constraints on solver for PDEs such as a posteriori stabilization of explicit time stepping terms via filtering, or extrapolation methods. Main applications will be in CFD.

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MS69
Teraflop Computational Materials Science

The LSMS method is an order-N approach best suited to calculating the electronic and magnetic structure of disordered alloys. It was the world's first application code to achieve sustained teraflop performance (1998); its current record is 4.6 teraflops. We show how it has been designed from first physical principles to achieve maximum locality and scalability to thousands of processors even when latencies are high.

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MS70
Parallel Preconditioned Newton-Krylov Methods for Inverse Wave Propagation

We study the performance of a parallel preconditioned Newton-Krylov method for inverse problems governed by wave propagation. The goal is to determine material coefficients of a heterogeneous medium, given a source and waveform observations at receiver locations on its boundary. Multiscale continuation and total variation regularization are employed to treat multiple local minima and layered media, respectively. Scalability results for up to 256^3 grids on up to 2048 processors of the PSC Terascale Computing System are presented.

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MS70
An All at Once Method for Time Domain Maxwell's Equations

We develop an inversion methodology for 3D electromagnetic data when the forward model consists of Maxwell's equations in which the permeability is constant but electrical conductivity can be highly discontinuous. The goal of the inversion is to recover the conductivity given measurements of the electric and/or magnetic fields in time. A standard Tichonov regularization is incorporated and we use an inexact, all-at-once methodology solving the forward problem and the inverse problem simultaneously in one iterative process. This approach allows development of highly efficient algorithms. Here we present the basic methodology for the all-at-once approach in the time domain. We then briefly review the time domain forward modeling equations, develop the linearized system of equations to be solved at each iteration, and show how these equations can be solved using a preconditioned QMR method.

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MS70
An Object Oriented Approach to Image Restoration in MATLAB

Image restoration is the process of minimizing or removing degradations from an observed image, which may be distorted by such things as blurring and noise. The mathematical and computational problem is a classical example of an ill-posed problem. Many algorithms have been developed for ill-posed problems, but they may differ in a variety of ways. For example, there are several different regularization methods one could use, and for each of these, various different methods for choosing a regularization parameter. There are direct and iterative methods, and still other schemes enforce nonnegativity or other bound constraints on the computed solution. For image restoration, as is the case for most ill-posed problems, the approach that produces the "best" computed solution is problem dependent. Another important issue that must be considered before attempting to restore an image is the determination of the blurring operator. In particular, the blur can be spatially invariant, spatially variant, and/or separable. The type of blur dictates the structure of the coefficient matrix, and often determines whether it is feasible to use a direct method, or whether an iterative method is more appropriate. All of these decisions require that we have a complex set of computational methods at our disposal, each likely having different input parameters and calling sequences. Even if we use a high level computing environment such as Matlab, research on such problems can be very time consuming. In

this talk we describe a set of Matlab tools that simplify this process, and which allow for easy adaptation of new problems and/or new methods. This is joint work with Katrina Palmer Lee and Lisa Perrone.

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MS70
Computational Methods for Adaptive Optics

Adaptive optics (AO) refers to the correction of wavefront, or phase, distortions due to atmospheric turbulence using deformable mirrors. An extension of AO called multi-conjugate adaptive optics (MCAO) requires the estimation of the "volume atmospheric turbulence profile" (3-dimensional index of refraction) from observations of "guide stars" (point sources) in various directions. In this talk we will discuss layer-oriented multigrid algorithms to solve this estimation problem. test

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MS71
Elements of Computational Science Education and Degree Programs

Education in computational science and education (CSE) has evolved through a number of stages, from recognition in the early 1980s to its present early growth. Now a number of courses and degree programs are being designed and implemented and students are beginning to receive degrees. This talk will discuss various aspects of this development, including impact on faculty and students, the intellectual content of CSE education, and comparisons of course requirements for programs in computational science, computer science, physics, and computational physics.

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MS71
Lessons from the National Computational Science Institute: Quantitative Reasoning Across the Curriculum

The National Computational Science Institute (www.computationalscience.net/) seeks to provide undergraduate faculty at small-to-medium sized schools an opportunity to explore new learning and teaching modes based on interactive explorations enabled by mathematical modeling and computational science tools in an undergraduate setting. This talk will discuss what has been learned during the first year's activities.

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MS71
Internships for Undergraduates in Computational Science

Internships can expose students to many new ideas, techniques, and applications that can greatly enhance their knowledge of computational science and make their classroom education more meaningful. Realizing the importance of such experiences, Wofford College's undergraduate Emphasis in Computational Science (www.wofford.edu/ecs) requires a summer internship. However, obtaining meaningful internships can be challenging. Committed to computational science education, the Krell Institute offers a website on internships (www.krellinst.org/ucse/internships.html) that provides valuable advice and links to other resources.

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MS71
An Assessment of Undergraduate Computational Science and Engineering Education

This presentation will first discuss the latest update to a survey of computational science education programs that Chuck Swanson has been maintaining since 1992 when he was in the University Marketing department of Cray Research, Inc. Then we will consider workforce requirements for undergraduates with computational science and engineering experience. This is related to the Department of Energy's Computational Science Graduate Fellowship Program that is designed to supply the DOE laboratories with qualified computational scientists.

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MS72
Adaptivity and Error Estimation for Inverse Problems Involving PDEs

Inverse problems (just as optimization problems) involving partial differential equations are computionally very demanding, especially if the parameters to be estimated are distributed functions. We present finite element methods that try to reduce the numerical effort as much as possible by choosing the computational mesh adaptively,

basing the refinement strategy on error estimates for the discretization. In particular, the meshes for state and adjoint variable will be chosen differently from those for the distributed variable to be identified.

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MS72

Robust Spectral Element Methods for Convection-Dominated Flows

High-order discretizations yield excellent transport properties and are well suited to modern cache-based computer architectures which favor data reuse. However, they are frequently unstable in underresolved situations and consequently often lack the robustness required of complex flows. We examine sources of these instabilities and provide practical remediies for simulation of transitional flows in complex geometries. Applications include biofluids and reactor core cooling.

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MS72

High-order Adaptive Discontinuous Galerkin Methods for Hyperbolic Systems

We describe several aspects of the discontinuous Galerkin method for solving hyperboic conservation laws including basis construction, flux limiting, local time stepping, data structures, parallel strategies, and a posteriori error estimation. Software for using this method is embedded into a general-pupose framework for solving partial differential equations and we illustrate its capabilities on several two- and three-dimensional compressible flow problems.

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MS72

Discontinuous Galerkin Methods for Modeling Biot's Consolidation Problem

Center for Subsurface Modeling at Texas Institute for Computational and Applied Mathematics, The University of Texas at Austin In this presentation, we describe the application of Discontinuous Galerkin methods for modeling a coupled system of equations known as Biot's model for consolidation of saturated porous media. Both theoretical and computational results will be presented.

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MS73

Separated Representations and Multiresolution Algorithms in Multiple Dimensions

In an ordinary representation, the cost of linear algebra operations, such as matrix-matrix or matrix-vector multiplications, increases exponentially with the underlying physical dimension. We have developed separated representations, a numerical generalization of separation of variables, to overcome this problem. We present relevant analytic results, briefly discuss applications, and illustrate our approach with several examples of separated multiresolution representations. For a number of physically significant operators, we generate separated representations using generalized Gaussian quaratures.

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MS73

Adaptive Multiresolution Solvers for a Class of Advection-Diffusion Equations

We use the separated multiresolution representations of operators to construct adaptive schemes for solving non-linear advection-diffusion equations with variable coefficients in two and three dimensions. Separated representation of operators is a numerical analogue of separation of variables which allows us to maintain efficiency in higher dimensions. We use multiwavelet bases and exponential operators as a tool to numerically solve these equations in the integral (semigroup) formulation.

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MS73

Efficient Representation of the Projector on Diver-

gence Free Functions

Divergence free vector fields are important in solving problems involving incompressible fluids as well as electric and magnetic fields in magneto-hydrodynamics. We derive an efficient construction using a multiwavelet representation of the projection operator on divergence-free functions in 3-D for arbitrary but finite precision accuracy. This representation is used to solve the Stokes equation as well as the Navier-Stokes equation.

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MS73

Multiresolution Quantum Chemistry

We describe our use of multiresolution analysis and multiwavelet bases to solve the 3-D density functional and Hartree-Fock models for general all-electron polyatomic atoms. Distinguishing features of this work include the use of an integral operator formulation of the DFT equations, and the use of separated forms for the kernel of integral operators (Poisson and bound-state Helmholtz). This solution scheme and the multiwavelet basis provide significant advantages over conventional atom-centered Gaussian basis sets.

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MS74

Quantum Perceptrons

There are several possible definitions for a quantum perceptron. We give a definition in which the "weights" as well as the inputs are quantum states, and the transformation from input to output is unitary. We investigate possible transformations, and also possible learning algorithms. Our completely unitary perceptron has two advantages: First, since the evolution is unitary, we have the possibility of interference within a Hilbert space with a tensor product structure, and hence can achieve behavior superior to classical perceptrons. Second, we can connect our perceptrons together into a quantum network.

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MS74

Control by Quantum Perceptrons

We consider situations in which a quantum perceptron learns by feedback from a second (teacher) quantum perceptron. This can equivalently be understood as a problem of quantum control, of one quantum system by another.

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MS74

Learning Problems Between Unstructured Search and Majority

Many of the oracle problems which have been studied in connection with quantum computation fall into the category of learning problems. Servedio and Gortler proved lower bounds on the number of quantum queries necessary to solve a quantum learning problem. In this talk, (joint work with D. Meyer), we state several conjectures which give upper bounds for the number of quantum queries required to solve any quantum learning problem. We analyze several examples of learning problems, in each case giving algorithms which satisfy our conjectures.

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MS74

Semi-Classical and Quantum Entangled Neural Networks

We construct small quantum neural networks with the nodes having more than two possible eigenstates, i.e., with multiqubits generalizing the $|0>, |1>$ two-state qubits. We then investigate analytically and by simulation the effect of different methods of internode connectivities, and also of a background control field.

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MS75

Nonlinear Aeroelasticity: Finite Element Formula-

tions and Parallel Solution Algorithms

Aeroelasticity is the study of the mutual interactions between aerodynamic, inertial and elastic forces on flexible structures, such as aircraft. The aerodynamic forces induced by the flow on an aircraft depend on the geometric configuration of the structure. On the other hand, the aerodynamic forces cause elastic deformations and displacements of the structure. Accurate prediction of aeroelastic phenomena such as static divergence and flutter is essential to the design and control of high performing and safe aircraft. This paper highlights some technical features of an analysis methodology being developed for nonlinear computational aeroelasticity. Finite element formulations for fluids, structures and mesh motion are presented. Several Fluid-Structure coupling algorithms are presented and analyzed. We particularly show a novel algorithm to tighten the coupling between all fields, which is based on a nonlinear version of GMRES. Implementation issues with some emphasis on distributed computing strategies are also discussed. The algorithms shown can be useful also to solve free surface flow problems. Numerical tests are finally shown to assess the efficiency of the methodology and the algorithms proposed.

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MS75

An Embedded Boundary Integral Solver for the Incompressible Navier Stokes with Moving Boundaries

We present a new method for the solution of the unsteady incompressible Navier-Stokes equations. Our goal is to achieve a robust and scalable methodology for two and three dimensional incompressible flows with moving boundaries. The spacial discretization of the Navier-Stokes operator is done using boundary integrals and structured-grid finite elements whereas the temporal discretization with a two step scheme. The convective term is discretized via a semi-Lagrangian formulation which not only results in a spatial constant-coefficient (modified) Stokes operator, but in addition is unconditionally stable. The Stokes operator is inverted by a double-layer boundary integral formulation. Domain integrals are computed via finite elements with appropriate forcing singularities to account for the irregular geometry. We use a velocity-pressure formulation which we discretize with bilinear elements (Q1-Q1), which give equal order interpolation for the velocities and pressures. Stabilization is used to circumvent the div-stability condition for the pressure space. The integral equations are discretized by Nyström's method. For the specific approximation choices the method is second order accurate. Our code is built on top of PETSc, an MPI based parallel linear algebra library. We will present numerical results and discuss the performance and scalability of the method.

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MS75

A Free Surface Updating Methodology for Marker-Function Based Eulerian Free Surface Capturing Techniques on Unstructured Triangular Meshes

The numerical modeling of industrial non-miscible free surface flows using a marker-variable based interface capturing strategy is popular in the computational science literature. Unfortunately, the price to pay for the simplicity of this approach is its limited accuracy. As the marker-function is advected, the region of transition of the marker gets deformed. A numerical methodology is proposed to help conserve mass, using a local least-squares based strategy. We are particularly interested in free surface flow simulations on highly adapted meshes, using the finite element method. Verification problems will be studied in order to assess the accuracy of the methodology for various free surface flows.

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MS75

Error Distribution Models for Strong Shock Interactions

John W. Grove and Yunghee Kang Computer and Computational Science Division Methods for Advanced Scientific Simulations Group Los Alamos National Laboratory A key problem in developing methods to quantify uncertainty in a numerical simulation is to understand the dynamic propagation and generation of solution error in a complex flow. For a given numerical method, the solution error for a specific realization can be regarded as the solution to a model equation obtained by the addition of the appropriate higher order diffusion and dispersion terms to the original set of PDE's being solved numerically. Since this model equation depends on the specific numerical method as well as the basic physical flow equations the utility of this abstract approach is limited in real problems, especially for complex nonlinear systems and complex numerical methods. In this talk we will discuss an alternative approach that attempts to build empirical models for error generation based on a stochastic analysis of wave interactions. For simplicity we will focus our attention on describing the probability distribution of error generated due to the interaction of two shock waves. The basic method is an extension to stochastic flows of the fundamental random choice numerical method. Briefly we seek to determine the probability distribution for solution error as a function of the probability distribution for the Riemann problem data. We model this error using a linear super-position of a deterministic component and a random component, where by deterministic we mean a pdf that is a deterministic function of the pdf of the data. The random component is then a function of the numerical method and is modeled as an independent Gaussian. This talk will describe the basic approach for performing the stochastic analysis, the evaluation of

specified fitting forms for the deterministic component of the solution error, and estimations of the variance of the random, numerical method dependent, component of the solution error.

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MS76
Discrete Element Simulation of Gas-Particle Flows

The dynamics of bubbles, the flow of gas and solids through the emulsion phase, and interchange of flowing gas between these two phases plays a dominant role in heat transfer, mass transfer and solid-catalyzed chemical reactions. This research is aimed at understanding the aspects of bed hydrodynamics, especially to investigate the effects of granular temperature and associated stresses on the gas flow patterns inside the bubbles, which play a crucial role in promoting gas-solid contacting. It was inferred through our recent investigations that the inter-particle friction also plays a critical role in determining the solid's resistance to the fluidizing gas. If the inter-particle friction is neglected or assumed to be negligibly small then one would expect an unrealistically elongated bubble because the solid's phase does not offer any resistance to the fluidizing gas. In the experiments and the Distinct Element Method (DEM) calculations, it is observed that the voidage on the lateral sides of the bubble and slightly above the bubble roof is smaller than the minimum fluidization voidage. In the present paper, we will incorporate the correlations for the particle pressure and associated stresses obtained from DEM in Two Fluid Model (TFM). The predicted characteristics of bubble formation, motion, and eruption at the bed surface from TFM then will be compared with the DEM predictions. In the absence of any available experimental data on the magnitude of granular stresses or granular temperature, we use the Distinct Element Model (DEM) of Tsuji et al. [1-2] to derive the magnitude of these normal stresses and granular temperatures from first principles in a fluidized bed. Tsuji's [1] DEM model, originally proposed in its primitive form by Cundall and Strack [3], is based on the soft sphere approach of molecular dynamics, which applies Newton's second law of motion to compute the contact forces between the colliding particles using a mass-spring-dashpot system. In general, discrete models are conceptually simpler but rely heavily on computing power when simulating medium-to-large scale systems. In this article, we discuss the effect of solid's pressure and granular temperature on the bubbling characteristics of a fluidized bed. REFERENCES [1] Tsuji, Y., Tanaka, T., and Ishida, T., Powder Technology, Vol. 71, pp. 239-50 (1992) [2] Tsuji, Y., Kawaguchi, T., and Tanaka, T., Powder Technology, Vol. 77, pp. 79-87 (1993) [3] Cundall, P.A., and Strack, O.D.L., Geotechnique, Vol. 29, pp. 47-65 (1979) ACKNOWLEDGMENTS The author would like to thank Prof. Yutaka Tsuji and his laboratory staff at Osaka University (Japan) for providing him with access to, and helping him understand, their DEM code. The author also gratefully acknowledges the access to MFIX code from National Energy Technology Laboratory (Morgantown, WV).

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MS76
Accurate Numerical Methods for the Solution of Two-Fluid Models

In recent years finite volume computations of two-fluid hydrodynamic models have been used in a number of numerical investigations of gas-solids fluidized bed and circulating fluidized bed processes. To avoid numerical diffusion from dominating simulation results, proper discretization of convective terms is critical i.e., higher-order methods should be used in the computation of convective terms at cell faces. It is well known that higher-order methods may give rise to nonphysical spatial oscillations. This problem is routinely addressed in single-phase theory by using flux limiters that satisfy certain constraints in order to obtain total variation diminishing schemes. However, applying these methods to multiphase flow problems is not straightforward and a critical look at these methods in a multiphase context is needed.

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MS76
Description of Fluidized Beds Using Proper Orthogonal Decomposition

Numerical simulations of the hydrodynamics of a fluidized bed are carried out to investigate complex interactions between gas and solid particles, and the derivation of a reduced order model based on the Proper Orthogonal Decomposition (POD). In simulations with a central air nozzle, the most dynamic region in the bed is confined to a central channel, in which the flow is successfully captured by a few POD eigenfunctions. Thus indicating low-dimensional dynamics.

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MS77

Estimating the Reliability of Optical Transmission Systems with Importance Sampling

Transmission errors in optical communication systems are typically required to be extremely rare. Because of this stringent requirement, it has been impossible so far to use numerical simulations to directly calculate bit error ratios and outage probabilities. Two of the most serious transmission impairments are amplifier noise and polarization mode dispersion, which are both stochastic in nature. We will show how, in both cases, use of importance-sampled Monte Carlo simulations allows one to speed up the simulations by several orders of magnitude, thus making it easy to observe events that would be beyond the reach of a brute force approach.

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MS77

Optical Transport Systems: Introduction and Simulation Directions

Optical transport system performance has outpaced Moore's law over the past two decades. This overview talk will introduce some of the key enabling technologies such as dense wavelength-division multiplexing, dispersion management, and new amplification methods that have enabled terabit-per-second transport over transcontinental distances. Simulation and modeling challenges will be discussed including the need for discrete events coupled to continuous physical layer simulators for the analysis and control of dynamic networks.

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MS77

Control and Design of Broadband Raman Amplifiers

Today's broadband DWDM (dense wavelength-division multiplexing) transmission systems can carry more than 100 signal channels on a single fiber. Raman amplifiers are ideally suited for compensating fiber loss in such broadband systems. These amplifiers employ multiple pump lasers, operating at different frequencies. The powers of these pumps need to be controlled dynamically, depending on the actual channel load. We present numerical techniques for the problems of design and control of broadband Raman amplifiers. We also discuss a simulation environment that allows us to test the performance of Raman control algorithms within complete transmission systems.

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MS77

Advances in Modeling High-data-rate Optical Fiber Communication Systems

Our recent advances in modeling high-data-rate optical fiber communications systems are reviewed. We first examine new methodologies that allow us to accurately calculate the evolution of the noise covariance matrix during transmission, the receiver's action on this noise, and from that the BER. We next examine the application of importance sampling to calculations of the eye closure penalty due to the combination of polarization effects and amplifier gain saturation in a wavelength-division-multiplexed system.

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MS78

The Impact of Computational Fluid Dynamics on Aerospace and Automotive Design

My remarks will review the recent developments in Computational Fluid Dynamics (CFD) modeling of applications in the Aerospace and Automotive industries via the following important themes: 1) The user environment for analysis including topics like interface, graphics, architecture, intelligent agents 2) CAD/Analysis integration and related geometry issues 3) Mesh generation 4) Mathematical models and solver algorithms 5) Error control and sensitivity 6) Optimization 7) Physical models 8) High performance computing 9) Visualization and results analysis

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MS78

Computer Simulation in the Automotive and Aerospace Industry: The Challenge of the Transition to a New Solution

Computer Aided Engineering (CAE) in the Automotive and Aerospace industries is changing very rapidly in response to developments in the HPC software and hardware industry. For example, the use of "domain decomposition" methods in the mainstream applications codes has dramatically altered the types of hardware being used for CAE. These modifications have repercussion across the whole CAE solution space. The discussion will highlight the changes and attempt to describe some of the near term

effects.

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MS78

Opening Remarks

Industrial global competitiveness requires the following actions: (1) The amount of physical prototyping must be reduced and replaced by realistic three-dimensional, math-based computer modeling; (2) Such models must employ very aggressive use of parallel hardware, software, and algorithmic technologies.To accomplish this requires extensive multidisciplinary interactions and sharing of resources within a company as well as amongst its suppliers. This panel session will focus on the aforementioned actions for several industrial applications.

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MS78

Web-Based Distributed Simulation of Aeronautical Propulsion System

Our application was developed to allow users to run and view the Numerical Propulsion System Simulation (NPSS) engine simulations from web browsers. Simulations were performed on multiple INFORMATION POWER GRID (IPG) test beds. The Common Object Request Broker Architecture (CORBA) was used for brokering data exchange among machines and IPG/Globus for job scheduling and remote process invocation. JavaServer Pages (JSP)performed Web server scripting. This application is a proven effective and efficient way to couple heterogeneous distributed components.

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MS78

Aspects of Computational Science in Advanced Material Manufacturing

Advanced composite materials are being aggressively proposed and developed to fill the need of new military and dual-use applications;however, the complexities of such systems are not well understood. Successful first-time manufacturing remains an elusive goal. The U.S. Army Research Laboratory is developing modeling and simulation tools to reduce the inherent risks with these non-monolithic structures. This talk will include details about simulation tools currently in development,numerical linear algebra solver issues, and application examples.

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MS79

SOCS: Software for Large, Sparse Optimal Control Problems

Optimal control problems arise in a number of applications, for example trajectory optimization, chemical process control, and multi body systems. To efficiently solve these problems, several different components need to work together, and influence each other. These range from methods for mesh refinement, discretization, to sparse nonlinear programming and linear algebra. The Boeing software SOCS combines all these disciplines into a powerful tool.

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MS79

DDAE: an integrator for ODEs, DAEs and DDEs

In addition to covering the problem classes mentioned in the title, the integrator offers a number of options that allow the user to take advantage of any structure present in their problem. Thus it will solve higher order equations directly, allow the user to provide extra derivatives, allow arbitrary interfaces for any linear algebra required, and allow stiff and nonstiff methods to be mixed. Grouping of equations plays a major role in the design.

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MS79

Software Development for Boundary Value Ordinary Differential Equations

Boundary value ordinary differential equations arise in a many applications and take on a variety of forms, including mixed order systems of nonlinear equations with multipoint conditions. In this talk we will briefly survey a number of software packages based on discrete and continuous implicit Runge-Kutta methods including subclasses such as the collocation methods and generalizations such as the Runge-Kutta-Nystrom methods.

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MS79

The Case for Implicit-Explicit Methods

Traditional numerical methods for solving ordinary differential equations are typically of two types: implicit or explicit. Explicit methods are easy to implement but are inefficient on stiff problems. Implicit methods are effective for stiff problems, but their implementation is not trivial. Recently there has been a lot of interest in hybrid solvers because many problems naturally have stiff and nonstiff parts. In this talk I will discuss how hybrid solvers can achieve the best of both worlds.

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MS80

Discrete Exterior Calculus

We present a theory and applications of discrete exterior calculus on simplicial complexes of arbitrary finite dimension. This can be thought of as calculus on a discrete space. Our theory includes not only discrete differential forms but also discrete vector fields and the operators acting on these objects. This allows us to address the various interactions between forms and vector fields (such as Lie derivatives) which are important in applications. Previous attempts at discrete exterior calculus have addressed only differential forms. We also introduce the notion of a circumcentric dual of a simplicial complex. The importance of dual complexes in this field has been well understood, but previous researchers have used barycentric subdivision or barycentric duals. We show that the use of circumcentric duals is crucial in arriving at a theory of discrete exterior calculus that admits both vector fields and forms. (Joint work with Mathieu Desbrun, Melvin Leok, Jerrold E. Marsden)

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MS80

Data Structures for CEM via Algebraic Topology

Given the success of simplicial data structures and Whitney forms in CEM, we examine the route that lead to current developments. Starting with de Rham's 1931 thesis, we consider: - The appearance of E-S axioms in the 40's, Andre Weil's 1952 criticism of axiomatics and Whitney's subsequent work. - Later uses of Whitney forms in rational homotopy theory, combinatiorial Hodge theory and torsion invariants in light of Milnor's theorem on CW complexes. - Semi-simplicial objects, and future consequences for data structures.

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MS80

Convergence of Mimetic Discretization Methods

The convergence of a mimetic discretization in rough grids is proven. The mimetic discretization method is based on discretizing the invariant operators divergence, gradient, and curl and then using these discretizations to discretize more general differential operators. Most importantly, mimetic method require that the discretization has exact analogs of many of the important theorems of vector calculus. For the grids, we only assume that the cells are convex. To study convergence, the family of grids under consideration are assumed to satisfy uniform convexity conditions. Because we are focused on convergence for rough grids, we use as a model problem the simple two-dimensional Laplace equation with Dirichlet boundary conditions so that the role of grid roughness is clear. In this case, the important theorem from vector calculus we mimic is the divergence theorem. To simplify the notation, the convergence is shown on logically rectangular grids with a lower bound on the angles in the cell corners and an upper bound on the cell aspect ratios. In this situation, the best convergence rate to be expected is first order, which is what proved.

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MS80

Lattice Subdivisions for Simplicial 3+1 Electrodynamics

Recognizing metric independent aspects of field theories is an important step to formulate discrete counterparts on arbitrary lattices (grids). This allows for a separate treatment (factorization) of the (quite distinct) topological and metric discretization problems. In the case of Maxwell's equations and using the exterior calculus framework, premetric properties can be associated with preconstitutive (i.e., medium independent) equations. This implies separate treatments for the purely topological (i.e., invariant under diffeomorphisms) dynamic equations and the constitutive equations (metric part). Metric dependent aspects are entirely encoded in the so-called (discrete) Hodge operators (generalized constitutive parameters), and the dynamic variables of the discrete theory (i.e., the cochains on the lattice) are governed by formally identical equations on dual instances, viz., (i) on a (particular) irregular lattice in a homogeneous medium and (ii) on a regular lattice in a (particular) anisotropic and inhomogeneous medium with identical (up to a constant) permeability and permittivity constitutive tensors. This factorization also provides a starting point to induce changes on the metric part of the theory for specialized purposes (e.g., to produce absorbing boundary conditions for simulation of unbounded geome-

tries). In this work, we will discuss aspects of this factorization and its relation to lattice subdivisions schemes for the discrete rendering of Maxwell's equations on a simplicial lattice. Emphasis will be given to metric-free subdivisions (standard subdivision and barycentric subdivision) and their role in the construction of the discrete Hodge operators. Implications on the design of numerical simulation methods and grid refinement strategies for complex media and/or geometries will be also be considered.

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MS81
Interactions of Load Balancing and Locality

The talk will present results concerning the interaction of load balancing with cache locality management in finite difference methods. It is shown that finer grain decompositions have the desirable property of enhancing load imbalance while simultaneously improving cache locality. An API is presented that supports a methodology for distributing non-uniform applications on heterogeneous clusters.

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MS81
Cache Aware Multigrid Algorithms and Their Implementations

For 10+ years, CPUs and memory caches have been coupled to counter data starvation for the CPU. Counting flops once was a good measure for an algorithm. Now, counting cache misses is a superior measure. We define cache aware multigrid algorithms that minimize cache misses and discuss their performance on unstuctured or patch based grids.

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MS81
Automated Introduction of User-Defined Locality Optimizations

ROSE is a programmable source-to-source transformation framework permitting the simple construction of sophisticated source-to-source preprocessors. ROSE provides an open access to the internals of many parts of a compiler, particularly the creation of the abstract syntax tree (AST) and the generation of source code from the AST. Additionally ROSE provides the user with both query and rewrite mechanisms for sophisticated analysis and general transformations of the AST. As a result, highly specialized optimizing compilers can be constructed as source-to-source preprocessors together with the vendor's compiler used as a backend to generate final executable code. Through the addition of architecture specific optimizations an existing vendor's compiler may be extended to address specific peculiarities of either a new computer architecture or high-level user-defined abstractions within a scientific application or library. Current research has targeted the optimization of high-level abstractions within object-oriented libraries, allowing ROSE to effectively turn any object-oriented library into a domain-specific language; in the sense that compile-time optimizations can be introduced based upon the semantics of the abstractions found within the library. The transformations we have defined are specific to the optimization of locality, our talk will report on the results from this research.

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MS81
Locality-optimized Iterative Algorithms

In order to mitigate the effects of the constantly growing gap between CPU speed and main memory performance, it is necessary that the codes respect the hierarchical memory design of today's computer architectures. This is particularly true for iterative algorithms that are used in the context of the numerical solution of partial differential equations, for example. Our previous research has focused on the development and the investigation of code transformations to enhance the cache performance of standard methods; e.g., Gauss-Seidel. These transformations cover both data layout as well as data access optimizations. Furthermore, we have studied the design of novel multilevel algorithms that exhibit a high potential of locality by construction. These algorithms are characterized by the idea that, in the course of the multilevel iteration, the computational work can be concentrated on those parts of the grid structures where a further reduction of the error is actually required. In our talk we will provide a survey on both research directions, covering practical performance results.

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MS82

Application of Differentiation-enabled Fortran 95 Compiler Technology

We present a novel approach to generating derivative code for mathematical models implemented as Fortran 95 programs using Automatic Differentiation inside the NAGWare Fortran 95 compiler. This technique allows us to combine the advantages of both operator overloading and source transformation based tools for Automatic Differentiation. Furthermore, the compiler's infrastructure for syntactic, semantic, and static data flow analysis can be built on. We will discuss a case study involving the application of the new differentiation enabled compiler to a tutorial problem from the PETSC test suite.

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MS82

Computing Periodic Orbits in Constrained Multibody Systems Using Automatic Differentiation and Taylor Series Integration

The techniques of automatic differentiation and Taylor series integration provide a convenient mechanism for computing highly accurate numerical simulations of constrained multi-body systems. These techniques can be coupled with a multiple shooting strategy to compute periodic orbits in multi-body systems to high accuracy using coarse discretizations. The algorithms are robust and can be further adapted to locate and track bifurcations of periodic orbits using a number of continuation strategies.

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MS82

Automatic Differentiation of Industrial CFD Codes: A Case Study with FLUENT

Automatic differentiation (AD) is a general technique for automatically augmenting a given computer program with statements for the computation of derivatives. A common misconception is that automatic differentiation is only applicable to small academic codes and does not scale to advanced industrial software packages. We demonstrate the scalability by applying AD to the FLUENT program, a widely used general-purpose CFD solver, and present various examples for the use of the AD-generated derivative code.

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MS82

Sensitivity Calculations for Elliptic Interface Problems

A Continuous Sensitivity Equation Methods is used to obtain sensitivity calculations for elliptic partial differential equations with discontinuous coefficients, or elliptic interface problems. The focus is on problems where the spatial location of the interface is parameter dependent. These PDEs have solutions which lack smoothness at the interface, and the corresponding sensitivity is discontinuous across the interface. The sensitivity equation is examined, and an iterative domain decomposition algorithm is used to numerically compute sensitivity approximations.

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MS83

Organization and Development of a General PDE Modeling Environment: Challenges and Issues

We will present the design goals of a modern, interactive, integrated environment for multiphysics modeling, including: - The ability to handle general systems of PDEs, described symbolically. - The flexibility to allow specification of several PDEs in terms of physical material parameters and to derive systems of PDEs automatically by adjoining derived equations. - The capacity to allow non-local couplings of PDEs, e.g., using the integral over a domain in the expression for a boundary condition in another domain.

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MS83

Implementing DASPK 2.0 in FEMLAB

Two software packages have been written for solving initial value problems for the DAE system—DASSL and an extension of it called DASPK. Both use variable-order variable-stepsize backward differentiation formulas. DASSL solves the linear systems that arise at each time step by dense or banded direct linear system methods. In DASPK, the linear systems that arise at each time step are solved with either direct linear system methods, or with a preconditioned Krylov iterative method, namely GMRES. Although DASPK has been widely used by computational science and engineering applications, it has not been incorporated into commercial integrated computing environments, e.g. MATLAB or FEMLAB. In this presentation, we describe a method how to implement DASPK in FEMLAB environment without rewriting the DASPK into the Matlab language. Moreover, the existing linear or nonlinear solvers in MATLAB and FEMLAB can be used to extend the capability of the DASPK solver. An approach to solve the complex DAE by the double version DASPK is also discussed. Several examples are tested. The numerical results demonstrate that our approach is very effectiv and efficient compared with other ODE/DAE solvers in Matlab and Femlab.

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MS83

Effective Graphical User Interfaces for Mathematical Modeling in Engineering and Science

The development of a graphical user interface (GUI) for modeling in engineering science must deliver a product that is easy to use for beginners while leaving all options open to the experienced user. Usability studies with paper prototypes help to redesign dialog boxes that are hard to use. Continuous integration, automatic test suites, and code reviews are important tools for assuring quality. The Java programming language is used to create a consistent cross-platform look and feel.

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MS83

Using FEMLAB as a Platform for Studying Time Integration Methods

We are using FEMLAB as a platform for studying time integration methods for systems of diffusion-reaction equations, in order to understand errors in production-level codes. While FEMLAB allows for quick prototyping of equations and easy modeling of a variety of physics, it is not designed for this type of numerical comparison. We will present how we adapted FEMLAB for this study and some results.

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MS84

Overview of Semiconductor Device Modeling and Astrophysical Jets

A brief introduction to semiconductor device modeling using the hydrodynamic model will be given. The semiclassical MESFET device and its operation will be described. Then an overview of supersonic astrophysical jets will be given, including Hubble Space Telescope images and the equations of gas dynamics with radiative cooling used to simulate the jets. Simulation results using the three different modern hyperbolic methods will be compared and contrasted.

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MS84

Simulation of a 2D MESFET Using the Tadmor Central Scheme

Simulations of the nonlinear conservation laws of gas dynamics with source terms coupled to Poisson's equation for a 2D MESFET (metal semiconductor field effect transistor) will be presented. The numerical method is based on the Nessyahu-Tadmor-Kurganov central scheme, which is described for the semiconductor partial differential equations. Special attention is paid to implementing mathematically correct boundary conditions. Simulations of an electron shock wave in a submicron GaAs MESFET will be presented.

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MS84

Well-posedness for the Initial Value Problem for the Maxwell-Hydrodynamic System

The Maxwell-Hydrodynamic model is a natural next step for applied and computational mathematicians. Its utility has already been established: in the simulation of microwave devices exhibiting electromagnetic effects, and in optical emission and detection, where optical fields are critical to the modeling. In this talk, we present: (1) A global approach, based on recent advances in conservation laws; and, (2) A local smooth solution theory for the Cauchy

problem, based on Kato's semigroup theory.

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MS84

WENO Simulation of High Mach Number Astrophysical Jets

The WENO method for gas dynamics will be reviewed, and simulations of high Mach number astrophysical jets with radiative cooling will be presented. The importance of radiative cooling in obtaining agreement between the Hubble measurements and the simulated densities and temperatures will be emphasized. In addition, the effect of radiative cooling on the jet morphology will be analyzed.

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MS85

Cellular Automata Model for a Continuous Mechanics Problem

The development of cellular automata models has increased considerably with the availability of powerful computers. In this work we explore CA approach to model a two-dimensional system with frictionless contact between an elastic body and a rigid foundation. We consider a microscopic description of the phenomena through the particles behaviour. We also extend the results to the case of a thermoelastic deformation. Simulation results based on an adaptation of Matlab code are presented.

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MS85

Analysis and Control of Distributed Parameter Systems Via Cellular Automata Application to Spreadability

A cellular automaton is a mathematical model that is perfectly suited to complex spatio-temporal systems with a large number of simple identical components having local interactions. DPS are commonly governed by PDE's and the aim of this work is to introduce cellular automata as an alternative modelling approach for DPS analysis. They are more convenient and more accurate for computation. They are applied to describe spreadability concept (see El Jai, 1994) and implemented for illustrative examples.

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MS85

Regional Analysis Via Cellular Automata Models

In DPS theory, regional analysis was introduced by El Jai and Zerrik (1992) and studied for continuous systems described by partial differential equations. The purpose of this paper is to consider regional analysis by means of cellular automata models. We present results that show how the main features of regional controllability may be simply described and implemented by cellular automata approach. Various examples are given involving appropriate optimization techniques.

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MS85

Modelling Vegetation Dynamics with Cellular Automata

We give an original modelling software for biogeographical systems, Lucas (LUcifer Cellular Automata Simulator) developed within a European programme. Lucas is based on coupling biological phenomena on a patch with space evolution described by cellular automaton model. The user has the opportunity to choose the dominant species, different parameters related to the considered landscape and to introduce fire interactions. The software has been applied to various examples of European landscapes.

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MS85

Coupling ODE and CA for Spatio-Temporal Sys-

tems

To describe spatio-temporal evolution of some natural phenomena, partial differential equations are common tools. For simulation, many mathematical techniques are proposed (finite elements method for example). This requires very huge and complex computations for their implementation. We propose, in this paper, two coupled models based on ordinary differential equations (for local dynamics) and cellular automata (for global space evolution) for modelling and simulating these systems. The approach is applied to model and simulate a vegetation dynamics system.

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MS86

Computation of Entanglement by a Quantum Neural Network

An outstanding problem in quantum computing is the calculation of entanglement, for which no general closed-form algorithm exists. Here we solve that problem, and demonstrate the utility of a quantum neural computer, by showing, in simulation, that such a device can be trained to calculate the entanglement of a general input state, something neither an algorithmic quantum computer nor a classical neural net can do.

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MS86

Quantum Neurons with Gate Output

We describe a model element able to perform universal stochastic approximations of continuous multivariable functions in both neuron-like and quantum form. The implementation of this model in the form of a multi-barrier, multiple-slit system is proposed and it is demonstrated that this single neuron-like model is able to perform the XOR function unrealizable with single classical neuron. For the simplified waveguide variant of this model it is proved for different interfering quantum alternatives with no correlated adjustable parameters, that the system can approximate any continuous function of many variables. This theorem is applied to the 2-input quantum neural model based on the use of the schemes developed for controlled nonlinear multiphoton absorption of light by quantum systems. The relation between the field of quantum neural computing and quantum control is discussed.

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MS86

On Quantum Learning of Small DNF Functions

The efficient learnability of Disjunctive Normal Form (DNF) functions has been of interest since Valiant initiated the computational study of learning. Although there is a nominally efficient classical algorithm for learning DNF from learner-selected examples, it is desirable to both speed up the algorithm and to enable it to learn from random examples. Quantum approaches to both of these problems that provide some improvement over known classical solutions will be presented.

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MS86

Quantum Versus Classical Learning

Imagine that you are given the task of extracting information from a "black box" which computes some unknown function. You can present inputs to the black box and receive the value of the function on those inputs, but have no other way of gathering information about the unknown function. Your mission is to obtain a complete description of the function computed by the black box, i.e. to exactly learn the unknown function. In the classical setting this problem has been studied by researchers in computational learning theory and is fairly well understood. This talk will consider the following question: does learning the unknown function become easier if you are dealing with a *quantum* black box? As we'll see, the answer is both yes and no depending on how we measure the difficulty of learning. First we'll show that the number of queries which need to be made to the black box is roughly the same in the classical and quantum models (up to a polynomial factor); so from a query complexity perspective quantum learning is not substantially easier than classical learning. (This is joint work with Steven Gortler.) However, we'll also show that from a computational complexity perspective – how much computation do we need to do in order to construct the desired description of the black-box function? – the quantum learning model does have a substantial (superpolynomial) advantage over the classical model. This computational separation relies only on general cryptographic assumptions (the existence of any one-way function).

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PP0

Optimization of Systems Governed by Pdes: Parallel Algorithms and Applications to Parameter Estimation, Optimal Control, and Optimal Design

The maturing of parallel PDE solvers for many classes of simulation problems invites pursuit of what is often of ultimate interest: the *inverse* problem of optimizing systems governed by PDEs. Such PDE-constrained optimization problems often arise as parameter estimation, optimal control, or optimal design problems. In this poster, we present

parallel algorithms for PDE-constrained optimization, and applications to optimal viscous flow control, inverse wave propagation, source inversion for convective-diffusive transport, and shape optimization.

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PP0

Effect of Slat Gap Width on the Performance of A Naca 0012 Airfoil: A Numerical Study

A steady, compressible turbulent flow around a NACA 0012 airfoil with and without slats was simulated. Three different slat gap sizes were used. The computation was carried out at Mach 0.3 and Re = 2.9x106. With clean configuration, the simulation predicted a stall condition. With the slat and a gap of 0.006c, major separation was observed. By doubling the gap, significant improvement in performance was predicted, including a 23% reduction in drag.

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PP0

Improving the Performance of Pde-Based Simulations by Using Multi-Method Solvers

The effective solution of nonlinear PDE-based simulations often depends on the performance of sparse linear solvers. We present a framework for multi-method linear solvers that can improve both execution time and reliability. We consider "composite solvers" with reliability tending to one in practice; these composites comprise a sequence of preconditioned iterative methods that are applied to solve a given system. We also consider "adaptive solvers" where the solution method is selected dynamically to match the changing attributes of linear systems. We present algorithms for developing these multi-method solvers and report on their performance in several CFD applications.

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PP0

Parallel Multiresolution Octree-Based Simulation of Earthquake Ground Motion in Heterogeneous Basins

This poster reports on parallel multiresolution octree-based finite element simulation of earthquake-induced ground motion in large, highly heterogeneous basins. We use the Tu-O'Hallaron out-of-core octree-based mesh generator, which allows us to generate meshes of essentially arbitrarily fine resolution, and an efficient parallel algorithm for solving the elastic wave propagation problem. Performance results on up to 2048 processors of the PSC Terascale Computing System demonstrate that, despite the highly irregular structure of the problem, teraflop performance and excellent scalability are achieved.

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PP0

Numerical Method for Time Reversal of Waves in Random Media

We simulate the time reversal refocusing of a pulse incident on a multi-layered scatterer with random variation. A windowed scattered wave is sent back into the scatterer and results in pulse refocusing The effect is enhanced when the scales of the layer, pulse wavelength and scatterer are well separated. This multi-scale problem is solved for the wave equation in the frequency domain using a boundary integral method that employs Green's functions for the Helmholtz equation.

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PP0

Geometric Completion of Circuit Dae Using Numeric-Symbolic Methods

Systems of differential algebraic equations (DAEs) arise quite naturally in electronic circuits simulation. Inclusion of more realistic models for circuit elements such as MOSFET transistor results in DAEs with higher order index. Moreover exact formulations of electronic circuits that take the second order effects and transmission line delays into account will result in systems of partial differential algebraic equations (PDAE). In high frequency integrated circuits for today's communications devices, these effects are highly significant. Consistent initial conditions are very difficult to obtain for an index > 1 DAE. Inconsistent initial conditions lead to wild zigzagging of the solution. Numerical jet geometry and numeric-symbolic methods for completion of differential systems are newly born methods that are used to find the constraints of the input differential algebraic system. Apart from the problem of circuit simulation, over and under-determined (non-square) systems of DAE arise in applications such as constrained multi body mechanics and control systems. They are becoming increasingly important in applications as more realistic models naturally lead to such constrained systems. Symbolic algorithms have been developed which use a finite number of exact differentiations and eliminations to reduce over and under-determined systems of polynomially non-linear differential equations to involutive form. The output involutive form enables the identification of consistent initial values, and eases the application of exact or numerical integration methods. However such differential-elimination algorithms, which usually incorporate Groebner bases, have poor complexity and are unsuited for application to systems with approximate coefficients. An underlying principle of the new numeric-symbolic approach is strong emphasis on geometry, in particular jet space geometry, the geometry of differential systems. In comparison to the symbolic differentiation-elimination approaches, where symbolic or algebraic manipulations of the equations figure heavily, new method focuses on the solutions of the system regarded as algebraic equations. A major principle of our approach is to replace what is usually a symbolic-preprocessing step with a variation of Newton's method, to locate points on the hidden constraints. This is quite natural since ultimately variants of Newton's method are used in solving the differential system. The new class of methods presented here can be compared to using an iterative method to solve systems (in our case Newton's method), instead of exact elimination (e.g. Gaussian Elimination, or its non-linear cousin Groebner Bases). The systems of polynomial equations involved in most physical phenomena are usually not square and generally have positive dimensional components (submanifolds) of solutions. Our treatment of such systems, using homotopy methods, is made possible by recent theoretical progress made by Sommese et al. in the developing area of numerical algebraic geometry. The new techniques rely on embedding the given systems in square polynomial systems, by the inclusion of extra (slack) variables and random linear equations if necessary. The key idea behind these methods is to reduce to the zero dimensional case (where there are only finitely many solutions), by slicing the solutions with a random linear space of the appropriate dimension. Enough points are located to interpolate the smooth components of a differential system by lowest degree polynomials. In this paper the physical problem in electronic circuit simulation is presented. Also the application and usefulness of the new numeric-symbolic algorithms to find hidden constraints in circuit differential system is examined.

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PP0

Microstructural Simulation of Blood Flow on Parallel Computers

The advent of multi-teraflop computers enables us to contemplate, for the first time, large-scale microstructurally-based simulations of blood flow. Such simulations, which resolve individual cell deformations and their interaction with surrounding plasma, are necessary to better understand blood damage and to develop more rational macroscopic blood models. This poster will summarize the efforts of the Sangria Project (www.cs.cmu.edu/~sangria) in developing the geometric algorithms and numerical models necessary for simulating complex blood flows in parallel.

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PP0

The Numerical Calculation of Electromagnetic Fields by Using Watson's Transformation Methods

Not only harmonic series representations but also the residue series representations are frequently used for representing fields scattered by a circular conducting cylinder. However, if the wavelength becomes much shorter than the radius of the cylinder, the convergence of the harmonic series becomes slow. In this study, the advantages and disadvantages of the residue series representations in comparison with the harmonic series representations are shown. Furthermore, the distinctive features and nature of the residue series representations will be given. The residue series representations are usually obtained by Watson's transformation. However, we will show that the residue series representations can also be obtained by the method of separating variables.

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PP0

A Method of Using Neumann Functions to Analyze Waveguides with Arbitrary Cross Section

Cutoff frequencies and modal fields in the waveguides with arbitrary shapes are calculated by the method of solving integral equations. Since the Green function used in the integral equation is the Hankel function $H_0^2(x)$, modal fields are given by complex numbers. When the Neumann function $N_0(x)$ is used, the fields are given by the real numbers, but so-called extraneous cutoff frequencies appear. Here the authors devised a method for suppressing the extraneous cutoff frequencies. By this method, the numerical calculation becomes simpler and offers more precise results.

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PP0

High-End Computer System Performance: Science and Engineering

We describe the research activities of the Performance Evaluation Research Center. PERC is an Integrated Software Infrastructure Center (ISIC) whose aim is to obtain the best possible performance of computational science and engineering applications on high-end computer systems. Our approach is three-pronged, including evaluation of application and hardware by using discipline-specific benchmarks, defining performance models of applications and architectures, and source- and machine-level tools for performance instrumentation, visualization, and optimization.

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PP0

The Estimation of Missing Data for Acute and Chronic Stress Arena, Duration and Stress Ratings

There is evidence that high levels of stress contribute to a weakened immune system. Two types of stress outcome are examined. These are the acute (short-term) stress and chronic (long-term) stress levels. The database consists of 200 subjects with blood draws taken at 4 time points. The acute stress ratings (ASR) and chronic stress ratings (CSR) data were used in the estimation of missing data for the acute and chronic stress arena, duration and ratings.

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PP0

The Modeling of Acute and Chronic Stress

Two types of stress outcome are examined. These are the acute (short-term) and chronic (long-term) stress levels. Seventeen independent variables are used to model acute and chronic stress levels. The variables include personality measures, social desirability scores, sociodemographic measures and a general health variable. Ten dif-

ferent model selection criteria are used and 200 subjects' data over 4 time periods are used to find 'best' fitting models. The SAS macros are available for download at http://pages.prodigy.net/johnsonp12/programs.html

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PP0

Projection-Based Parallel Delaunay Meshing Algorithms

Quality mesh generation of complex domains is required for finite element calculations. Many problems require frequent remeshing as the solution evolves; i.e. problems involving dynamic interfaces. This calls for large-scale, efficient and robust quality mesh generators. We present a general strategy to parallelize Delaunay based mesh refinement algorithms on distributed memory machines. At the heart of the algorithm lies a projection based partition of the mesh. This partition gets dynamically updated as new points get added to the mesh. Using properties of the Delaunay triangulation we can establish a high level of asynchronicity and keep communication at the necessary minimum.

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PP0

Terascale Optimal Pde Simulations

The nine-institution Terascale Optimal PDE Simulations (TOPS) project is developing methods for PDE-based simulations on distributed hierarchical memory computers, and related methods, including optimization of PDE-constrained systems, sensitivity analysis, eigenanalysis, and adaptive time integration, as well as the core implicit linear and nonlinear solvers. Most PDE simulation is ultimately a part of some larger scientific process that can be hosted by the same data structures and carried out with many of the same optimized kernels as the simulation, itself. We describe early accomplishments and work in progress.

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PP0

Robust Algebraic Multigrid

Substantial effort has recently focused on developing methods capable of solving very large linear systems that arise from discretizing partial differential equations, especially on unstructured grids. Algebraic multigrid (AMG) is of particular interest because of its promise of optimal performance without the need for explicit knowledge of the problem's origin. We introduce an extension of AMG based on an adaptive process that achieves good convergence on a broader class of problems than the original algorithm.

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PP0

Large-Scale Methods for Calculating Exact Cumulative Reaction Probabilities

The calculation of reaction rate coefficients can be obtained from exact quantum cumulative reaction probabilities (CRP) by computational intensive methods that are rarely applied. We are using PETSc to parallelize time independent CRP methods that involve iteratively obtaining the eigenvalues of the probability operator by the iterative evaluation of two Green's functions in each eigenvalue iteration. Initial tests show the code is scalable to a hundred or more processors.

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PP0

Least-Squares Finite Element Methods for Hyperbolic Pdes

We consider partial differential equations of hyperbolic type and allow for discontinuities in the solution. The problem is posed as a least-squares minimization principle and we seek numerical solutions in a finite element setting for non-grid aligned flows. An appropriate finite element space is proposed and we discuss the convergence of the numerical approximation. Finally, we detail the performance of the Algebraic Multigrid solver applied to the resulting linear system.

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PP0

Parallel Bipartite Matching for Sparse Matrix Computations

Practical and efficient methods exist for parallelizing the numerical work in sparse matrix calculations. The initial symbolic analysis is now becoming a sequential bottleneck, limiting problems' sizes. One such analysis is the weighted bipartite matching used to achieve scalable, unsymmetric *LU* factorization in SuperLU. Applying a mathematical optimization algorithm produces a distributed-memory implementation with explicit trade-offs between speed and matching quality. We present accuracy and performance results for this phase alone and in the context of SuperLU.

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PP0

Managing Biological Concept Maps With The Heuristic Entity Relationship Building Environment (herbe) Eric Stephan, George Chin, Heidi Sofia

The Heuristic Entity Relationship Building Environment (HERBE) prototype will allow biologists to use an open visual environment to collect diverse, complex data and construct models graphically. As data are entered, HERBE captures the data, then integrates and heuristically interprets underlying concepts into an enhanced entity relationship model. HERBE creates a database from the model in an underlying layer for querying. We are initially focusing our research efforts in the field of biology and systems biology.

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PP0

Computational Simulation Environments

Reaction Engineering is developing three computational workbench environments for various applications. The first targets the optimization of reduced chemical mechanisms. The second provides capabilities for modeling one of the Army's chemical weapons incineration facilities. The third is used for simulation of the Department of Energy's Vision21 systems. Each of these environments uses the University of Utahs SCIRun software as their framework. Special attention has been paid to making use of HPC technologies including CCA.

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PP0

Uncertainty in Numerical Prediction Models: the Lack of Convergence of the Lorenz Equations

Most computational models are non-linear and it is usually implicitly assumed that the solutions of the numerical algorithms in which they are based converge to the analytic solutions of the underlying differential equations, for small time-steps and grid-sizes. The Lorenz equations are used to show that for highly non-linear systems there is no apparent convergence.

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PP0

Automatic Performance Tuning of Sparse Matrix Kernels

We consider the problem of generating high-performance implementations of the sparse matrix operations automatically. Tuning is a tedious and time-consuming task because performance is a complicated function of the underlying computer architecture, compiler, kernel, and matrix. We present recent results in which we combine a variety of performance optimization techniques—register blocking, cache blocking, multiple vectors, matrix reordering, and matrix splitting, among others—to several important kernels: sparse matrix-vector multiply, sparse triangular solve, and $A^TA \cdot x$.

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PP0

Robust Optimal Design for Biological Systems Via the Laplace Approximation

The Expected Determinant (ED) criterion can be more robust for designing experiments than the D-optimality criterion because it requires less precise prior knowledge of system parameters. However, ED-optimality involves a

multi-dimensional integral that is computationally expensive for biological system models, which are nonlinear, often involve differential equations, and include substantial variability. We describe an algorithm that implements a variation of the Laplace approximation for the integral and present an application to the design of population pharmacokinetic experiments.

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PP0

First-Order System Least Squares for Geometrically Nonlinear Elasticity

In this research we develop a first-order system least squares (FOSLS) method to solve the equations of geometrically-nonlinear elasticity. We follow a Newton-FOSLS algorithm where each linear step is solved as a two-stage, first-order system under a least squares finite element discretization. We show H^1 equivalence of the FOSLS functional norm in the case of pure displacement boundary conditions for deformations allowed by the model. Numerical results are given for both pure displacement and mixed boundary conditions.

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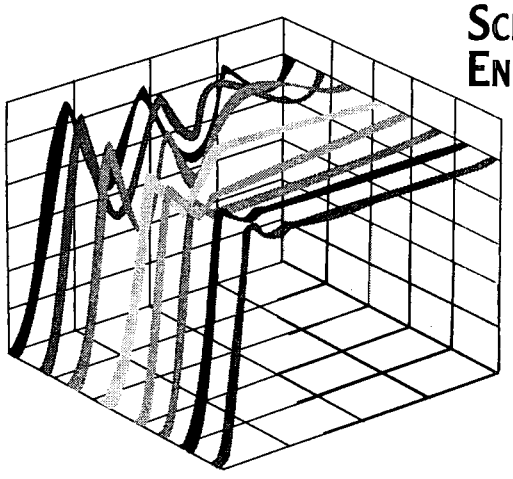

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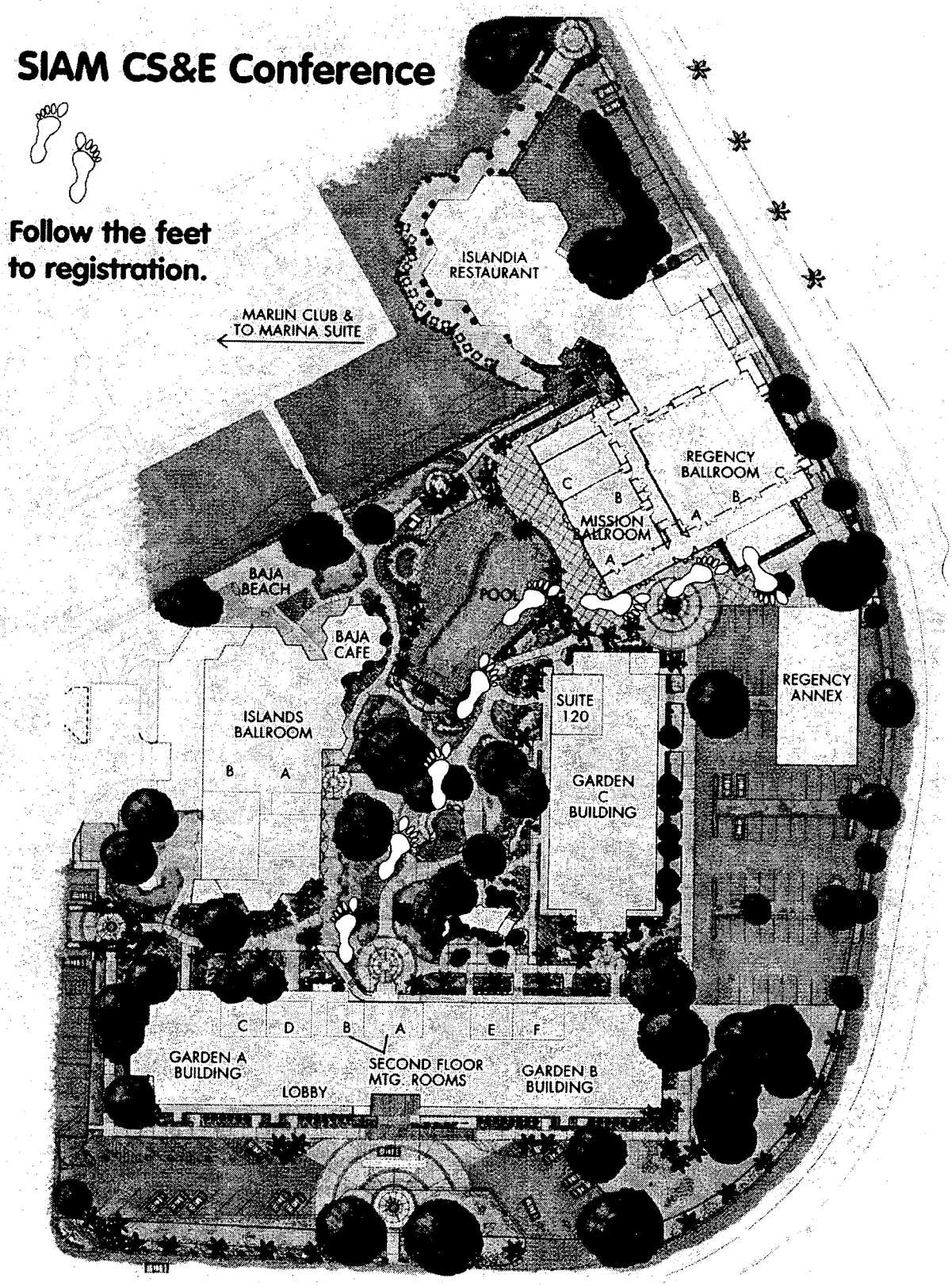
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