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Critical issues in High End Computing

Final Report

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Summary and Objectives

High-End computing (HEC) has been a driver for advances in science and engineering for the past four decades. Increasingly HEC has become a significant element in the national security, economic vitality, and competitiveness of the United States. Advances in HEC provide results that cut across traditional disciplinary and organizational boundaries. This program provides opportunities to share information about HEC systems and computational techniques across multiple disciplines and organizations through conferences and exhibitions of HEC advances held in Washington DC so that mission agency staff, scientists, and industry can come together with White House, Congressional and Legislative staff in an environment conducive to the sharing of technical information, accomplishments, goals, and plans. A common thread across this series of conferences is the understanding of computational science and applied mathematics techniques across a diverse set of application areas of interest to the Nation.

The specific objectives of this program are:

Program Objective 1. To provide opportunities to share information about advances in high-end computing systems and computational techniques between mission critical agencies, agency laboratories, academics, and industry.

Program Objective 2. To gather pertinent data, address specific topics of wide interest to mission critical agencies.

Program Objective 3. To promote a continuing discussion of critical issues in high-end computing.

Program Objective 4. To provide a venue where a multidisciplinary scientific audience can discuss the difficulties applying computational science techniques to specific problems and can specify future research that, if successful, will eliminate these problems.

Accomplishments

The Computational Engineering and Science Conference (CESC), the first conference in a series to be funded through this contract, was held in Washington DC at the Marriott Wardman Park Hotel on April 26 - 27, 2005. It focused on combustion and featured participation by the Department of Defense, the Department of Energy, and the National Aeronautics and Space Administration as the primary organizing agencies.

This meeting provided an opportunity to bring people together to gather information about the state of the art of combustion research and the technical (hardware and software) barriers that they face in scaling up their research studies to take advantage of current and future high end computing resources.

To assist with the third program objective, a website was created to host the series of workshops and to promote continuing dialog between workshop participants.

The second CESC meeting was held in Washington DC at the Marriott Wardman Park Hotel on April 10-12 2007. CESC2007 is designed to bring together disciplinary scientists and engineers focused on nuclear energy and reactor simulation with computer and computational scientists to identify barriers and opportunities for the effective use of high-end computing on nuclear energy research. A significant goal of this conference is to encourage collaboration across disciplinary and organizational boundaries on this global technical challenge.

To assist with the third program objective, a website was created to host the series of workshops and to promote continuing dialog between workshop participants.

A third meeting in the series with the working theme ASCR Software Development Tools for Improved Ease-of Use-of Petascale Systems was planned as a principal investigators meeting to be held at Cliff Lodge, Snowbird, Utah August 5 – 6, 2010. Extensive effort was put into planning the meeting including securing a venue. For a variety of reasons this meeting was cancelled by HQ.

The diversity and scope of the technical exchanges can be seen in the meeting agendas below. The program goals were clearly met.

APPENDIX:

April 25 – 27, 2005

April 10-12, 2007

2010 Draft

Meeting Agenda

MONDAY, APRIL 25

5:00 - 7:00pm Registration

TUESDAY, APRIL 26

7:00 - 8:00am Registration and Continental Breakfast

8:00 - 8:30am Opening Remarks

8:30 - 10:30am **Ground Transportation**

Session Chair: Robert Carling, Sandia National Laboratories

John Dec, Sandia National Laboratories

High-Efficiency and Low-Emissions Engines: the Need for High End Computing [abstract]

Jacqueline Chen, Sandia National Laboratories

Direct Numerical Simulation of Fundamental Processes in Engines [abstract]

Christopher Rutland, University of Wisconsin - Madison

Simulation in IC Engine Applications [abstract]

Angela Violi, University of Utah

Nanoparticle formation and transformation in diesels: a multiscale computational tool [abstract]

10:30 - 11:00am Break

11:00 - 12:00pm **Enabling Technologies, part 1**

Session Chair: William Gropp, Argonne National Laboratory

Christopher Johnson, University of Utah/ASC Alliance Center

Computational Multi-Field Visualization [abstract]

James R. Taft, Sienna Software/NASA Ames Research Center

Preliminary Science Results from NASA's 60 TFLOP Columbia System [abstract]

12:00 - 1:30pm Lunch (provided)

1:30 - 3:00pm

Agency Perspective

Session Chair: C. Edward Oliver

Associate Director, Advanced Scientific
Computing Research; Department of Energy

Dimitri Kusnezov

Director, Office of Advanced Simulation and Computing
Department of Energy

Charles Holland

Deputy Under Secretary of Defense, Science and Technology
Department of Defense

Raymond Orbach

Director, Office of Science
Department of Energy

Walter Brooks

Division Chief, Advanced Supercomputing Division
National Aeronautics and Space Administration

3:00 - 3:30pm Break

3:30 - 5:00pm ***High-End Computing and Science***

Session Chair: Richard Hilderbrandt, DOE Office of Science

Sidney Karin, University of California - San Diego

History and Future of High-Performance Computing and Science

John B. Bell, Lawrence Berkeley National Laboratory

Simulation of Reacting Flow [abstract]

Thomas L. Jackson, University of Illinois—Urbana-Champaign

*Recent Advances in the Numerical Simulation of Heterogeneous
Solid Propellant Combustion* [abstract]

Charles A. Wight, University of Utah

*Interdisciplinary Advanced Scientific Computing in Partnership with
DOE: A Worthwhile Exercise in Herding Cats* [abstract]

5:00 - 7:00pm Poster Session/Reception

WEDNESDAY, APRIL 27

7:00 - 8:30am Continental Breakfast

8:30 - 10:30am **High Speed Combustion**

Session Chair: Thomas Jackson, Air Force Research Laboratory

Robert Baurle, NASA Langley Research Center

High Performance Computing Issues Related to the Simulation of Scramjet Flow Fields [abstract]

K. Kailasanath, Naval Research Laboratory

Detonative Combustion – Science and Technology [abstract]

Joseph Oefelein, Sandia National Laboratories

Large Eddy Simulation of Liquid Rocket Injection and Combustion Processes [abstract]

Neeraj Sinha, Combustion Research & Flow Technology, Inc.

High Fidelity Simulation of Threat Ballistic Missile Plume Signature & Scramjet Propulsion Flow Fields [abstract]

10:30 - 11:00am Break

11:00 - 12:00pm **Enabling Technologies, part 2**

Session Chair: William Gropp, Argonne National Laboratory

Adolfy Hoisie, Los Alamos National Laboratory

Performance Modeling of Extreme-Scale Systems and Applications [abstract]

David Keyes, Columbia University

Letting Physicists be Physicists, and other Goals of Scalable Solver R&D [abstract]

12:00 - 1:30pm Lunch (on your own)

1:30 - 3:30pm **Gas Turbine Combustion**

Session Chair: Paul Bartolotta, NASA Glenn Research Center

Nan-Suey Liu, NASA Glenn Research Center

Comprehensive Combustion Modeling & Simulation [abstract]

Heinz Pitsch, Stanford University

Large-Eddy Simulation of Realistic Gas-Turbine Combustors [abstract]

Mel Roquemore, Air Force Research Laboratory/Wright Patterson
*Development of Simulations/Diagnostics and Their Use as a
Combustor Design Tool* [abstract]

Clifford E. Smith, CFD Research Corporation
Needed: A Next Generation Combustion LES Code [abstract]

3:30 - 4:00pm Break

4:00 - 5:00pm **Program Manager Session**
Session Chair: Michael Strayer, DOE Office of Science

Linda Blevins
Program Director, Combustion and Plasma Systems
National Science Foundation

Eric Rohlffing
Team Leader for Fundamental Interactions
Basic Energy Sciences, Department of Energy

Wing Tsang
NIST Fellow, Physical and Chemical Properties Division
National Institute of Standards and Technology

Julian Tishkoff
Program Manager, Combustion and Diagnostics
Air Force Office of Scientific Research

5:00pm Concluding Remarks

April 10-12, 2007
Omni Shoreham Hotel
Washington DC

CESC
COMPUTATIONAL ENGINEERING AND SCIENCE CONFERENCE

Agenda

MONDAY, APRIL 9

5:00 – 7:00pm Registration - *Empire Room foyer*

TUESDAY, APRIL 10

7:00 – 8:15am Registration and Continental Breakfast - *Empire Room foyer*

Technical Program - *Empire Room*

8:15 – 8:30am **Opening Remarks**

Conference Co-Chairs:

Alan Laub (University of California, Los Angeles)

Richard Martineau (Idaho National Laboratory)

8:30 – 9:15am **Keynote Talks**

Session Chair: Richard Martineau (Idaho National Laboratory)

Nuclear Reactor Simulation within GNEP

Speaker: Kathryn McCarthy (Idaho National Laboratory)

The Role of Modeling and Simulation in the Global Nuclear Energy Partnership

9:15 – 10:00am **Nuclear Reactor Simulation Technical Barriers**

Speaker: Marvin Adams (Texas A&M University)

Technical Barriers to High-Fidelity Reactor Simulations

10:00 – 10:30am Break

10:30 – Noon **Neutronics**

Session Chair: Robert Hill (Argonne National Laboratory)

Speakers: Jim Morel (Texas A&M University)

Deterministic Neutronic Barriers

Temitope A. Taiwo (Argonne National Laboratory)

Fast Reactor Applications

William R. Martin (University of Michigan)

Monte Carlo Methods

12:00 – 1:30pm Lunch (provided) - *Diplomat Room*

Speaker: Kord S. Smith (Studsvik Scandpower, Inc.)

Obstacles and Challenges for High End Computing in Nuclear Reactor Simulation – A Practical Perspective

1:30 – 3:00pm **Uncertainty Analysis**

Session Chair: Paul Turinsky (North Carolina State University)

Speakers: Giuseppe Palmiotti (Argonne National Laboratory)

Sensitivity and Uncertainty Analysis

William J. Rider (Sandia National Laboratories - Albuquerque)

What Can the Computational Modeling for GNEP Learn from the DOE ASC Program?

Dan G. Cacuci (Commissariat à l'Énergie Atomique)

Open Issues in Sensitivity and Uncertainty Analysis: A European Perspective

3:00 – 3:30pm Break

3:30 – 5:00pm **Structural Mechanics**

Session Chair: Gil Weigand (Oak Ridge National Laboratory)

Speakers: Ted Belytschko (Northwestern University)

Challenges in Computation of the Failure of Solids and Structures

Srdjan Šimunović (Oak Ridge National Laboratory)

Algorithmic/Simulation Opportunities in Modeling of Thermo-Mechanics of Nuclear Fuels

Paul Maudlin (Los Alamos National Laboratory)

Thermodynamically Consistent Material Modeling Involving Elastoplasticity, Damage and Thermal Effects

5:00 – 7:00pm Poster Session and Reception - *Diplomat Room*

Session Chair: Kimberlyn Mousseau (Idaho National Laboratory)

April 10-12, 2007
Omni Shoreham Hotel
Washington DC

CESC
COMPUTATIONAL ENGINEERING AND SCIENCE CONFERENCE

Agenda (cont'd)

WEDNESDAY, APRIL 11

7:00 – 8:30am Continental Breakfast - *Empire Room foyer*

Technical Program - *Empire Room*

8:30 – 10:00am **CFD/Heat Transfer**

Session Chair: Ray Berry (Idaho National Laboratory)

Speakers: Richard Saurel (Polytech Marseille and Institut Universitaire de France, France)

The Importance of Physically, Mathematically and Numerically Well-Designed Multiphase Flow Models

Simon Lo (CD-adapco, UK)

Requirements and Challenges in CFD and Multi-Physics Modeling for the Next Generation of Advanced Nuclear Reactors

Rainald Löhner (George Mason University, USA)

High-End Multi-Disciplinary Computing: Barriers, Challenges and Opportunities

10:00 – 10:30am Break

10:30 – Noon **Applied Mathematics and Algorithms**

Session Chair: David Keyes (Columbia University and Lawrence Livermore National Laboratory)

Speakers: John Shadid (Sandia National Laboratory)

Solution Methods for Multi-Time-Scale Multiphysics Systems

Phil Colella (Lawrence Berkeley National Laboratory)

Structured-Grid Adaptive Methods for Partial Differential Equations in Complex Geometries

Barry Smith (Argonne National Laboratory)

Multigrid/Multilevel Solvers

12:00 – 1:30pm Lunch (on your own)

1:30 – 3:00pm **Mesh Generation and Visualization**

Session Chair: Gary Miller (Carnegie Mellon University)

Speakers: Jonathan R. Shewchuk (University of California at Berkeley)

Why Mesh Generators with Correctness Proofs Will Win Out

Glen A. Hansen (Idaho National Laboratory)

Mesh Generation for Nuclear Reactor Simulation

Henry (Hank) Childs (Lawrence Livermore National Laboratory)

On the Importance of a Flexible Integrated Visualization and Analysis Environment

3:00 – 3:30pm Break

3:30 – 5:30pm **Policy Maker session – Federal Agency and Administration Perspective**

Session Chair: Alan Laub (University of California, Los Angeles)

Speakers: Peter B. Lyons (United States Nuclear Regulatory Commission)

Victor H. Reis (Office of the Secretary, United States Department of Energy)

Christopher King (Committee on Science and Technology, U.S. House of Representatives)

Kathryn Clay (Committee on Energy and Natural Resources, U.S. Senate)

5:30 – 7:00pm Reception - *Diplomat Room*

2010 ASCR CS PI Meeting

Generic Agenda

Day 1

7:30 am - 8:15 am Registration and Breakfast

8:15 am - 8:30 am Osni Marques –Opening Remarks

Session 1: Lightweight and Statistical Techniques for Petascale Debugging – *Meeting Room 1*

Session chair/moderator:

8:30 am - 9:15 am Invited speaker

Session 2: Correctness Tools for Petascale Computing - *Meeting Room 1*

Session chair/moderator:

9:15 am – 10:00 am Invited speaker

10:00 am - 10:30 am Break

Session 3: Fortran Transformational Tools in Support of Scientific Application Development for Petascale Computer Architectures - *Meeting Room 1*

Session chair/moderator:

10:30 am - 11:15 am Invited speaker

Session 4: A Scalable Development Environment for Peta-Scale Computing - *Meeting Room 1*

Session chair/moderator:

11:15 am - 12:00 pm Invited speaker

12:00 pm - 1:00 pm Lunch (group lunch provided) - *Meeting Room 2*

Session 5: A Multi-Language Environment for Programmable Code Optimazation and Empirical Tuning - *Meeting Room 1*

Session chair/moderator:

1:00 pm - 1:45 pm Invited speaker

Session 6: Automatic Transformation of MPI Programs to Asynchronous, Graph Driven Form – *Meeting Room 1*

Session Chair/moderator:

1:45 pm – 2:30 pm Invited speaker

Session 7: Composite Parallelisms: Creating Interoperatbility Between PGAS Languages, HPCS Languages and Message Passing Libraries - *Meeting Room 1*

Session chair/moderator:

2:30 pm – 3:00 pm Invited speaker

3:00 pm – 3:30 pm Break

**Session 8: Software Construction and Composition Tools for Petascale Computing –
*Meeting Room 1***

Session chair/moderator:

3:30 pm - 4:15 pm Invited speaker

Session 9: Model-Oriented Global Optimization of Petascale Applications – *Meeting Room 1*

Session chair/moderator:

4:15 pm - 5:00 pm Invited speaker

Poster Reception 6:00 pm - 8:00 pm

Day 2

7:30 am - 8:30 am Registration and Breakfast

Session 10: Performance Health Monitoring for Large-Scale Systems - *Meeting Room 1*

Session chair/moderator:

8:30 am – 9:15 am Invited speaker

**Session 11: An Optimizing Compiler for Petascale I/O on Leadership Class Architectures
- *Meeting Room 1***

Session chair/moderator:

9:15 am - 10:00 am Invited speaker

Session 12: Foundational Tools for Petascale Computing - *Meeting Room 1*

Session chair/moderator:

10:00 am - 10:45 am Invited speaker

10:45 am - 11:15 am Break

**Session 13: Building a Community Infrastructure for Scalable On-Line Performance
Analysis Tools Around Open SpeedShop - *Meeting Room 1***

Session chair/moderator:

11:15 am - 12:00 pm Invited speaker

12:00 pm - 1:00 pm Lunch and closing comments