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PROCEEDINGS
Fifth LACSI Symposium
October 12 – 14, 2004
Santa Fe, NM USA

### INTRODUCTION

The Fifth Symposium of the Los Alamos Computer Science Institute (<u>LACSI</u>) was held in Santa Fe, NM on October 12 –14, 2004. LACSI was formed at <u>Los Alamos National Laboratory</u> to conduct research in computer science issues relevant to DOE's Accelerated Strategic Computing Initiative (renamed <u>ASC</u>). The Institute focuses on research with a longer time frame than the operational requirements of ASCI, and supports work both at LANL and at LACSI-associated universities.

The technical program for 2004 addressed the current and future state of high performance computing in several ways.

- 9 peer-reviewed technical papers were presented to the Symposium and reproduced in this proceedings.
- 9 posters were presented at the poster session.
- The keynote address, titled "On Demand Processing, Query and Exploration of Distributed Petascale Datasets", was delivered by Professor Joel Saltz of the Ohio State University.
- Four panel discussions focused on important issues for researchers and managers in high performance computing.
- Ten workshops were held focusing on technical areas of particular importance to the LACSI community.





### TECHNICAL PROGRAM

The Fifth Symposium offered participants a wide variety of opportunities to discuss and learn about technical and policy issues in high-performance computing.

# **Tuesday, October 12: Workshop Sessions**

All Day Workshops: 9:00am - 5:30pm

*Open Source Development and Software Engineering Practices* Rod Oldehoeft (rro@lanl.gov; 505-665-3663)

Mimetic Methods for PDEs and Applications

Mikhail Shashkov (misha@t7.lanl.gov; 505-667-4400)

Python for High Productivity Computing

Craig E. Rasmussen (rasmussn@lanl.gov; 505-665-6021)

Performance and Productivity of Extreme-Scale Parallel Systems

Adolfy Hoisie (hoisie@lanl.gov; 505-667-5216)

Clustermatic: An Innovative Approach to Cluster Computing

Gregory Watson (gwatson@lanl.gov; 505-665-0726)

Path to Extreme Supercomputing

Erik P. DeBenedictis (epdeben@sandia.gov; 505-284-4017)

High Availability and Performance Computing Workshop

Stephen L. Scott (scottsl@ornl.gov; 865-574-3144)

Taking Your MPI Application To The Next Level: Threading, Dynamic Processes, &

Multi-Network Utilization

Richard L. Graham (rlgraham@lanl.gov; 505-665-5685)

# Morning Workshop: 9:00am - 12:30pm

Adaptive Mesh Refinement (half day AM)

Bobby Philip (bphilip@lanl.gov; 505-667-3844)

Michael Pernice (pernice@lanl.gov; 505-665-7119)

# Afternoon Workshop: 2:00pm - 5:30pm

Building Scalable Simulations of Complex Socio-Technical Systems (half day, PM)

James P. Smith (jpsmith@lanl.gov; 505-665-0921)





# Welcoming Reception and Poster Presentations: 6:00pm – 7:00pm

Workshops/tutorials on subjects of special interest to attendees, and the Welcome Reception and Poster Exhibit were featured. The posters were also made available over the next two days for additional inspection.

# POSTER PRESENTATIONS

Using Generic Programming Techniques with Procedural Finite Element Codes Fehmi Cirak and Julian C. Cummings (California Institute of Technology)

Cost-effective Performance-scalable Workstation Accelerators for High-resolution Volumetric Imaging

Robert Michael Lea, Aby Jacob Abraham, and Pawel Tomil Tetnowski (School of Engineering & Design, Brunel University, UK)

Reliability, Availability and Serviceability Management for HPC Linux Clusters: Self-awareness Approach

Stephen L Scott (ORNL); Chokchai Leangsuksun, Tong Liu, and Yudan Liu (Louisiana Tech University); Richard Libby (Intel); Ibrahim Haddad (Ericsson Research)

Design and Development of High Performances Parallel Particle in Cell (PIC) Stefano Markidis, Giovanni Lapenta, and W. Brian VanderHeyden (LANL)

#### MPI Collective Operation Performance Analysis

Jelena Pjesivac-Grbovic, Thara Angskun, George Bosilca, Graham Fagg, Edgar Gabriel, and Jack Dongarra (Innovative Computing Laboratory, University of Tennessee, Knoxville)

High Performance Simulation of Developmental Biology on a Hybrid Grid Frederic R. Fairfield (Fairfield Enterprises); Giovanni Lapenta and Stefano Markidis (LANL)

# A Sample-Driven Call Stack Profiler

Nathan Froyd, John Mellor-Crummey, and Robert J. Fowler (Rice University)

#### Reliability Costs in LA-MPI

Galen M. Shipman, Arthur B. Maccabe, and Patrick G. Bridges (The University of New Mexico)

Design and Implementation of Adifor90: Preliminary Results Michael Wayne Fagan (Rice University)





# Wednesday, October 13:

9:00am Welcoming remarks

9:30am: Keynote Address – "On Demand Processing, Query, and Exploration of Distributed Petascale Datasets"

Dr. Joel Saltz, Ohio State University

#### **Abstract:**

Increasing numbers of applications communities are demanding infrastructure to support efficient on-demand analysis and query of very large heterogeneous collections of distributed data. We will focus on recent developments that support high level language queries directed at very large datasets consisting of large numbers of files, mechanisms for global management of grid-based metadata definitions, and mechanisms for rapid definition and instantiation of databases used to cache grid-based data. We will describe application scenarios in biomedical research, earth science, and climate modeling. These application scenarios will be used to provide a broad view of what advances in systems software are needed to make this vision a reality; the application scenarios will also motivate a variety of focused performance studies that explore tradeoffs associated with different methods of optimizing performance of on-demand computations and queries.

#### 10:30am Break

# 11:00am - Reviewed Papers I: Systems

How To Build A Fast And Reliable 1024 Node Cluster With Only One Disk Erik Arjan Hendriks, Ronald Minnich, Los Alamos National Laboratory

An Event-driven Architecture for MPI Libraries

Supratik Majumder, Scott Rixner, Rice University; Vijay S. Pai, Purdue University

Layout Transformation Support for the Disk Resident Arrays Framework

Sriram Krishnamoorthy, Gerald Baumgartner, Chi-Chung Lam, The Ohio State University; Jarek Nieplocha, Pacific Northwest National Laboratory; P Sadayappan, The Ohio State University

12:30pm - 2:00pm Lunch





### 2:00pm - Reviewed Papers II: Compilation and Program Transformation

Exploring the Structure of the Space of Compilation Sequences Using Randomized Search Algorithms

Keith D. Cooper, Alexander Grosul, Timothy J. Harvey, Steve Reeves, Devika Subramanian, Linda Torczon, Todd Waterman, Rice University

Experiences with Sweep3D Implementations in Co-array Fortran Cristian Coarfa, Yuri Dotsenko, John Mellor-Crummey, Rice University

Automatic Tuning of Whole Applications Using Direct Search and a Performance-based Transformation System

Apan Qasem, Ken Kennedy, John Mellor-Crummey, Rice University

# 3:30pm - 4:00pm Break

### 4:00pm Reviewed Papers III: Applications and Performance

Rapid Prototyping Frameworks for Developing Scientific Applications: A Case Study Christopher D. Rickett, South Dakota School of Mines and Technology; Sung-Eun Choi, Craig E. Rasmussen, Matthew J. Sottile, Los Alamos National Laboratory

On the Use of a Two-Grids Method in the Numerical Simulation of Free Boundary Problems

Alexandre Caboussat, Roland Glowinski, University of Houston

Memory Performance Profiling via Sampled Performance Monitor Event Traces
Diana Villa, Jaime Acosta, Patricia Teller, The University of Texas at El Paso; Bret
Olszewski, IBM Corp.; Trevor Morgan, Exxon/Mobil Corp.

#### **ADJOURN**





# Thursday, October 14: Panel Discussions

Four panel discussions took place focusing on important issues for researchers and managers in high performance computing and a Closing Reception ended the LACSI Symposium.

#### 8:00am Breakfast

#### 9:00am - Panel I

# FPGAs in High Performance Computing

Use of Field-Programmable Gate Arrays is expanding from specialized embedded systems to more general-purpose application accelerators. Panelists will consider software support aspects and applications using FPGAs.

Wim Bohm, Colorado State University, Burton Smith, Cray, Inc., Maya Gokhale, Los Alamos National Laboratory, Keith Underwood, Sandia National Laboratories, Jeffrey Hammes, SRC Computers, Inc.

Moderator: Rod Oldehoeft, Los Alamos National Laboratory

#### 10:30am Break

#### 11:00am - Panel II

# Computer Science Innovations in ASC ASAP Centers

The ASC Academic Strategic Alliance Program Centers pursue advances in computational science, computer systems, mathematical modeling, and numerical mathematics important to Advanced Simulation and Computing. The panelists will discuss innovations in computer science that are contributing to the success of their Centers.

Michael Aivazis, California Institute of Technology, Tom Henderson, University of Utah, Eric Darve, Stanford University, Sanjay Kale, University of Illinois at Urbana-Champaign, Anshu Dubey, University of Chicago

**Moderator**: Karl-Heinz Winkler, Los Alamos National Laboratory

#### 12:30pm Lunch

2:00pm - Panel III

Panel III: HPC Languages of the Future

3:30pm Break

4:00pm - 5:30pm Panel IV

Panel IV: TBA at Production Time

5:30pm – 7:00pm Closing Reception





# SUPPLEMENTAL MATERIALS

VISTAR group, Electronic and Computer Engineering School of Engineering & Design Brunel University, UK

- Cost-effective performance-scalable workstation accelerators for high-resolution volumetric imaging
- Cone-beam X-ray CT reconstruction

Bobby Philip (bphilip@lanl.gov)
Michael Pernice (pernice@lanl.gov)
Computer and Computational Sciences Division
Los Alamos National Laboratory
P.O. Box 1663, MS B256
Los Alamos, NM 87545

• Workshop on Adaptive Mesh Refinement





#### SUPPORTING CAST

The 2003 LACSI Symposium was successful because of the combined efforts of many people.

#### **LACSI Co-Directors**

Andy White, Los Alamos National Laboratory Ken Kennedy, Rice University

# **Organizing Committee**

Rob Fowler, Program Chair, Rice University; Rod Oldehoeft, General Chair, LANL; Barney Maccabe, Local Arrangements Chair, University of New Mexico

# **Program Committee**

Rob Fowler, Rice University; Rod Oldehoeft, LANL; Michael Fagan, Rice University; Daniel Chavarria, Rice University; Patrick Bridges, University of New Mexico; Lennart Johnsson, University of Houston; Darren Kerbyson, LANL; Celso Mendes, University of Illinois at Urbana-Champaign; Shirley Moore, University of Tennessee

#### **External Reviewers**

Chuck Koelbel, Rice University; William Symes, Rice University; Alan Cox, Rice University; Lawrence Musson, Sandia National Laboratory; Manjunath Gorentla, University of New Mexico; Sinan Al-Saffar, University of New Mexico; Wenbin Zhu, University of New Mexico

### **Conference Arrangements**

Deborah G. Cole, Registration Coordinator, University of New Mexico; Barbara Daniels, Meeting Coordinator, Local Arrangements, University of New Mexico

### **Submission and Review Management Software and Service**

John Konkle, Linklings

### Symposium Web Pages and LACSI CDROM

Sarah Gonzales Rice University; John Konkle, Linklings

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