2008 e Science

4th IEEE International Conference on e-Science

Workshops and Special Sessions Detailed Programs

Monday, December 8, 8 a.m.–5 p.m. IUPUI Library, Room 1130

Riding the Geoscience Cyberinfrastructure Wave of Data: Real Time Data Use in Education

Organizers

- Beth Plale, Indiana University, USA
- Kelvin Droegemeier, Oklahoma University, USA
- Sepi Yalda, Millersville University, USA
- Cathy Brown, Indiana University, USA

Program

9–9:15 a.m.

Opening remarks: Beth Plale, School of Informatics, Indiana University

9:15–10 a.m.

Southeastern Universities Research Association (SURA) Coastal Ocean Observing and Prediction (SCOOP)
Sandra Harper, University of Alabama Huntsville

10–10:30 a.m.

Environmental Data on the Web: Really, How Valuable Is it In the Classroom Today?
Moderator: Adam Maltese, School of Education and Geology Department, Indiana University

10:30–10:45 a.m.

Break

10:45–Noon

The Potential of Grid-Enabled Learning for High Impace Weather with LEAD
Sepideh Yalda, Millersville University; Rich Clark

Noon–1 p.m.

Lunch
On your own

1–1:45 p.m.

Online CReSIS and Polar Resources for Education
Ryan Bowman, University of Kansas; Linda Hayden

1:45–2:30 p.m.

MAEviz: Exploring Earthquake Risk Reduction Strategies
Christopher Navarro, NCSA, University of Illinois at Urbana-Champaign; Jim Myers

2:30– 3:30 p.m.

How Cyberinfrastructure Can Facilitate STEM Education—Panel of Educators and Technologists
Moderator: Cathy Brown, School of Education, Indiana University; Adam Maltese; Polly Baker

3:30–4 p.m.

Closing Keynote

Monday, December 8, 1–5:00 p.m. Room 232

Project Management and User Engagement

Organizers

- Dimitrina Spencer, University of Oxford, UK
- Sharon Lloyd, University of Oxford, UK
- Marina Jirotka, University of Oxford, UK
- David Abramson, Monash University, Australia

Program

1–1:15 p.m.

Opening: **Why Project Management and User Engagement?**
Dimitrina Spencer, OeRC, Uiversity of Oxford, UK; Sharon Lloyd, Computing Laboratory, University of Oxford, UK; Marina Jirotka, OeRC, University of Oxford, UK; David Abramson, Monash e-Research Centre (MERC), Monash University, Australia

1:15–1:45 p.m.

Introduction: **Beyond Being There: How to Apply Lessons Learned about Virtual Organizations for Successful e-Science Projects**
Thomas Finholt, Crew, School of Information, University of Michigan, USA

Session 1: The Challenges of Distributed eResearch Projects

1:45–2 p.m.

Good Partners are Hard to Find: The Search for and Selection of Collaborators in the Health Sciences
Heiko Spallek, School of Dental Medicine, Titus Schleyer, School of Dental Medicine, and Brian Butler, Joseph M Katz Graduate School of Business, University of Pittsburgh, USA

2–2:15 p.m.

The Challenges of Distributed Scientific Collaboration among Top Scientists—A Case Study
Airong Luo, Office of Enabling Technologies, University of Michigan Medical School, USA

2:15–2:30

Why good software sometimes dies&mdash and how to save it
Neil Chue Hong, OMII-UK, ECS, University of Southampton; Alex Voss, National Centre for e-Social Science, University of Manchester, UK

2:30–3 p.m.
Session 1 Discussion
3–3:15 p.m.
Coffee Break
3:15–3:45
Keynote: Transforming Research
Stephen P. Meacham, Sr. Science and Technology Advisor, Office of Cyberinfrastructure, National Science Foundation, USA

Session 2: Case Studies in Project Management and User Engagement

3:45–4 p.m.
The Power of Cyberinfrastructure in Building Grassroot Networks: A History of the Pacific Rim Applications and Grid Middleware Assembly (PRAGMA) and Lessons Learnt in Developing Global Networks
Peter Arzberger, Chair PRAGMA Steering Committee, University of California, San Diego, USA; Grace S. Hong, London School of Economics
4–4:15 p.m.
Trials and Tribulations of a National Grid
Gillian Sinclair, UK National Grid Service (NGS)
4:15–4:30 p.m.
Managing and Engaging through the UK e-Science Program
Tony Hey, Microsoft and Anne Trefethen, OeRC, University of Oxford, UK
4:30–5 p.m.
Session 2 Discussion and Closing

Tuesday, December 9, 8 a.m.-5 p.m. Room 216

Introduction to Computational Science Resources and Tools

Organizers

- Shawn T. Brown, Pittsburgh Supercomputing Center (PSC) and Carnegie Mellon University, USA
- Scott Lathrop, TeraGrid, USA
- Laura F. McGinnis, Pittsburgh Supercomputing Center (PSC), USA
- Robert M. Panoff, Shodor Education Foundation, Inc., USA
- Charlie Peck, Earlham College, USA

Abstract

The participants in this full-day, hands-on workshop will learn about existing models and simulations available across a range of science, technology, engineering, and mathematics disciplines to engage students in interactive learning and scientific discovery. The participants will learn about resources they can directly apply in their classrooms. The participants will explore models that span a range of computing platforms from desktop level problem solving to high-performance computing solutions. The participants will also receive information on how to access high-performance computing resources via TeraGrid for class accounts and research projects.

Tuesday, December 9, 8 a.m.–Noon Room 232

International Grid Interoperability and Interoperation Workshop 2008 (IGIIW 2008)

Organizers

- Morris Riedel, Jülich Supercomputing Centre, Germany

Program

8–8:10 a.m.
Welcome and short IGIIW 2007 Reflection
Morris Riedel

TALK TOPICS: Interoperability in General

8:10–8:35 a.m.
Invited Talk: To be confirmed
8:35–9 a.m.
Talk 1: **Modeling and Evaluating Interoperable Grid Systems**
Ivan Rodero; Francesc Guim; Julita Corbalan
9:00–9:25 a.m.
Talk 2: **Integration of GridFTP as an Alternative File Transfer in UNICORE for the DEISA Infrastructure**
Michael Rambadt; Andrea Vanni; Ralph Niederberger
9:25–9:35
Break

TALK TOPICS: Interoperability of Infrastructures and Middleware

9:35–10 a.m.
Talk 3: **Towards Making BOINC and EGEE Interoperable**
P. Kacsuk; Z. Farkas; G. Fedak

10–10:25 a.m.
Talk 4: **Interoperability between ARC and gLite—Understanding the Grid-job Life Cycle**
M. Grønager; D. Johansson; J. Kleist; C. Søttrup; A. Wäänänen; L. Field; D. Qing; K. Happonen; T. Linden
10:25–10:50 a.m.
Talk 5: **Cross-Domain Middlewares Interoperability for Distributed Aircraft Design Optimization**
Yongjian Wang; D'Ippolito Roberto; Mike Boniface; Depei Qian; Degang Cui; Jiyun Jiang
10:50–11 a.m.
Break

TALK TOPICS: Interoperability of Information Services and Models

11–11:25 a.m.
Talk 6: **Functional Analysis and Architecture for Interoperable and DVO-specific Grid Monitoring Services**
Timo Baur
11:25–11:50 a.m.
Talk 7: **Grid Information System Interoperability: The Need For A Common Information Model**
Laurence Field; Sergio Andreozzi; Balazs Konya
11:50 a.m.–12:00 p.m.
Workshop Closing
Morris Riedel

Tuesday, December 9, 8 a.m.–12:45 p.m. Room 236

PRAGMA Workshop on e-Science Highlights

Organizers

- Kum Won Cho, Korea Institute of Science and Technology Information, South Korea
- Peter Arzberger, University of California, San Diego, USA

Program

8–8:15 a.m.
Introduction to Session
Kum-Won Cho and Peter Arzberger

Resources and Data Working Group Activities

8:15–8:40 a.m.
Interfacing SCMSWeb with Condor-G—A Joint PRAGMA-Condor Effort
Somsak Sriprayoonsakul; Putchong Uthayopos (TNGC); Jysoo Lee (KISTI); Cindy Zheng (SDSC); Miron Livney; Jaime Frey (U WI)
8:40–9:05 a.m.
Grid Workflows and Data-aware Plugins for Improved Metaschedulers CSF4
Zhaohui Ding; Xiaohui Wei, Yifan Zhu, Yaoguang Yuan (Jilin); Wilfred Li (NBCR, UCSD); Osamu Tatebe (U Tsukuba)
9:05–9:30 a.m.
Grid Interoperability: An Experiment in Bridging Grid Islands
Blaire Bethwaite; David Abramson; Ashley Buckle (Monash U)

Applications Using PRAGMA Grid Resources

9:30–9:55 a.m.
CFD Cyber Education Service Using Cyberinfrastructure
Jongbae Moon; Chongam Kim (SNU); Yoonhee Kim (Sookmyung); Kum Won Cho (KISTI)
9:55–10:20 a.m.
Identification of a Specific Inhibitor for the Dual-Specificity Enzyme SSH-2 via Docking Experiments on the Grid
Phil Pham; Marshall Levesque (UCSD); Kohei Ichikawa; Susumu Date (Osaka); Jason Haga (UCSD)
10:20–10:45 a.m.
Virtual Screening for SHP-2 Specific Inhibitors Using Grid Computing
Simon X Han; Marshall Levesque (UCSD); Kohei Ichikawa; Susumu Date (Osaka); Jason Haga (UCSD)

Biosciences, Telescience, Education

11 a.m.–11:25 p.m.
Bioscience: **Service Oriented Architecture for Managing Workflows of Avian Flu Grid**
Luca Clementi; Sriram Krishnan; Wesley Goodman; Jingyuan Ren; Wilfred Li (SDSC); Peter Arzberger (UCSD); Guillaume Vareille; Sargis Dallakyan; Michel Sanner (TSRI)
11:25–11:50 a.m.
Telescience: **Optimized Rendering for a Three-Dimensional Videoconferencing System**
Rachel Chu; Daniel Tenedorio; Jurgen Schulze (UCSD); Susumu Date; Seiki Kuwabara; Atsushi Nakazawa; Haruo Takemura (Osaka); Fang-Pang Lin (NCHC)
11:50 a.m.–12:15 p.m.
Education: **PRIUS: An Educational Framework on PRAGMA toward Fostering of Globally-leading Researchers in Integrated Sciences**
Susumu Date; Shoji Miyanaga; Kohei Ichikawa (Kansai); Shinji Shimojo (Osaka, NIICT); Haruo Takemura; Toru Fujiwara
12:15–12:45 p.m.
Discussion

Wednesday, December 10, 10 a.m.–12:30 p.m., Reconvening 1:30–6 p.m., Auditorium

e-Humanities—An Emerging Discipline

Organizers

- Peter Wittenburg (Chair), MPI, Nijmegen, The Netherlands
- Laurent Romary, MPDL, Berlin, Germany
- Sheila Anderson, AHDS, London, UK
- Peter Doorn, DANS, Den Haag, The Netherlands
- Tamas Varadi, Academy of Science, Budapest, Hungary
- Steven Krauwer, University Utrecht, The Netherlands

Program

9 a.m.
Keynote talk
10 a.m.
Introduction to the Workshop
P. Wittenburg
10:15 a.m.
No Claims for Universal Solutions
T. Blanke, A. Aschenbrenner, M. Küster, and C. Ludwig
11:15 a.m.
Coffee Break
11:30 a.m.
Managing and Integrating Very Large Multimedia Archives
D. Broeder, E. Auer, M. Kemps-Snijders, H. Sloetjes, P. Wittenburg, and C. Zinn
12:30 p.m.
Lunch Break
1:30 p.m.
The e-Linguistics Toolkit
S. Farrar and S. Moran
2:30 p.m.
Visualization of Dialect Data
E. Hinrichs and T. Zastrow
3:30 p.m.
Putting Data Categories in their Semantic Context
M. Kemps-Snijders, M. Windhouwer, and S. Wright
4:30 p.m.
eAQUA—Bringing Modern Text Mining Approaches to Two Thousand Year-old Ancient Texts
M. Buechler, G. Heyer, and S. Gründer
5:30 p.m.
Discussion and Conclusions
6 p.m.
End Workshop & Start Poster Session

Wednesday, December 10, 10 a.m.–Noon, Reconvening 1–5 p.m., Room 232

SWBES08: Challenging Issues in Workflow Applications

Organizers

- Adam Belloum, University of Amsterdam, The Netherlands
- Carole Goble, University of Manchester, UK
- Zhiming Zhao, University of Amsterdam, The Netherlands

Program

Session I

10–10:30 a.m.
A Tale of Two Workflows
Roger Barga
10:30–11 a.m.
Resource Provisioning Options for Large-Scale Scientific Workflows
Gideon Juve; Ewa Deelman
11–11:30 a.m.
Build Grid Enabled Scientific Workflows Using gRAVI and Taverna
Kyle Chard; Cem Onyuksel; Wei Tan; Dinanath Sulakhe; Ravi Madduri
11:30–Noon
Kairos: An Architecture for Securing Authorship & Temporal Info. of Provenance Data in Grid-Enabled Workflow Management Systems
Luiz Gadelha, Marta Mattoso

Session 2

1–1:30 p.m.
Where Experimental Work Flows
David de Roure
1:30–2 p.m.
Lattice QCD Workflows: A Case Study
Luciano Piccoli
2:30–3 p.m.
StrainInfo.net web services: Enabling Microbiologic Workflows Such as Phylogenetic Tree Building & Biomarker Comparison
Bert Versylppe; Bram Slabbinck; Wim De Sme; Paul De Vos; Bernard De Baets; Peter Dawyndt
3–3:30 p.m.
MRGIS: A MapReduce-Enabled High Performance Workflow System for GIS
Liqiang Wang; Qichang Chen; Zongbo Shang

Session 3

3:30–4 p.m.
A High-Level Distributed Execution Framework for Scientific Workflows
Jianwu Wang; Ilkay Altintas; Chad Berkley; Lucas Gilbert; Matthew Jones

4–4:30 p.m.
Capturing Workflow Event Data for Monitoring, Performance Analysis & Management of Scientific Workflows
Matthew Valerio; Satya Sahoo; Roger Barga; Jared Jackson

4:30–5 p.m.
On the Use of Cloud Computing for Scientific Workflows
Christina Hoffa; Gaurang Mehta; Ewa Deelman; Timothy Freeman; Kate Keahey; Bruce Berriman; John Good

5 p.m.
Discussion

Thursday, December 11, 10–11:30 a.m. Auditorium

Panel Discussion: Assessing the Potential Impact and Challenges of ManyCore Processors on eScience

Moderator

- Dennis Gannon

Panelists

- Jack Dongarra
- Satoshi Matsuoka
- Dan Reed
- Geoffrey Fox

Abstract

This panel will address the challenges that a shift to manycore architectures on eScience. Manycore refers to designs with 32 or more standard core or advanced hybrid architectures and GPUs. The panel will consider both opportunities and challenges.

Thursday, December 11, 1–5 p.m. Auditorium

Advances in High-Performance E-Science Middleware and Applications

Organizers

- Robert van Engelen, Florida State University, USA
- Madhu Govindaraju, SUNY Binghamton, USA
- Massimo Cafaro, University of Salento, Italy

Program

Session 1—Chair: Robert van Engelen

1–1:30 p.m.
Parallel Multidimensional Scaling Performance on Multicore Systems
Seung-Hee Bae

1:30–2 p.m.
Analysis of Cache Performance for Processing XML-based Application Data on Multi-core Processors
Rajdeep Bhowmik and Madhusudhan Govindaraju

2–2:15 p.m.
Break

Session 2—Chair: Madhusudhan Govindaraju

2:15–2:45 p.m.
DAGDA: Data Arrangement for the Grid and Distributed Applications
Gael Le Mahec, Eddy Caron, and Frédéric Desprez

2:45–3:15 p.m.
Coordinated Co-allocation Scheduling on Heterogeneous Clusters of SMPs
Ivan Rodero and Julita Corbalan

3:15–3:30 p.m.
Break

Session 3—Chair: Massimo Cafaro

3:30–4 p.m.
Resource Availability Prediction for Improved Grid Scheduling
Brent Rood and Michael J. Lewis

4–4:30 p.m.
An Adaptive XML Parser for Developing High-Performance Web Services
Wei Zhang and Robert van Engelen

Thursday, December 11, 10 a.m.–4 p.m. Room 236

Innovative and Collaborative Problem Solving Environments (PSE) in Distributed Resources: PSE Workshop08

Organizers

Co-Chairmen

- Soonwook Hwang, Korea Institute of Science and Technology Information (KISTI), Daejon, Korea
- Mo Mu, Dept. of Mathematics, Hong Kong University of Science and Technology, Hong Kong

Committee Members

- Ron Boisvert, Mathematics and Comput Sciences Division, NIST, USA
- Stratis Gallopoulos, University of Patras, Greece
- Ryutaro Himeno, RIKEN, 2-1, Hirosawa, Wako-shi, Saitama, Japan
- Elias Houstis, Department of Computer Eng and Comm, University of Thessaly, Greece
- Yoshimasa Kadooka, Fujitsu Lab, Fujitsu Co. LTD, Japan
- Shigeo Kawata, Graduate School of Engineering, Utsunomiya University, Japan
- David Meredith, Science and Technology Facilities Council, eScience Centre Daresbury Laboratory, UK
- Kimio Miyazawa, Fujitsu Lab, Fujitsu Co. LTD, Japan
- Naren Ramakrishnan, Department of Computer Science, Virginia Tech, USA
- Calvin J. Ribbens, Department of Computer Science, Virginia Tech, USA
- Yukio Umetani, Department of Computer Science, Shizuoka University, Japan
- Nancy Wilkins-Diehr, San Diego Supercomputer Center, University of California at San Diego, United States
- Heon-Young Yeom, Department of Computer Science and Engineering, Seoul National University, Korea
- Wu Zhang, School of Computer Science and Engineering, Shanghai University, China

Program

10–10:30 a.m.

The Problem Solving Environments of TeraGrid, Science Gateways, and the Intersection of the Two
Jim Basney, Stuart Martin, JP Navarro, Marlon Pierce, Tom Scavo, Leif Strand, Tom Uram, Nancy Wilkins-Diehr, Wenjun Wu, Coonhan Youn

10:30–11:00 a.m.

A Login Shell for Computing Grid
Xiaoning Wang, Jian Lin, Li Zha

11–11:30 a.m.

A Grid-enabled Problem Solving Environment for Supporting Collaboreative Aerodynamic Engineering Process
Junehawk Lee, Dukyun Nam, Soonwook Hwang, Ok-hwan Byeon

11:30 a.m.—1:30 p.m.

Lunch

1:30–2:00 p.m.

Jylab Meets Eclipse: Integrating PSEs with Multi-component Platforms
Giorgos Kollias, Kostantinos Georgiou, Strajs Gallopoulos

2:00–2:30 p.m.

Studies of Agent Composition Model of PSE- Bio Workflow
Jiang Xie, Wu Zhang, Guoyong Mao, Jian Mei

2:30–3:00 p.m.

e-Science Workbench: An Approach to Build Domain-specific Problem Solving Environments
Dongsoo Han, Soonwook Hwang

3–3:30 a.m.

A Distributed Linkage Method for a Large Amount of Event Data
Hiromichi Kobashi, Riichiro Take, Shigeo Kawata

Thursday, December 11, 10 a.m.–5 p.m. Room 232

Abstractions for Distributed Applications and Systems

Organizers

- Shantenu Jha, Louisiana State University and e-Science Institute, Edinburgh, USA and UK
- Murray Cole, University of Edinburgh, UK
- Dan Katz, Louisiana State University, USA
- Manish Parashar, Rutgers University, USA
- Omer Rana, Cardiff University, UK
- Jon Weissman, University of Minnesota, USA

2008 e-Science

4th IEEE International Conference on e-Science

Program

10:00 - 10:30 a.m.

Programming Models for Instrument-driven e-Science Workflows : Experiences with LEAD Science Gateway

Beth Plale (Indiana)

10:30 - 11:00 a.m.

Classification of Different Approaches for e-Science Applications in Next Generation Computing Infrastructures

Morris Reidel

11:00 - 11:30 a.m.

Using Small Abstractions to Program Large Distributed systems

Doug Thain

11:30 a.m.-1:00 p.m.

Lunch

1:00 - 1:30 p.m.

Towards Computational Abstractions over a RESTful Architecture

Dave de Roure

1:30 - 2:00 p.m.

LEAD

Surresh Marru

2:00 - 2:30 p.m.

Wool

Matthew Sottile

2:30 - 3:00 p.m.

Break

3:00 - 3:30 p.m.

Programming Abstractions for Multicore Clouds

Geoffrey Fox

3:30 - 4:00 p.m.

Applications and Classification of Workflows

Ewa Deelman

4:00 -5:00 p.m.

Informal Question and Answer

Friday, December 12, 9:30 a.m. – 11:30 a.m. Room 236

eScience for Cheminformatics and Drug Discovery

Organizers

- David Wild, Indiana University, USA
- Rajarshi Guha, Indiana University, USA
- Marlon Pierce, Indiana University, USA

Program

9:30-10:00

An Automatic Drug Discovery Workflow Generation Tool using Semantic Web Technologies

Xiao Dong, David Wild

10:00-10:30

SQMD: Architecture for Scalable, Distributed Database System built on Virtual Private Servers

Kangseok Kim, Rajarshi Guha, Marlon Pierce

10:30-11:00

DrugScreener-G: Towards an Integrated Environment for Grid-based Large-scale Virgual Screening & Drug Discovery

Jincheol Kim, Nhan Nguyen Dang, Sehoon Lee, Soonwook Hwang, Vincent Breton

11:00 – 11:30

Open Drug Discovery in Malaria Research

Jean-Claude Bradley, Rajarshi Guha, Philip Rosenthal, Khalid Mirza, Jiri Gut

Friday, December 12, 9:30 a.m.–Noon, Reconvening 2–3:30 p.m. Room 232

eBioinformatics

Organizers

- Mehmet Dalkilic, Indiana University—Bloomington, School of Informatics
- Jake Chen, Indiana University, School of Informatics; Purdue University, Department of Computer & Information Science
- Daisuke Kihara, Purdue University, Computer Science, Biological Sciences

Friday, December 12, 9:30 a.m.–Noon, Reconvening 2–5:00 p.m. Auditorium

Adding Value to Data—Digital Repositories in the e-Science World

Organizers

- Andreas Aschenbrenner, University of Göttingen, Germany
- Tobias Blanke, King's College London, UK
- Mark Hedges, King's College London, UK

Program

9:30–10:30 a.m.

Keynote by David de Roure, title TBC

10:30–10:45 a.m.

Virtual Poster Presentation: Synergies between Grid and Repository Technologies—A Methodical Mapping
Andreas Aschenbrenner, Tobias Blanke, Mark Hedges

10:45–11 a.m.

Break

11 a.m.–Noon

Paper: Rethinking Metadata Creation & Management in a Data-Driven Research
Ross Wilkinson, Andrew Treloar

Paper: A Wiki for Collaboration & Publication in Research
Christoph Von Hinten, Andreas Hense, Matthias Razum

2–4 p.m.

Expert panel on Adding value to data–Digital Repositories in an e-Science world
Confirmed presentation:

- Adil Hasan: SHAMAN
- Roger Barga: Microsoft Activities
- Reagan Moore: Preservation Management Policies
- Matthias Razum: eSciDoc
- Andrew Treloar: The Australian Programme

4–5 p.m.

Informal Networking and Discussion