



THE UNIVERSITY OF TEXAS AT AUSTIN
TEXAS ADVANCED COMPUTING CENTER

Supercomputing '09: TACC Demonstrates Largest Presence to Date

Visit TACC Booth #1545!

The Texas Advanced Computing Center (TACC) will have its largest presence to date at Supercomputing '09 (SC09), the international conference for high-performance computing, networking, storage and analysis, which runs from November 16-20 in Portland, Oregon. Emphasis on Scientific Visualization

“This is an exciting year for scientific visualization at SC09,” said Kelly Gaither, director of data & information analysis at TACC. “We’re in the process of constructing and deploying Longhorn, the largest hardware accelerated visualization cluster for use in the national open science community. The National Science Foundation has done a tremendous job of recognizing the importance of visualization resources to the advancement of science and engineering. We’re excited to deploy the first NSF XD Visualization resource.”

The visualization resources and capabilities that will be on display in TACC’s Booth are:

* **Colt:** A tiled display powered by a Dell graphics cluster that comprises multiple LCD panels and enables viewing of very large data sets at high resolution. Colt demonstrates the procedures and software used by TACC for the highest resolution single-tiled display in the world, Stallion, housed in its visualization laboratory at The University of Texas at Austin. These procedures are detailed in a white paper that will be distributed in the TACC booth.

* **Longhorn:** Soon to be the largest, hardware-accelerated visualization cluster in the world, capable of producing visualizations of data at unprecedented scale. TACC will showcase a subset of Longhorn with live demonstrations of remote and interactive large-scale visualizations to be displayed on Colt.

TACC staff will be available to discuss visualization, remote collaboration, high-speed data transfer, and to provide hands-on guidance

Top Computational Scientists to Provide Talks in TACC's Booth #1545

Some of the nation's top computational scientists will be in TACC's booth to discuss how access to TACC systems helps advance science. They will share their experiences and insights learned computing at the petascale level. The speakers include:

Omar Ghattas (The University of Texas at Austin), "Parallel Scalable Adaptive Mesh Methods for Solid Earth Geophysics Problems"

Tuesday, November 17, 10:30-11:15am.



Adaptive mesh refinement and coarsening (AMR) is essential for the numerical solution of partial differential equations (PDEs) that exhibit behavior over a wide range of length and time scales. Ghattas is developing a library for dynamic mesh adaptation of PDEs, called ALPS, that is designed to scale to hundreds of thousands of compute cores. Ghattas will present scalability

and performance results for several problems in solid earth geophysics.

Klaus Schulten (University of Illinois at Urbana-Champaign), "The Computational Microscope"

Tuesday, November 17, 1:30-2:30pm.



Over the past three decades computational biology has made great strides into simulating biomolecules at ever more relevant time scales and length scales. Today biomolecular assemblies can be followed for many microseconds and at multi-million atom size. This methodology will be demonstrated for the case of the ribosome, a machine in cells that

reads genetic information and synthesizes accordingly new proteins. The computational microscope will also be demonstrated as a key imaging technology in nanotechnological sensor development.

Diego Donzis (Texas A&M University), "High-Resolution Computations for Studies of Scaling in Turbulence and Turbulent Mixing"

Tuesday, November 17, 3:00-3:45pm.



Turbulence is very important to many fields of science and technology that depend on efficient transport of mass, momentum, and heat or chemical species as a result of disorderly fluctuations over a wide range of scales in space and time. The deployment of the 500-Teraflop system, *Ranger*, provided a timely opportunity for Donzis and his

collaborators to surpass the present "world-record" turbulence

TACC Presentations: Tutorials, Paper Presentations & BOFs

Several members of TACC's staff will give tutorials, present papers, and lead Birds-of-a-Feather discussions that highlight TACC's R&D and education and outreach efforts. The presentations are as follows:

"Hybrid MPI and OpenMP Parallel Programming," Gabriele Jost Tutorials Session, Monday, November 16, 8:30am-12:00pm, Room E141-142.



Most HPC systems are clusters of shared memory nodes. Such systems can be PC clusters with dual or quad boards and single or multi-core CPUs, but also "constellation" type systems with large SMP nodes. Parallel programming may combine the distributed memory parallelization on the node interconnect with the shared memory parallelization inside of each node. This tutorial analyzes the strength and weakness of several parallel programming models on clusters of SMP nodes.

"Composing and Executing Parallel Data-flow Graphs with Shell Pipes," Edward Walker, Weijia Xu and Vinoth Chandar

Paper presentation as part of the "Workshop on Workflows in Support of Large-Scale Science," Monday, November 16, 4:20-4:45pm.



This paper describes the design and implementation of the language extensions in Bourne Again Shell (BASH), and examines the performance of the system using micro and macro benchmarks. The implemented system is shown to scale to thousands of processors, enabling high throughput performance for millions of processing tasks on large commodity compute clusters.

"Developing and Teaching Courses in Computational Science," Brad Armosky

Birds-of-a-Feather Session, Tuesday, November 17, 12:15-1:15pm, Room D133-134.



The computational power and science potential of the new NSF-funded HPC resources are growing faster than the pool of talent who can use them. The Grand Challenges facing our world demand scientific discovery that will only be possible with new talent to apply these resources in industry and academia. During this 90-minute BoF, an expert panel will discuss their experiences and lead a dialogue

focused on how colleges and universities can develop courses for students to apply computational science and advanced computing.

"Data Curation," Chris Jordan

Birds-of-a-Feather Session, Tuesday, November 17, 5:30-7:00pm, Room D137-138.

simulation, while probing important physics with greater precision than before.

Martin Berzins (University of Utah), "Scalability of Adaptive Mesh Simulations of Fires and Explosions"

Wednesday, November 18, 10:30-11:15am.



Recently, NSF has funded two projects based on the Uintah software developed by multidisciplinary C-SAFE DOE project at Utah. The projects aim to show that the adaptive mesh and particle methods in Uintah can scale to the largest machines available and model a wide variety of challenging physical problems related to fluid-structure interaction, including some that arise from the transport of hazardous materials. The methods being used to solve these challenging problems will be discussed.

Rob Farber (Pacific Northwest National Laboratory), "Rounding Up a Full Posse with Ranger: 363 TF/s and Near-Linear Scaling to 60k Cores"

Wednesday, November 18, 1:30-2:30pm.



Ranger delivered over one third of a petaflop (363 TF/s) of useful floating-point throughput Farber's facial-recognition application and exhibited near-linear scaling to 60,000 processing cores. Additionally, he was able to fully exploit the Barcelona processor architecture to deliver 4 floating-point operations per clock during the computational phase.

Farber will discuss how having early access to the full machine emphasized the importance of the administrative and consulting staff in making large supercomputers perform well at scale.

Scott Callaghan (Southern California Earthquake Center), "Many-Task Computing on Ranger: The SCEC CyberShake Project"

Thursday, November 19, 10:30am-11:15am.



The Southern California Earthquake Center (SCEC) CyberShake project is using *Ranger* to calculate probabilistic seismic hazard curves using 3D ground motion simulations to replace empirically-based attenuation relationships. The hazard curves produced using 3D ground motion simulations can provide scientists, engineering groups, and emergency

responses organization with more accurate understanding of the seismic hazards in areas studied.



Management, utilization, and preservation of large datasets is a topic of growing importance to the scientific and HPC community. Increasingly more HPC centers are planning or implementing data curation services for certain classes of data collections. How will researchers work across collaborative organizations to enable HPC access for their long-term curated data? What can the researcher expect in terms of support for data curation both short-term and long-term within these data curation partnerships? This BOF will discuss these issues along with topics related to sustainable data curation arising from expanded HPC partnerships working with humanities, social sciences, and cultural heritage collections.

"iPlant Collaborative: Computational Scaling Challenges in Plant Biology," Dan Stanzione

Birds-of-a-Feather Session, Wednesday, November 18, 5:30-7:00pm, Room B117.



The Plant Science Cyberinfrastructure Collaborative (PSCIC) program is intended to create a new type of organization: a cyberinfrastructure collaborative for the plant sciences - that would enable new conceptual advances through integrative, computational thinking. To achieve this goal, we have developed the iPlant Collaborative (iPC). This session will provide a forum for members of the HPC community to learn more about the iPC, and how to become involved. We will particularly focus on the barriers to computational scalability in plant biology.

"Communicating Virtual Science," Aaron Dubrow

Birds-of-a-Feather Session, Wednesday, November 18, 5:30-7:00pm, Room E147-148



The conduct of computational science is an esoteric activity, but the results of that research are of interest and importance to everyone. "Communicating Virtual Science" will address the myriad ways writers communicate complex ideas about math, computer programming and discipline-specific research to lay and scientific audiences. Experts will debate which communication models are most suitable to

the changing media environment and what's at stake if we fail to make the case for science as a societal imperative.

"Evolving Interfaces to Impacting Technology: The Mobile TeraGrid User Portal," Rion Dooley

Grid Computing Environments Workshop, Friday, November 20, 11:20-11:40am, Room D139.



This 20 minute talk will detail experiences developing the mobile version of the TeraGrid User Portal.