SEARCH FOR NEW CRYSTAL STRUCTURES ON THE TERAGRID
- PI: Michael Deem (Rice) and David Earl (UPitt)
- Science goal: Generate > 2 million novel Zeolite crystal structures.
- Science progress: > 700k structures found using Purdue/TG resources so far.
- Running across multiple resources including Condor pool and multiple Resource Provider sites using MyCluster and GridShell.

MIXING ACROSS THE TURBULENT SHEAR LAYER IN A STAR
- PI: Woodward and Porter (U MN), TG: R Reddy (PSC/GIG)
- Pioneering explorations of the large-scale effects of small-scale turbulence.
- PPM code on 1025 PEs of XT3 at PSC sustains 1 TFLOP.
- Application sustained ~120 MB/s over 1 lambda using PDIO for visualization/steering.

REMOTE, REAL-TIME VISUALIZATION OF MULTIDIMENSIONAL BIOLOGY
- PI: Chris Gilpin, University of Texas Southwestern Medical Center
- Remote visualization of electron tomography data imaging neural synapses stained with phosphotungstic acid.
- Now visualizing structures scientists have never seen before.
- Visualizing the data using 64 bit parallel Paraview and currently looking at EnSight as a possible solution.

SOUTHERN CALIFORNIA EARTHQUAKE CENTER
- PI: David Okaya (USC), Kim Olsen (SDSU), TG Embeds Cui (SDSC), Reddy (GIG/PSC)
- Goal: Workflow tools to enable work at a scale previously unattainable.
- CyberShake workflow expanded to include both parallel jobs and post-processing jobs that run as Condor glide-ins.
- TeraShake code scaled up to 2048 processors, run time reduced from 4-5 days to 8 hours, and I/O time improved by 7x as well.
- Earthworks Science Gateway portal, grid-based workflow using Pegasus, file management using MCS/RLS, storage using SRB.

GRID INTEROPERATION: H-DIFFUSION IN ALUMINA
- Goal: building a Japan/TeraGrid Ninf/GT4 architecture to enable direct calculation of the energy states through a relatively long H-diffusion path in an inhomogeneously nano-stressed g-alumina, by combining the NEB (nudged elastic band) method and the hybrid MD-QM methods.

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Office of Cyberinfrastructure
THE MISSION IS TO ENGAGE LARGER AND MORE DIVERSE COMMUNITIES OF RESEARCHERS, EDUCATORS AND LEARNERS IN DISCOVERING, USING, AND CONTRIBUTING TO TERAGRID.

### Education
**Applying TeraGrid for Teaching and Learning Among All Ages.**
- Professional development
- Hands-on workshops
- Internships and fellowships
- On-line Learning
- Tools and Resources
- Life-long Learning
- Student Competitions
- Faculty and Teacher Awards
  - SC Education Program
  - Teacher@TCH
  - Clipyngo
  - Research Experiences for Undergraduates (REU)
  - Girls Engaged in Math and Science (GEMS)
  - Curriculum materials
  - Tutorials
  - Software

### Outreach
**Engaging People in Learning About and Using Cyberinfrastructure.**
- Science Gateways
- TeraGrid '07 Conference
- TeraGrid Science Highlights
- TeraGrid Speaker’s Bureau
- Engaging New Communities
- Campus Partnerships
  - Science Gateways
  - TeraGrid '07 Conference
  - Hands-on workshops
  - Self-paced Tutorials
  - Access Grid Seminars
  - Campus Training

### Training
**Applying TeraGrid for Teaching and Learning Among All Ages.**
- TeraGrid Institute Series
- TeraGrid '07 Conference
- Hands-on workshops
- Self-paced Tutorials
- Access Grid Seminars
- Campus Training
  - Parallel programming
  - Grid computing
  - Web services
  - Virtual Data System
  - Science Gateways
  - Curriculum development

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CHIPS TO GO
U.S.-Japan grid testbed links six supercomputers for quantum simulations of chip fabrication.

BOSON MATES
Physicists prepare for the Large Hadron Collider to come online with the help of TeraGrid resources and expertise.

THE REAL DEAL
With innovative algorithms and TeraGrid resources, economists are getting real with the life-cycle model.

THE BIG PICTURE
Massive mosaics let astronomers see the whole sky.

MAKING THE EARTH MOVE
TeraShake and Cybershake move seismology toward predictive science.

FEEL THE BIRN
TeraGrid-powered mapping tool distinguishes Alzheimer’s from normal brains.

KNOCK, KNOCK. WHO’S THERE?
TeraGrid simulations reveal new information about the gateway to the cell nucleus.

DUSTLING FLOW
TeraGrid resources power ground-breaking arterial simulations, providing insight into cardiovascular disease.

KETCHUP ON THE GRID
Transatlantic linked grids produce new understanding of liquid crystals.

NOVEL IMAGING
TeraGrid’s imaging resources provide new insights into proteins, leading to drugs that cure diseases.

NO' BETTER STORMWARNINGS
TeraGrid resources produce detailed, accurate storm forecasts a full day in advance.

STEP UP TO THE BAR DOMAIN
One of the largest biological simulations ever shows how banana-shaped proteins induce membranes to curve.

CAPTURED IN ICE
TeraGrid research helps validate data from a new kind of telescope and rules out some neutrino theories.

NOTHING TO SNEEZE AT
Nature publication shows the effectiveness of pandemic mitigation strategies.

INDUSTRY DARLINGS
A two-million-item database of zeolite structures is born of distributed computation using TeraGrid.

FUEL, CELL COMETH
By exploring some of fuel cell's most basic reactions, researchers are on their way to reducing costs and improving efficiency.

SPECIAL SECTION: TERAGRID’S IMPACT ON SCIENCE EDUCATION
With nanoHUB, a TeraGrid science gateway, simulation meets education.
TeraGrid provides some of the world’s most powerful computational resources, enabling deep computation that leads to scientific discovery.

More than 150 teraflops of peak computational capacity, over 30 petabytes of data storage, over 100 scientific databases, advanced workflow applications, and visualization services.

TeraGrid Science Gateway partners harness TeraGrid through discipline-specific portals, desktop applications, and community grid systems to support wide community access.

- Over 20 Science Gateways and workflow applications for researchers and educators to access TeraGrid capabilities with tools tailored to their own communities
- Education, Outreach and Training programs, workshops, on-line tutorials, and resources.

TeraGrid is an expanding, open, service-oriented architecture leveraging open standards, with strategic partnerships involving resource providers, researchers, technologists, educators, and campuses.

- National and international collaboration to address grid interoperability.
- Campus Partnerships are being developed with the goal of enabling campuses to extend TeraGrid resources to local communities, and to extend local resources to the national community.

RESOURCE PROVIDERS

- Indiana University
- National Center for Supercomputing Applications
- National Center for Atmospheric Research
- Oak Ridge National Laboratory
- Pittsburgh Supercomputing Center
- Purdue University
- San Diego Supercomputer Center
- Texas Advanced Computing Center
- The University of Chicago/Argonne National Laboratory

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CALL FOR PARTICIPATION

MADISON, WISCONSIN
JUNE 4-8, 2007
JOIN US FOR THE 2ND ANNUAL TERAGRID CONFERENCE!

CONFERENCE THEME:
BROADENING PARTICIPATION IN TERAGRID

PAPERS ARE BEING ACCEPTED IN FOUR TRACKS:
→ Science
→ Technology
→ Education, Outreach and Training
→ Demonstrations

STUDENT SUBMISSIONS ARE BEING ACCEPTED FOR TWO COMPETITIONS:
→ What is Cyberinfrastructure
→ Research posters

The competitions are open to high school students, undergraduate students and graduate students.