TeraGrid: Enabling Terascale Science

Jay Boisseau
Texas Advanced Computing Center
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“Initial Conditions”

• Computation is increasingly important in sci/eng R&D
• High-end computing is increasingly important within computational science
  – Many important problems are resource-limited (CPU, memory, disk)
  – Access to massive computing (HPC, grid) is crucial for advancement, but bottlenecked
• Data explosion is real—from instruments and from simulation
  – Data collections are ‘expensive’ and often unique
  – Visualization is a primary method of scientific data analysis
• Research often requires diverse types of resources (serial, HPC, storage, data, visualization, instruments)
• Integrating diverse resources through software and networking can increase capability, effectiveness, impact
• Cyberinfrastructure includes all these components
What is the TeraGrid?

• TeraGrid is the largest cyberinfrastructure (CI) project in the US, connecting computing, storage & visualization systems, data collections, and instruments with high speed networks and grid computing software.

• The TeraGrid mission is to enable and facilitate DEEP Science and make a WIDE impact with an OPEN infrastructure.
TeraGrid Objectives

• DEEP Science: Enabling Terascale Science
  – Make Science More Productive through an integrated set of very-high capability resources.

• WIDE Impact: Empowering Communities
  – Bring TeraGrid capabilities to the broad science community.

• OPEN Infrastructure, Open Partnership
  – Provide a coordinated, general purpose, reliable set of services and resources.
# TeraGrid Resources

<table>
<thead>
<tr>
<th>Compute Resources</th>
<th>ANL/UC</th>
<th>IU</th>
<th>NCSA</th>
<th>ORNL</th>
<th>PSC</th>
<th>Purdue</th>
<th>SDSC</th>
<th>TACC</th>
</tr>
</thead>
<tbody>
<tr>
<td>Itanium 2 (0.5 TF)</td>
<td>Itanium2 (0.2 TF)</td>
<td>Itanium2 (10.7 TF)</td>
<td>IA-32 (0.3 TF)</td>
<td>XT3 (10 TF)</td>
<td>Hetero (1.7 TF)</td>
<td>Itanium2 (4.4 TF)</td>
<td>X86-64 (55 TF)</td>
<td></td>
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<tr>
<td>IA-32 (0.5 TF)</td>
<td>IA-32 (2.0 TF)</td>
<td>SGI SMP (7.0 TF)</td>
<td>IA-32 (11 TF)</td>
<td>TCS (6 TF)</td>
<td>IA-32 (11 TF)</td>
<td>Power4+ (15.6 TF)</td>
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<tr>
<td></td>
<td></td>
<td>Dell Xeon (17.2 TF)</td>
<td>Marvel (0.3 TF)</td>
<td></td>
<td>Marvel (0.3 TF)</td>
<td>Blue Gene (5.7 TF)</td>
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<tr>
<td></td>
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<td>IBM p690 (2 TF)</td>
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<tr>
<td></td>
<td></td>
<td>Condor Flock (1.1TF)</td>
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</tbody>
</table>

<table>
<thead>
<tr>
<th>Storage</th>
<th>20 TB</th>
<th>32 TB</th>
<th>1140 TB</th>
<th>1 TB</th>
<th>300 TB</th>
<th>26 TB</th>
<th>1400 TB</th>
<th>50 TB</th>
</tr>
</thead>
</table>

<table>
<thead>
<tr>
<th>Mass Storage</th>
<th>1.2 PB</th>
<th>5 PB</th>
<th>2.4 PB</th>
<th>1.3 PB</th>
<th>6 PB</th>
<th>2 PB</th>
</tr>
</thead>
</table>

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<tr>
<th>Net Gb/s, Hub</th>
<th>30 CHI</th>
<th>10 CHI</th>
<th>30 CHI</th>
<th>10 ATL</th>
<th>30 CHI</th>
<th>10 CHI</th>
<th>40 LA</th>
<th>10 CHI</th>
</tr>
</thead>
</table>

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<tr>
<th>Data Collections</th>
<th>5 (&gt;3.7 TB)</th>
<th>&gt; 30 Col.</th>
<th></th>
<th>4 (7 TB)</th>
<th>&gt;70 (&gt;1 PB)</th>
<th>4 (2.35 TB)</th>
</tr>
</thead>
</table>

| Instruments | Proteomic X-ray Cryst. | SNS | | | | |
|-------------|------------------------|-----|--------|---|---|

<table>
<thead>
<tr>
<th>Visualization Resources</th>
<th>RI, RC, RB</th>
<th>RI-32, 96</th>
<th>RB</th>
<th>RI, RB</th>
<th>RI, RB</th>
<th>RB</th>
<th>RI, RC, RB</th>
</tr>
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<tbody>
<tr>
<td></td>
<td>GeForce 6600GT</td>
<td>SGI Prism, 32 graphics pipes; IA-32</td>
<td>980 XGL</td>
<td>IA-32 + Quadro4 Nodes</td>
<td>IA-32, 48 Nodes</td>
<td>USPARC IV, 512GB SMP, 16 gfx cards</td>
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TeraGrid Approach

- **A single point of contact** for user assistance.
- **A common allocation process** that includes a currency usable on all systems, while preserving the need to provide specific machine access to users with specific needs.
- **A common access service and environment** on all platforms, allowing users to readily move from machine to machine as needed. *Learn Once; Run Anywhere.*
- **Services to assist users in harnessing the right TeraGrid platforms for each part of their work**, ranging from tightly-coupled applications (MPICH-G2) to workflow (Condor-G, GridShell), file staging (GridFTP/RFT) and remote file I/O (GPFS), supported by common authentication (GSI), and in 2006 Web services via GT4.
- **New capabilities driven** by tight feedback loop with **users** via surveys and hands-on projects.
- **Science Gateways** build on this architecture (common definitions, interfaces) to reach communities.
Delivering User Priorities in 2005

Results of in-depth discussions with 16 TeraGrid user teams during first annual user survey (August 2004).
TeraGrid Use

- Biology: 26%
- ENG: 12%
- Physics: 15%
- Astronomy: 9%
- Materials: 5%
- Math: 1%
- CS/Eng: 7%
- GEO: 4%
- Social Sciences: 0%
- Chem: 21%

Annual Growth ~33%

Monthly Usage (Millions of NU)

Total Monthly Usage

Monthly Roaming Usage
Predicting Severe Weather
Droegemeier (OU) and LEAD

Earthquake Simulation
Olsen (SDSU), Okaya (USC), Southern California Earthquake Center
Turbulent Fluid Dynamics

Woodward (UMinn)

Full Body Arterial Tree Simulation

Karniadakis (Brown)
TeraGrid Science Support

- Two primary methods for advanced support:
  1. ASTA Support for facilitating DEEP science
  2. Science Gateways for enabling WIDE impact to a broad science community
Advanced Support for TeraGrid Applications (ASTA)

- Inaugurated 6/1/05; 10 projects now underway
- Already enabled remarkable new science using TG-deployed software … including the SC05 Analytics Challenge winner.
- Help users to:
  - Achieve their science objectives
  - Utilize TeraGrid resources interestingly and effectively
- Improve the quality of the TeraGrid infrastructure
  - Provide feedback to staff when testing, piloting and exercising TeraGrid capabilities
- Selection by TG staff, NSF, PIs willing and able to assign developer time from within their project.
<table>
<thead>
<tr>
<th>Project</th>
<th>Discipline</th>
<th>End Date</th>
</tr>
</thead>
<tbody>
<tr>
<td>Cellulose + Cellulase interactions using CHARMM, PI Brady</td>
<td>Molecular Dynamics</td>
<td>3/31/2006</td>
</tr>
<tr>
<td>Port, Scale and Optimize Code</td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>MD Data Repository, PI Jakobsson</strong></td>
<td>Molecular Dynamics</td>
<td>3/31/2006</td>
</tr>
<tr>
<td>Implementation of architectural components</td>
<td></td>
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</tr>
<tr>
<td><strong>Liquid Rocket Engine Coaxial Injector Modeling, PI Heister</strong></td>
<td>Computational Fluid Dynamics</td>
<td>3/31/2006</td>
</tr>
<tr>
<td>Computational model development and implementation</td>
<td></td>
<td></td>
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<tr>
<td><strong>NekTar Arterial Tree Simulations, PI Karniadakis</strong></td>
<td>Computational Fluid Dynamics</td>
<td>3/31/2006</td>
</tr>
<tr>
<td>Code porting and optimization; MPICH-G2 and visualization support</td>
<td></td>
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<tr>
<td><strong>Vortonics: CFD with Vortex Degrees of Freedom, PI Boghosian</strong></td>
<td>Computational Fluid Dynamics</td>
<td>3/31/2006</td>
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<tr>
<td>MPICH-G2 and visualization support</td>
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</tr>
<tr>
<td><strong>SPICE Non-Equilibrium Simulations, PIs Coveney and Boghosian</strong></td>
<td>DNA Modeling</td>
<td>3/31/2006</td>
</tr>
<tr>
<td>Code deployment, grid and steering implementation support</td>
<td></td>
<td></td>
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<tr>
<td><strong>ENZO Cosmic Simulator, PI Norman</strong></td>
<td>Cosmology</td>
<td>3/31/2006</td>
</tr>
<tr>
<td>Code optimization and scaling, network data handling and archiving</td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>SCEC TeraShake-2 and CyberShake, PI Olsen</strong></td>
<td>Seismology</td>
<td>3/31/2006</td>
</tr>
<tr>
<td>Code optimization, TG data handling and archiving, task flow mapping</td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>CIG: Cyberinfrastructure for Geodynamics, PI Gurnis</strong></td>
<td>Geophysics</td>
<td>5/31/2006</td>
</tr>
<tr>
<td>Develop software framework, repository, portal and training</td>
<td></td>
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</tr>
<tr>
<td><strong>BIRN (Biomedical Informatics Research Network), PI Ellisman</strong></td>
<td>Biomedical Imaging</td>
<td>9/30/2006</td>
</tr>
<tr>
<td>Develop and optimize codes; map task flows to TG</td>
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</table>
Simulation of Blood Flow in Human Arterial Tree on the TeraGrid

Supported by NSF and TeraGrid

Team Members

**Brown University:** S. Dong, L. Grinberg, A. Yakhot, G.E. Karniadakis

**Imperial College, London:** S.J. Sherwin

**Argonne National Lab:** N.T. Karonis, J. Insley, J. Binns, M. Papka

**ASTA:** D.C. O’Neal, C. Guiang, J. Lim
Simulating & Visualizing Human Arterial Tree

Computation

USA
- TACC
- NCSA
- TERAGRID

UK
- CSAR

Visualization

ANL
- Viz servers

Viewer client

SC05, Seattle, WA
Science Gateways

Achieving Wide Impact

- Increasing investment by communities in their own cyberinfrastructure, but heterogeneous:
  - Resources
  - Users – from expert to K-12
  - Software stacks, policies
- Science Gateways
  - Provide “TeraGrid Inside” capabilities
  - Leverage community investment
- Three common forms:
  - Web-based Portals
  - Application programs running on users' machines but accessing services in TeraGrid
  - Coordinated access points enabling users to move seamlessly between TeraGrid and other grids.
# Science Gateways Span Communities

<table>
<thead>
<tr>
<th>Science Gateway Prototype</th>
<th>Discipline</th>
<th>Science Partner(s)</th>
<th>TeraGrid Liaison</th>
</tr>
</thead>
<tbody>
<tr>
<td>Linked Environments for Atmospheric Discovery (LEAD)</td>
<td>Atmospheric</td>
<td>Droegemeier (OU)</td>
<td>Gannon (IU), Pennington (NCSA)</td>
</tr>
<tr>
<td>National Virtual Observatory (NVO)</td>
<td>Astronomy</td>
<td>Szalay (Johns Hopkins)</td>
<td>Williams (Caltech)</td>
</tr>
<tr>
<td>Network for Computational Nanotechnology (NCN) and “nanoHUB”</td>
<td>Nanotechnology</td>
<td>Lundstrum (PU)</td>
<td>Goasguen (PU)</td>
</tr>
<tr>
<td>Open Life Sciences Gateway</td>
<td>Biomedicine and Biology</td>
<td>Schneewind (UC), Osterman (Burnham/UCSD), DeLong (MIT), Dusko (INRA)</td>
<td>Stevens (UC/Argonne)</td>
</tr>
<tr>
<td>Biology and Biomedical Science Gateway</td>
<td>Biomedicine and Biology</td>
<td>Cunningham (Duke), Magnuson (UNC)</td>
<td>Reed (UNC), Blatecky (UNC)</td>
</tr>
<tr>
<td>Neutron Science Instrument Gateway</td>
<td>Physics</td>
<td>Cobb (ORNL)</td>
<td>Cobb (ORNL)</td>
</tr>
<tr>
<td>Grid Analysis Environment</td>
<td>High-Energy Physics</td>
<td>Newman (Caltech)</td>
<td>Bunn (Caltech)</td>
</tr>
<tr>
<td>Transportation System Decision Support</td>
<td>Homeland Security</td>
<td>Stephen Eubanks (LANL)</td>
<td>Beckman (Argonne)</td>
</tr>
<tr>
<td>Open Science Grid [GrPhyN/ivDGL/Grid3]</td>
<td>Multiple</td>
<td>Pordes (FNAL), Huth (Harvard), Avery (UFlorida)</td>
<td>Foster (UC/Argonne), Kesselman (USC-ISI), Livny (UW)</td>
</tr>
</tbody>
</table>
Science Gateway Examples

Nano-technology: nanoHUB.org

NCN PI: Mark Lundstrom, Gerhard Klimeck, Purdue University
TeraGrid PI: Sebastian Goosguen, Purdue University

NVO Service Framework

co-PI: Roy Williams, Caltech
co-PI: Julian Bunn, Caltech

National Microbial Bioinformatics Resource Center (NMBR)

PI: Rick Stevens, Argonne National Laboratory / University of Chicago
PI: Dint Schneeewind, University of Chicago

Open Science Grid

Bioinformatics Science Gateway

PI: Daniel A. Reed, RENCI

Flood Modeling

Project Lead: Bill Barth, TACC
Project Members: David Guzman, Patrick Hurley Tomsilov Urban, TACC

LEAD Gateway

PI: Dennis Gannon, Indiana University

Grid Portals for LHC Particle Physics

Co-PIs: Julian Bunn & Roy Williams, California Institute of Technology

TACC
TeraGrid Campus Partnerships

- Campus (organization) CI is ‘fundamental’
  - Increasing emphasis on effective utilization of ‘owned’ resources
  - Campuses have
    - 10K+ CPUs
    - unique data and instruments
    - in-person opportunities for vis, support
    - education, training
  - Campuses are appropriate for identify authentication

- TeraGrid exploring methods for campus partnership
  - Make it easier for campus users to use TG
  - Enable campuses to contribute resources to TG
TeraGrid Industrial Partnerships

• No formal TG-wide program yet, but
  – Some resource providers (RPs) have some industrial partners program
  – NSF encourages academic/industry cooperation
  – TeraGrid provides resources of scale attractive even to large companies
    • Very large HPC (50-100 Tflops very soon))
    • Remote large-scale visualization, massive data storage
    • EXPERTISE (optimization, data analysis, training, etc.)
  – Forthcoming Track2 system may have % of cycles for industrial partners…
Final Comments

- HPC now mainstream, and parallel computers now ‘all computers’ (multi-core)
- I/O and data analysis is increasingly a bottleneck as HPC systems grow
- Network bandwidth has made remote data usage & remote visualization possible
- Increased capability, but increased usage complexity. Need:
  - More gateways, community apps, frameworks, libraries
  - More education & training
  - More funding for high-end apps development
  - More algorithm R&D (fault/latency/bandwidth tolerance, asynchronous distributed computing, etc.)
More Information & Questions

- TeraGrid web site: www.teragrid.org
- TeraGrid User Portal: portal.teragrid.org
- User support: help@teragrid.org

Feel free to contact me:
Jay Boisseau, boisseau@tacc.utexas.edu