Overview of HPC at LONI

Le Yan
HPC Consultant
User Services @ LONI
What Is HPC

- High performance computing is to use supercomputers to solve problems computationally
  - The most powerful supercomputer today can execute more than $10^{15}$ floating point operations per second (1 Petaflops)
  - Top 500 list: the semi-annually published list of most powerful supercomputers (http://www.top500.org)
- May also involve
  - Massive storage space
  - High speed network
  - Large-scale visualization
Why Uses HPC

- HPC may be the only way to achieve specific computational goals in a given time
  - Size: Many problems that are interesting to scientists and engineers cannot fit on a PC - usually because they need more than a few GB of RAM, or more than a few hundred GB of disk.
  - Speed: Many problems that are interesting to scientists and engineers would take a very long time to run on a PC: months or even years; but a problem that would take a month on a PC might only take a few hours on a supercomputer
Louisiana Investments in IT (NSF Report: The Louisiana Model)

- Multiple Layers: Each reinforces the next
  - 2001-3: Vision 2020
    - Gov. Foster: $25M annual across 5 campuses
    - 2003: CCT, $9M annual at LSU, LITE Center, ULL
  - 2004: Louisiana Optical Network Initiative (LONI)
    - Gov. Blanco: $40M + $10M infrastructure
  - 2007: CyberTools and LONI Institute and beyond
    - Develop software and recruit people
  - 2007: $16M FCC grant connects over 100 hospitals to LONI
What is LONI

• LONI Base
  • A state-of-the-art fiber optics network that runs throughout Louisiana and connects Louisiana and Mississippi research universities
  • $40M Optical Network, 4x 10 Gb lambdas (10 Gb Ethernet over fiber optics)
  • $10M Supercomputers installed at 6 sites, centrally maintained by HPC @ LSU
What is LONI

- Cybertools ([http://cybertools.loni.org](http://cybertools.loni.org))
  - Tools on top of LONI base
  - $12M statewide NSF/EPSCOR Cyberinfrastructure project
- LONI Institute ([http://institute.loni.org](http://institute.loni.org))
  - Collaborations on top of LONI base and Cybertools
  - $15M statewide project to recruit computational researchers
LONI Members

- 8 LONI member institutions
  - LSU, ULL, LaTech, Tulane, UNO, Southern, LSUHSC at New Orleans, LSUHSC at Shreveport
- 19 LONI associate institutions in Louisiana and Mississippi
- 50 community and technical colleges
- 2 LONI partners
  - Louisiana Public Broadcasting (LPB)
  - Louisiana Department of Transportation and Development (DOTD)
LONI Fiber Routes

- LSU HSC @ 20 Gbps
- La Tech @ 40 Gbps
- ULL @ 60 Gbps
- SU @ 40 Gbps
- LSU @ 40 Gbps
- UNO @ 40 Gbps
- LSU HSC @ 20 Gbps
- Tulane @ 40 Gbps
LONI Network Connections
LONI Links to NLR

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LONI High Performance Computing Workshop – Tulane University
April 13, 2009
LONI Supercomputing Grid

• 12 supercomputers hosted at seven campuses
  • 11 currently online
LONI Dell Linux x86 clusters

- Queen Bee: 50 TeraFlops centerpiece
  - 77th in the Nov 2008 Top 500 list
  - Hosted at the state's Information Systems Building
  - 668 nodes with 8 Intel Xeons cores @ 2.33 GHz, 8 GB RAM
  - 192 TB storage
- Six 5 TeraFlops clusters
  - Online: Eric(LSU), Oliver(ULL), Louie(Tulane), Poseidon(UNO), Painter (LaTech)
  - To be installed: Satelite(Southern)
  - 128 nodes with 4 Intel Xeons cores @ 2.33 Ghz, 4 GB RAM
LONI IBM p575 clusters

• Five p575 systems
  • Bluedawg(LaTech), Dukcy(Tulane), Zeke(ULL), Neptune(UNO), Lacumba(Southern)

• Hardware info
  • 14 nodes with 8 IBM Power 5 processors @ 1.9 GHz, 16 GB RAM, 2 146GB HDD, 1 Federation switch, 4 1Gb Ethernet
  • 0.851 TeraFlops theoretical peak each; a total of 4.256 total TeraFlops
LONI HPC System Usage

LONI Supercomputers Usage Statistics

- Total Usage (SU Hours)
- Total Available SU Hours (95% Total Machine SU Hours)

Month: Aug-06, Sep-06, Oct-06, Nov-06, Dec-06, Jan-07, Feb-07, Mar-07, Apr-07, May-07, Jun-07, Jul-07, Aug-07, Sep-07, Oct-07, Nov-07, Dec-07, Jan-08, Feb-08, Mar-08, Apr-08, May-08, Jun-08, Jul-08

SU Hours: 0, 500000, 1000000, 1500000, 2000000, 2500000, 3000000, 3500000, 4000000, 4500000, 5000000, 5500000, 6000000
Who Uses LONI HPC Resources

From 7/1/07 to 9/30/08

- Astronomy/Astrophysics: 40%
- Computational Fluids/Hydro: 25%
- Chemistry: 8%
- Biology Systems/Biophysics: 4%
- Math & Computer Science: 19%
- Atmos/Earth/Ocean Science: 12%
- Physics: 8%
- Material Science: 8%
- Biochemistry: 4%
- Grid/Portals: 4%
- Training: 4%

LONI High Performance Computing Workshop – Tulane University
April 13, 2009
Who Uses TeraGrid Resources

- Louisiana biology researchers are catching up
  - Louisiana Biology Research Network (LBRN)
  - http://lbrn.lsu.edu/portal/
LONI User Services

- Provided by LSU HPC User Services group
  - User support
  - Software management and maintenance
  - Portal development and maintenance (http://portal.loni.org)
  - User training
- Where to seek for help
  - LONI website: http://www.loni.org
  - LONI user documentation: http://docs.loni.org
  - LONI ticket system: sys-help@loni.org
  - Live help: lsuhpchelp (AIM, GoogleTalk, Yahoo Messenger)
Introduction to TeraGrid

Thanks go to Dr. Honggao Liu, Raju Gottumukkala (and everyone else they acknowledged in their presentations)
Outline

- TeraGrid overview
- Science highlight of TeraGrid
- Getting started on TeraGrid
What Is TeraGrid

- NSF-sponsored computational environment for scientists
- World's largest open scientific discovery infrastructure
  - An Integrated persistent computational platform
    - High Performance Networks, Computers (>1090 TFlops) & Visualization (>60 TFlops), Data (>30 PB)
    - Science Gateways
    - User Portal & Services
- CPU Cycles allocated through a national peer-review process
Operation and Research

- **Operations**
  - Facilities/services on which users rely
  - Infrastructure on which other providers build

- **Research**
  - Learn how to do distributed, collaborative science on a global, federated infrastructure
  - Learn how to run multi-institution shared infrastructure
TeraGrid Resource Providers
TeraGrid Supercomputers
TeraGrid Usage

TeraGrid by Discipline, Q3 2007

- All 18 Other Disciplines
- Advanced Scientific Computing
- Chemical, Thermal Systems
- Cross-Disciplinary Activities
- Earth Sciences
- Materials Research
- Astronomical Sciences
- Chemistry
- Physics
- Molecular Biosciences
TeraGrid Science Highlight

How To Use TeraGrid

TeraGrid Infrastructure
(Accounting, Network, Authorization,...)

POPS (for now)
User Portal
Science Gateways
Command Line

RP

Compute Service
Viz Service
Data Service
TeraGrid Allocations

- POPS (https://pops-submit.teragrid.org) is the online system used for the allocations process
  - Requests
  - Peer reviews
  - Usage information
- Two types of allocation

<table>
<thead>
<tr>
<th>Meeting</th>
<th>Service Units (SUs) range (K=1000)</th>
<th>Open submissions</th>
<th>Close submissions</th>
<th>Allocations begin</th>
<th>Review Cycle</th>
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<td>SAC Startup/Educational</td>
<td>Up to 200K (Variable: systems under 100 TFLOPS are less.)</td>
<td>Year round</td>
<td>n/a</td>
<td>Usually 2-3 weeks after submitted</td>
<td>Year round</td>
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</table>
User Portal

- One stop shopping for TeraGrid users

Welcome to the TeraGrid User Portal

About

The TeraGrid User Portal is a Web interface for making TeraGrid account management easier, for getting information about TeraGrid resources, and for accessing many of the existing TeraGrid services in a single place.

While users may utilize many features of the User Portal without logging in, authenticating provides access to a full set of services available on the TeraGrid. All new users will receive a "New User Form" via U.S. postal mail containing a User Portal username and password along with their other TeraGrid system account usernames and passwords.

Feature Spotlight

TeraGrid ’08
June 9-13, 2008
Las Vegas
# User Portal – Resource Information

## High Performance Computing Systems

<table>
<thead>
<tr>
<th>Name</th>
<th>Institution</th>
<th>System</th>
<th>CPUs</th>
<th>Peak TFlops</th>
<th>Memory TBytes</th>
<th>Disk TBytes</th>
<th>Load</th>
<th>Jobs*</th>
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<td>IBM Itanium2 Cluster</td>
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## High Throughput Computing Systems

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<tr>
<th>Name</th>
<th>Institution</th>
<th>Active/Available Nodes</th>
<th>Active/Available CPUs</th>
<th>Peak TFlops</th>
<th>Memory GBytes</th>
<th>Disk GBytes</th>
<th>Resource Details</th>
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<tbody>
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<td>Condor Pool</td>
<td>Purdue</td>
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<td>13044 / 16229</td>
<td>14</td>
<td>10506</td>
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<tr>
<td>Total:</td>
<td>4877 / 5828</td>
<td>13044 / 16229</td>
<td>14</td>
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## Advanced Visualization Systems

<table>
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<th>System</th>
<th>CPUs</th>
<th>Peak TFlops</th>
<th>Memory TBytes</th>
<th>Disk TBytes</th>
<th>Graphics HW</th>
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<tr>
<td>TeraGrid Cluster</td>
<td>UC/ANL</td>
<td>Intel Xeon Cluster</td>
<td>192</td>
<td>0.61</td>
<td>0.38</td>
<td>4.00</td>
<td>nVIDIA GeForce 6600GT AGP graphics cards</td>
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<tr>
<td>Maverick</td>
<td>TACC</td>
<td>Sun E25K</td>
<td>128</td>
<td>0.27</td>
<td>0.50</td>
<td>0.56</td>
<td>16 nVIDIA QuadroFX 3000G graphics cards</td>
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<tr>
<td>Total:</td>
<td></td>
<td></td>
<td>320</td>
<td>0.88</td>
<td>0.88</td>
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</tbody>
</table>

*Jobs Key: R - Number of Jobs Running, Q - Number of Jobs Queued, O - Number of Jobs in an Other State
*Detailed job information available upon login.
User Portal – Access Resources

![System Accounts Table](image)
User Portal – A Lot More

- Knowledge Base for quick answers to technical questions
- Documentation
- Science Highlights
- News and press releases
- Education, outreach and training events and resources
Scientific Gateways

• A natural extension of Internet developments
  • Provide a community of scientists with access to a specific set of tools, applications and data collection that are tailored to meet their needs.

• A customized interface for accessing supercomputers
  • Hide the low level details and focus on analysis
  • Capabilities
    • Workflows
    • Visualization software
    • Data access
    • Data analysis

• Example Gateways
  • LEAD (Atmospheric sciences)
  • GEON (Geo sciences)
  • Earth System Grid
Questions?