TACC’s Perspective on Data in Science

Jay Boisseau, Director
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Computational Science is Relatively New

- Experimental science – for a few millennia
- Theoretical science – for a few centuries
- Computational science – several decades

- Computers are fast and accurate: scientists need them in all domains
- Big problems require massive equation solving -> big computers (storage, vis)
Computational Science is Not Just Modeling and Simulation

• Modeling & simulation
  – Simulation of mathematical models
  – Must store, visualize/analyze simulation output

• Data-enabled science
  – Facilitated by digital data collection
  – Often, no formal mathematical laws -> statistics
  – Mine/analyze data (then work towards models)
  – “Physics & stamp collecting” – not true (Rutherford)
  – “End of science (simulation)” – even less true 😊

(Wired)
TACC Mission

To enable discoveries that advance science and society through the application of advanced computing technologies.
TACC Vision

• *Provide the most powerful, capable computing technologies and techniques* that enable people—researchers, educators, developers, engineers, businessmen, etc.—to advance science and society.

• *Provide leadership in the advanced computing community* in technology R&D, support, education, and expertise to ensure maximum impact of current and future technologies in diverse applications.

• *Enable transformational science and societal achievements* that change, influence, and improve our understanding of the world, and the world itself.
TACC Strategic Approach

• **Resources & Services**
  – Deploy best possible systems for entire open science community
  – Provide excellent support, ensure effective usage for science

• **Research & Development**
  – Conduct technology R&D that maximizes resources, users
  – Collaborate on applications R&D that uses our technologies

• **Education & Outreach**
  – Focus education on who we know: higher education
  – Increase public awareness of importance, impact of advanced computing
Some of TACC’s Major Computing System Successes…

<table>
<thead>
<tr>
<th>System Deployed</th>
<th>Year</th>
<th>Resource</th>
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<tbody>
<tr>
<td>First Power4 system in PACI (IBM)</td>
<td>2002</td>
<td>Longhorn</td>
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<tr>
<td>First terascale Linux cluster in PACI (Cray-Dell)</td>
<td>2004</td>
<td>Lonestar2</td>
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<td>Largest SMP remote visualization system (Sun)</td>
<td>2004</td>
<td>Maverick</td>
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<tr>
<td>Most powerful per-core performance cluster in TG (Dell)</td>
<td>2006</td>
<td>Lonestar3</td>
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<tr>
<td>First petascale (&gt; ½ PF) Linux cluster (Sun)</td>
<td>2008</td>
<td>Ranger</td>
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<td>First integrated visualization subsystem on a massive HPC system (Sun)</td>
<td>2008</td>
<td>Spur</td>
</tr>
<tr>
<td>First petascale (½ PF single precision) GPU-based visualization/compute system (Dell)</td>
<td>2010</td>
<td>Longhorn</td>
</tr>
<tr>
<td>First large-scale comprehensive capability (HPC, shared memory, vis) cluster in TeraGrid/XSEDE</td>
<td>2011</td>
<td>Lonestar4</td>
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Ranger: World-Class Supercomputing Capability
Longhorn: Most Powerful Interactive Remote Vis System in the World

• NSF “XD Visualization” award to TACC for $7M to
  – deploy world-class visualization services for US open science research
  – also offers tremendous GPU computing capability
  – provide advanced support for 3 years

• Longhorn specs
  – 256 Dell Quad-core Intel Nehalem Nodes
    • 8 cores/nodes, 2048 total cores
  – 128 NVIDIA Quadroplexes
    • 4GPUs/node, 512 total GPUs
  – QDR InfiniBand Interconnect
Stallion - Highest Resolution Display Environment in the World
Storage for Simulation-Based Science

Past data importance varies greatly:

• Research codes constantly changing
  – old data may no longer be useful
  – but still some value, for some timescale, for regression purposes

• Production codes more stable, focused on scientific results than research into ‘physics’ and algorithms
  – Old data much more likely to be useful
  – New production code versions can still reduce value of old data
Storage for Simulation-Based Science

• Remember: storage costs, but compute costs
  – Cheaper to store, or recompute?
  – Not just a function of technology costs, but also availability/scarcity/competitiveness
Storage for Data-Enabled Science

• Growth in computing and digital detectors increases amount of data
• Fortunately, growth in computing and storage can help us deal with explosive data growth—and has to.
• As data continues to grow exponentially, but processors cores, spindle latencies, etc. don’t grow much, data intensive world faces the same transition as simulation: **parallelism**
Advanced Computing for Archivists

- Archivists will need to use advanced computing technologies and/or work with advanced computing centers
  - Scale of data requires parallelism for storage, access, analysis
  - Centers have tremendous storage capabilities, diverse user requirements, need for general solutions
  - Computing technologies do not replace archivists, they augment them (same as scientists!)
TACC’s Evolution to Support Data Collections and Archiving

• Huge expansion of Ranch tape-based archival systems
  – to 50PB now, 100PB soon

• Establishment of Corral disk-based collections management system
  – 1 PB now
  – 5PB imminent through UT Research Cyberinfrastructure project
  – 25+ PB and beyond through new private support
TACC’s Evolution to Support Data Collections and Archiving

- Hiring of new staff
  - Maria Esteva: digital archives and preservation expert
  - Chris Jordan: data management expert
  - Weijia Xu: data mining expert
  - 3 other staff, 2 more senior openings coming
One Big Challenge: Making Archives Generally Useful

• Archives are only useful if accessible! Must solve this problem
  – Interfaces –necessary but not enough
  – Trust/confidence – also necessary, also not enough
  – Network bandwidth (in some cases)
  – Guidance/expert help in finding the needed data!

• We expect TACC to play a huge role in these issues in 2012+
A More Pragmatic Challenge: Data Management Plans

- NSF awards require DMPs, but don’t fund long-term storage
  - Universities can provide long-term storage
  - Centers like TACC are NSF-supported but university-based
- No DMP fits all cases, but centers have options to help tailor plans
- DMPs are not enough—need to have persistent storage, expert support, etc.
TACC’s Data Collections Hosting System - Corral

• Corral specs and services:
  – 1.2 Petabytes of Lustre + dedicated database and service storage
  – Web, Database, and File System applications
  – iRODS-based data management

• Corral usage has grown to over 700TB of new data 2009-2012
  – 20 "data collections" proper
  – numerous less-organized datasets
An interesting note on the growth of Corral usage and the UTRC is that:

Genome data is our biggest growth area by far at the moment. We granted over 100TB in allocations for genomics data in the last quarter of 2011 alone, and we haven't even started receiving requests from most of the health campuses yet.
TACC’s Data Collections Hosting System – Corral+

- Corral + UTRC (early 2012)
  - 6 Petabytes total, 5 Petabytes replicated GPFS storage
  - All the current Corral services plus
    - Hierarchical storage with multiple disk speeds
    - Multiple encryption and data protection mechanisms for HIPAA and other high-security data
    - Cross-campus authentication and improved collaboration tools
TACC’s Data Collections Hosting System – Corral++

- Corral + /new $$$ configs (early 2013):
  - Smart/Cloud archive - 100 nodes @ 180TB storage per node, 18PB raw capacity
  - 150GB/sec max I/O throughput
  - Gateways farm - 32 nodes, 24 cores & 128GB per node, 768 cores & 4TB of RAM total capacity
  - 80GB/sec of Network capacity, 320GB/sec I/O capacity
TACC’s Archival System - Ranch

• Ranch configuration:
  – Solaris SAM-FS Archival System
  – Two Sun Storagetek SL8500 tape libraries
    • 20,000 tape slots total, current loaded with mix of 1TB and 5PB tapes, 16 T10000C tape drives, and 200TB disk cache
    • Sun x4600, 8-socket, 32-core system, 64GB
    • 10GigE and 4Gb fibre-channel cards
    • Four Sun x4600 data-mover nodes

• ~10PB of user data on tape
• Over 15,000 user accounts on the system
Summary

• Digital data explosion is exponential
• Archiving scientific data is crucial for
  – Future research that is often unanticipated
  – Verification of past research
  – Regression testing for current/future efforts
• Archivists will need to embrace advanced computing to storage, manage, make available, and analyze vast quantities of digital data, in new ways
Summary

- Challenges are many, but big categories include
  - Availability/capacity/performance
  - standards/interfaces
  - awareness/trust
  - expertise on accessing and using data
- We want to work with researchers to understand data preservation issues from DMPs to data reuse, integration, etc.
Opportunity

Science has never before had access to anywhere near this scale and variety of data, or anywhere near this potential for data reuse and integration.

It’s not the dusk of ‘old’ computational methods, but the dawn of new complementary methods that will accelerate science in many fields!
Thanks

• To the many staff at TACC who are helping us develop and implement our vision of data intensive computing, especially:
  – Maria Esteva
  – Weijia Ju
  – Chris Jordan
  – Tommy Minyard
  – Dan Stanzione
  – Tomislal Urban, David Walling, and others