Report of the Colorado State University
ISTeC Research Computing Committee
November 30, 2014

Background
To address how to provide CSU researchers with the high-performance computing (HPC) capabilities they need to support, expand, and enhance their research, the Vice President for Information Technology (Pat Burns) and the Vice President for Research (Alan Rudolph) established the “ISTeC Research Computing Committee.” The members of this committee are listed in Appendix A. This report summarizes our committee’s findings.

On April 28, 2014, our committee received its charge from the VP for Information Technology. Our job was to determine a strategy for providing HPC for research at CSU. We were tasked to consider alternatives for research computing systems, both on-campus and off-campus. We were asked to analyze the range and scope of the research computing being done at CSU that needs HPC. We were also asked to determine if the ISTeC Cray, CSU’s current HPC system, is being used efficiently and effectively.

The current CSU HPC system was installed in December 2010 (please see Appendix B). Specifically, Cray installed an XT6m HPC system at CSU under a $640K MRI National Science Foundation grant awarded to ISTeC (the CSU Information Science and Technology Center). The system has experienced great growth in usage, and is now overfull. In 2014, we have had over 200 active users. Today, four years since the ISTeC Cray was installed, there are significant unmet needs for HPC in a variety of areas at CSU, including applied mathematics, atmospheric science, bioinformatics, ecological and environmental science, energy, groundwater modeling, life sciences, mechanical and aerospace engineering, microwave sensing, optimization, robustness, signal processing, and statistics. Several major emergent areas also need an expanded HPC resource at CSU, including computational biology, carbon sequestration, disease spread, economics, and robotics. Based on our committee’s discussions with the ISTeC Cray support staff and users, efforts are continually made to help users employ the ISTeC Cray in a way that effectively and efficiently exploits its capabilities.

The fact that the current HPC system technology is now almost four years old, and the user base is outgrowing its capacity, leads us to consider how to best provide HPC to CSU researchers in the future. A strong HPC environment is an enabler for CSU to attract the best new faculty and retain and sustain its existing excellent faculty, and we have simply fallen behind our peers. In the Rocky Mountain region, the University of Utah, the Colorado School of Mines, the University of Wyoming, and the University of Colorado at Boulder all have invested several millions of dollars in their HPC systems, and each exhibits an order of magnitude greater performance than our current ISTeC Cray. Indeed, except for Kansas State University, all of our peer institutions that
responded to our survey also have much larger systems and invest much more in HPC than does CSU.

Process
We established the following definition for needing HPC as a loose guideline for our committee’s work: “Any computer program or software application that requires or would benefit from the use of numerous processors and/or computers to process some volume of data within a reasonable timeframe that would be beyond the capabilities of a single laptop/desktop/workstation computer.” There is also a need on campus for storage that is higher performance and/or larger in scale than is found with a typical desktop. However, there is a separate ISTeC Data Management Committee that has a representative on our committee so we can be sure data issues are not ignored.

Our committee surveyed over 50 top CSU users of HPC on their current and future projected needs (please see Appendix E). Our committee analyzed alternatives such as clouds (please see Appendix F), national lab facilities (please see Appendix G), and methods used by peer institutions (please see Appendices C and D).

On Friday September 26, 2014, from 1 pm to 3 pm, our committee held the “ISTeC Research Computing Open Forum,” which was attended by about 80 people. The poster used to advertise that open forum is in Appendix I. Alan Rudolph, the VP for Research, and Pat Burns, the VP for Information Technology, welcomed the attendees and gave introductory comments. The objective of this open forum was to present our committees findings and gather feedback from CSU faculty, staff, and students to help our committee determine how CSU could best provide HPC for their research. This includes equipment, software packages, education, and consulting.

Findings
Our committee found that we need to increase the capacity to accommodate approximately 1,000 researchers within two to three years, based on the current growth rate. We need the ability for researchers to process bigger, more complex, higher resolution, large-data applications. We also need an HPC system of a size such that it will be possible to allow users to have large subsystems for a week at a time, which cannot be done now. We need to have the latest hardware technology (e.g., accelerators) that can give users an order of magnitude or more improvement on the performance of their applications. We need our HPC system to have the latest internal interconnect among processing elements and storage, which is especially important for large, complex, multi-physics problems. We need to provide users memory/storage that is fast and can accommodate big data analyses.

CSU needs to provide support for continuing to teach courses on how to use HPC systems effectively and efficiently (please see Appendix H). We need CSU support for establishing an HPC consulting service, possibly similar to the successful model used by the Statistics Department (also discussed in Appendix H). We need to address the fact that CSU is now behind other institutions in the state, where these institutions have significant internal financial support, such as University of Colorado at Boulder and the Colorado School of Mines.
We summarize some of committee’s findings in the appendices to this report, where we have the slides we presented at the open forum, expanded to clarify points discussed and feedback received. In Appendix B, we describe the current ISTeC Cray system, and its use. Our committee hosted a visit and open seminar by the CIO of Purdue University, Dr. Gerry McCartney. Appendix C summarizes what we learned from numerous detailed discussions with Dr. McCartney about the very successful “condominium model” used by Purdue and other universities; this model is discussed later in the report. Appendix D contains the results of a survey of HPC at peer institutions conducted by Pat Burns, VP for Information Technology, in cooperation with our committee. The survey showed that CSU was quite low compared to our peers in the metrics of number of HPC cores (processing elements), university internal funding to support HPC, and university supported HPC staff. Our survey of HPC needs at CSU in Appendix E shows the broad need for HPC support across numerous disciplines on campus. Our analysis of cloud computing in Appendix F shows that costs can be prohibitive at well-known sites, and file transfer rates can be a serious bottleneck, showing that today commercial cloud solutions are not as cost-effective as having an internal CSU HPC system. Furthermore, these commercial cloud systems are currently not designed for HPC. We present our findings about using NSF or national lab machines in Appendix G. Difficulties that make this approach a problem for many users include: the problem type and/or size must match compute center’s interests, usually hard for small to medium sized applications to get time on these systems, getting compute time awarded is competitive, moving data back and forth can be time-consuming, and the need to submit an application (usually) a few months in advance. Finally, in Appendix H we recommend a model similar to that used by the Statistics Department to provide consulting support for CSU HPC users.

Recommendations
As a result of our analyses, inquiries, discussions, examinations of existing cloud and federal computing sites, surveys of peer institutions, and surveys of CSU researchers, we believe the best way for CSU to provide HPC support for research at CSU is to adopt the emerging “condominium model,” which has been extraordinarily successful at Purdue and other institutions. The success of the condominium model at these institutions is in part due to the level of HPC support staff provided internally by the institution. The number of HPC staff at our peer institutions ranged from four to 15, while we currently have 0.75 FTE. We recommend increasing the HPC staff to two to six FTEs, and some GRAs to work with and support users, under the guidance of HPC staff.

As part of this condominium model, each year a new HPC system is purchased, following the technology curve upward and the cost curve downward. In the condominium model, the university needs to provide (possibly through an NSF, NIH, or DoD MRI grant) the basic framework (e.g., service nodes, networking, interconnect, operating system, power supplies, and shared storage), support staff, and a limited number of compute nodes for each new system in years 1 through 3. Researchers then extend the basic framework by buying nodes using funds from their grants and contracts, from their start-up packages, and from their department. Buying in is voluntary, and researchers get a “hardware back” guarantee if they are not satisfied with
the HPC services they receive with this approach. Researchers can get started with just a single, inexpensive node, or buy hundreds of nodes, where each node consists of multiple “cores.” Typically, research teams do not use their nodes 24/7, and under this model, other participants can access unused nodes, giving each research team access to much, much more compute power than they purchased. Purchases are bundled up, and done centrally to obtain the most value for the investment. Every year a new cluster is added, and the cluster that is five-years old is decommissioned. Each new cluster will consist of the most current technology needed to support the latest CSU research. The buy-in annually by CSU researchers to new systems, as well as some central IT and grant support, will perpetuate the five-year cycle, and continually provide researchers with state-of-the-art HPC.

One advantage of the condominium model over a single supercomputer, such as our current ISTeC Cray, is the ability to easily and continually increase the system size as more researchers purchase nodes to join. Another advantage is that the condominium model is built with commodity parts, allowing an initial cost-effective system to be purchased at smaller cost. Furthermore, the condominium model allows a mixture of processor types that can be customized to CSU user needs. There needs to be a discussion about the implementation of this model at the campus-level, including the Provost, the VPR, the Deans, the department heads/chairs, and the faculty.

This HPC ecosystem we recommend above will allow CSU faculty, students, and staff to implement and employ application packages and techniques that will support existing and new research and discovery, and allow our faculty to be competitive in their future proposals. Furthermore, it would allow us to expand classes and instruction on big data, using state-of-the-art parallel architectures.

Summary of recommendations:

1. Adopt the Purdue University buy-in condominium model. There needs to be a discussion about the implementation of this model at the campus-level, including the Provost, the VPR, the Deans, the department heads/chairs, and the faculty.

2. Increase the staffing support for HPC.

3. Add some GRA’s to work with and support users, under the guidance of the HPC staff.

4. Submit a proposal to the next NSF MRI that will support the implementation of the condominium model.
List of Appendices

Appendix A: ISTeC Research Computing Membership
Appendix B: Brief Overview of the ISTeC Cray
Appendix C: Purdue University Condominium Approach to HPC
Appendix D: Survey of HPC at Other Universities
Appendix E: Survey of HPC Needs at CSU
Appendix F: Using Cloud Computing
Appendix G: Using NSF or National Lab Machines
Appendix H: Model for HPC Consulting
Appendix I: Poster for Research Computing Open Forum
Appendix A - ISTeC Research Computing Committee

Prof. H.J. Siegel, Electrical & Computer Engineering Dept., COE - Chair
Prof. Wim Bohm, Computer Science Dept., CNS
Prof. Randy Boone, Ecosystem Science and Sustainability Dept., WCNR
Prof. Ray Browning, Health and Exercise Science Dept., CAHS
Dr. Richard Casey, Infectious Disease research Center (IDRC)
Prof. Dan Cooley, Statistics Dept., CNS
Prof. Mark Enns, Animal Sciences Dept., CAS
Prof. Xinfeng Gao, Mechanical Engineering Dept., COE
Dan Hamp, ACNS
Bhavesh Khemka, student representative and ISTeC Cray user
Scott Novogoratz, CIO, CVMBS
Prof. Tony Rappe, Chemistry Dept., CNS
Prof. Dan Turk, Computer Information Systems Dept., COB
ISTeC CSU Cray XT6m
High-Performance Computer
Rick Casey

• Funding
  - $627K NSF MRI grant; “Acquisition of the ISTeC High Performance Computing Infrastructure for Science and Engineering Research Projects”; awarded 09/01/2009
  - 50/50 engineering & life sciences content
  - PI's: HJ Siegel & Pat Burns

• Specs
  - 2,016 CPU cores
  - 2.5 TB RAM
  - 32 TB disk
  - 19 Teraflops / sec.

• 500+ CSU user accounts + Woodward Governor & Boeing grant
• Many colleges and departments, diverse disciplines
• Publications, grants, conference proceedings
• Software/Databases: ca. 150 apps & DB’s

• Staff
  - ½-FTE manager
  - ¼-FTE sysadmin
  - ½-FTE grad student (occasional)

• Total Cost of Ownership: ca. $200K / yr.
• Steady, consistent increase in user accounts over time
 ISTeC Cray Usage by College
 Nov. 2013: 495 Total Users

- Engineering - 179
- Nat. Sciences - 161
- CVMBS - 65
- Nat. Resources - 30
- Ag. Sciences - 26
- Woodward - 20
- Health&Human Sci. - 5

• Representation across numerous colleges and departments
# Applications & Databases Installed on ISTeC Cray

<table>
<thead>
<tr>
<th>Applications &amp; Databases Installed on ISTeC Cray</th>
</tr>
</thead>
<tbody>
<tr>
<td>“R” statistical package &amp; 50+ “R” modules</td>
</tr>
<tr>
<td>MACS</td>
</tr>
<tr>
<td>PyCogent</td>
</tr>
<tr>
<td>WRFV3</td>
</tr>
<tr>
<td>Rmpi</td>
</tr>
<tr>
<td>Mercurial</td>
</tr>
<tr>
<td>Python</td>
</tr>
<tr>
<td>Xcms</td>
</tr>
<tr>
<td>Abyss</td>
</tr>
<tr>
<td>Metacomponent</td>
</tr>
<tr>
<td>Qiime</td>
</tr>
<tr>
<td>Zylib</td>
</tr>
<tr>
<td>Allinea</td>
</tr>
<tr>
<td>MetaVelvet</td>
</tr>
<tr>
<td>RayDenovo</td>
</tr>
<tr>
<td>Ampliconoise</td>
</tr>
<tr>
<td>Migrate</td>
</tr>
<tr>
<td>RayMeta</td>
</tr>
<tr>
<td>ANSYS</td>
</tr>
<tr>
<td>Mira</td>
</tr>
<tr>
<td>ARDB</td>
</tr>
<tr>
<td>Mono</td>
</tr>
<tr>
<td>ATLAS</td>
</tr>
<tr>
<td>Mothur</td>
</tr>
<tr>
<td>BioPerl</td>
</tr>
<tr>
<td>MPE</td>
</tr>
<tr>
<td>BLAS</td>
</tr>
<tr>
<td>mpiBLAST</td>
</tr>
<tr>
<td>Boost</td>
</tr>
<tr>
<td>MUMmer</td>
</tr>
<tr>
<td>Bowtie</td>
</tr>
<tr>
<td>MySQL</td>
</tr>
<tr>
<td>Breeze</td>
</tr>
<tr>
<td>NCBI databases</td>
</tr>
<tr>
<td>CFDPlus</td>
</tr>
<tr>
<td>NCBI-Blast</td>
</tr>
<tr>
<td>Converge</td>
</tr>
<tr>
<td>NETcdf</td>
</tr>
<tr>
<td>CPLEX</td>
</tr>
<tr>
<td>Numpy</td>
</tr>
<tr>
<td>Cufflinks</td>
</tr>
<tr>
<td>NWchem</td>
</tr>
<tr>
<td>Egenix</td>
</tr>
<tr>
<td>Oases</td>
</tr>
<tr>
<td>Expat</td>
</tr>
<tr>
<td>OpenBUGS</td>
</tr>
<tr>
<td>Fastx Toolkit</td>
</tr>
<tr>
<td>Openeye</td>
</tr>
<tr>
<td>GAMESS</td>
</tr>
<tr>
<td>OpenEye Suite</td>
</tr>
<tr>
<td>GDAL</td>
</tr>
<tr>
<td>OpenFOAM</td>
</tr>
<tr>
<td>Genbank</td>
</tr>
<tr>
<td>OpenMPI</td>
</tr>
<tr>
<td>GHC</td>
</tr>
<tr>
<td>Parallel-NETcdf</td>
</tr>
<tr>
<td>Greengenes</td>
</tr>
<tr>
<td>Pasha</td>
</tr>
<tr>
<td>GSR</td>
</tr>
<tr>
<td>pBWA</td>
</tr>
<tr>
<td>Hwloc</td>
</tr>
<tr>
<td>RevSeq</td>
</tr>
<tr>
<td>JSpecies</td>
</tr>
<tr>
<td>PeakSplitter</td>
</tr>
<tr>
<td>Knitro</td>
</tr>
<tr>
<td>Plexos</td>
</tr>
<tr>
<td>LAPACK</td>
</tr>
<tr>
<td>PostgreSQL</td>
</tr>
<tr>
<td>WGS</td>
</tr>
</tbody>
</table>
ISTeC Cray Used in Courses

GRAD511:  "High Performance Computing and Visualization“
          (Introduction to parallel computing on CSU’s Cray XT6m)
GRAD510:  "Fundamentals of High Performance Computing“
          (Parallel computing concepts using OpenMP & MPI)
CS475:    "Parallel Programming“
          (Basic concepts of designing/writing/debugging/analyzing parallel code)
CS675:    "Advanced Parallel Computing“
          (Compare programming models and evaluate performance of GPU’s and multicore systems)
CS560:    "Foundations of Fine-Grained Parallelism“
          (Develop applications that best exploit emerging computing architectures)


Journals: 36
Book chapters: 3
Theses/Dissertations: 2
Conference papers: 45
Other: 2
CSU MIC Cluster

- Launched August 2014
- $25K grant
  - Research and Creative Artistry Infrastructure Proposal, Core and Specialized Facilities, High Performance Computing (HPC) Expansion
- 8 CPU cores
- 180 MIC cores – Intel Phi Coprocessor
- 24 GB RAM
- 8 TB disk

- Makes new accelerator computing available to CSU community
Benefits of Campus Resources – One Alternative

- Research computing hardware
  - Attractor for new faculty
  - Supports advanced education
- Stable hardware & software environment needed for multi-year development efforts
  - HPC is hard and requires sustained effort
  - Foundation for intellectual development
- Data locality for tasks that use “big data”
- Tech support staff install software apps at user requests, custom for CSU researchers
- Computing resources
  - Free, no charge for services
  - Easily & quickly available
  - No one is refused an account
  - No grant proposal requirements
  - No periodic reporting requirements
Purdue HPC
Scott Novogoratz

• Developed “condo” HPC model, permitting faculty to buy in at (1) node costing ~ $1600, with ability to utilize any idle nodes
• Organized procurement, to get volume purchase pricing, saving money for all HPC participants
• IT group takes responsibility for running the HPC and providing infrastructure (data center, components, etc.) for the nodes
• No “new” money used to fund HPC, as funds were reallocated to HPC from other IT sources
BETTER THAN REMOVING YOUR APPENDIX WITH A SPORK: DEVELOPING FACULTY RESEARCH PARTNERSHIPS

Dr. Gerry McCartney
Vice President for Information Technology and System CIO
Olga Oesterle England Professor of Information Technology
PURDUE’S IT MISSION

Implement novel business models for the acquisition of computational infrastructure to support research
2007 at PURDUE: BEFORE CLUSTER PROGRAM

• Faculty purchase computers in a variety of platforms from multiple vendors
• Research computers housed in closets, offices, labs and other spaces
• Grad students support computers rather than focus on research
• Inefficient utility usage
• Wasted idle time cycles
• Redundant infrastructures for scattered sites
2008: STEELE
A New, Collaborative Model

- IT negotiates “bulk” research computer purchase
- Existing central IT budget funds investment
- Researchers buy nodes as needed/access other, idle nodes as available
- Infrastructure/support provided centrally at no cost to researchers
- Money-back guarantee
“I’d rather remove my appendix with a spork than let you people run my research computers.”
2008: STEELE

*Results*

- 12 early adopters increase to over 60 faculty
- 1,294 nodes purchased in 4 rounds
  - $600 savings per node (40%)
  - Collective institutional savings more than $750K
- Ranking: 104 in Top 500; 3 in Big Ten
- No one acted on money-back guarantee
“IT completely took care of the purchasing, the negotiation with vendors, the installation. They completely maintain the cluster so my graduate students can be doing what they, and I, want them to be doing, which is research.”

— Ashlie Martini
associate professor of mechanical engineering, University of California Merced

“In a time when you really need it, you can get what you paid for and possibly more, when available. And when you don’t need it, you share with others so they can benefit from the community investment.”

— Gerhard Klimeck
professor of electrical and computer engineering and Reilly Director of the Center for Predictive Materials and Devices (c-PRIMED) and the Network for Computational Nanotechnology (NCN)
### SIX COMMUNITY CLUSTERS

<table>
<thead>
<tr>
<th>Cluster</th>
<th>Installed/Month</th>
<th>Cores</th>
<th>Departments</th>
<th>Faculty</th>
<th>Performance Cost Per GFLOP</th>
</tr>
</thead>
<tbody>
<tr>
<td>STEELE</td>
<td>May 2008</td>
<td>7,216</td>
<td>13</td>
<td>26</td>
<td>$27.02</td>
</tr>
<tr>
<td>COATES</td>
<td>July 2009</td>
<td>8,032</td>
<td>20</td>
<td>60</td>
<td>$21.84</td>
</tr>
<tr>
<td>ROSSMANN</td>
<td>Sept. 2010</td>
<td>11,088</td>
<td>17</td>
<td>37</td>
<td>$16.58</td>
</tr>
<tr>
<td>HANSEN</td>
<td>Sept. 2011</td>
<td>9,120</td>
<td>13</td>
<td>26</td>
<td>$13.28</td>
</tr>
<tr>
<td>CARTER</td>
<td>April 2012</td>
<td>10,368</td>
<td>20</td>
<td>60</td>
<td>$10.52</td>
</tr>
<tr>
<td>CONTE</td>
<td>Aug. 2013</td>
<td>9,280</td>
<td>20</td>
<td>51</td>
<td>$2.86</td>
</tr>
</tbody>
</table>

**STEELE**
- Installed May 2008
- Retired Nov. 2013

**COATES**
- Installed July 2009
- Retired Sept. 2014

**ROSSMANN**
- Installed Sept. 2010
- 17 departments
- 37 faculty

**HANSEN**
- Installed Sept. 2011
- 13 departments
- 26 faculty

**CARTER**
- Installed April 2012
- 26 departments
- 60 faculty
- #282 on June 2014 Top 500

**CONTE**
- Installed Aug. 2013
- 20 departments
- 51 faculty (as of Aug. 2014)
- #39 on June 2014 Top 500
2013: CONTE

- Intel/HP offer next generation chips with Phi accelerators
- Max speed 943.38 teraflops
- Peak performance 1.342 petaflops
- 580 nodes
- 78,880 processing cores (the most in a Purdue cluster to date)
- Ranked 28th in TOP500 (June 2013 rankings)
“We've been running things on the Conte cluster that would have taken months to run in a day. It's been a huge enabling technology for us.”

— Charles Bouman
Showalter Professor of Electrical and Computer Engineering and Biomedical Engineering and co-director of the Purdue Magnetic Resonance Imaging (MRI) Facility

“For some of the tasks that we’re looking at, just running on single cores we estimated that my students would need a decade to graduate to run all their simulations. That’s why we’re very eager and dedicated users of high-performance computing clusters like Conte.”

— Peter Bermel
assistant professor of electrical and computer engineering
NUMBER OF PRINCIPAL INVESTIGATORS

157 out of 160-200
# Top Ten Campus Supercomputers in the Nation

**June 2014 Top 500**

<table>
<thead>
<tr>
<th>U.S. Campus Ranking</th>
<th>University</th>
<th>Name</th>
<th>World Ranking</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>Purdue</td>
<td>Conte</td>
<td>39</td>
</tr>
<tr>
<td>2</td>
<td>Rensselaer Polytechnic Institute</td>
<td>AMOS</td>
<td>43</td>
</tr>
<tr>
<td>3</td>
<td>Indiana University</td>
<td>Big Red II</td>
<td>62</td>
</tr>
<tr>
<td>4</td>
<td>Clemson University</td>
<td>Palmetto 2</td>
<td>66</td>
</tr>
<tr>
<td>5</td>
<td>USC</td>
<td>HPCC</td>
<td>71</td>
</tr>
<tr>
<td>6</td>
<td>Texas A&amp;M</td>
<td>Neumann</td>
<td>110</td>
</tr>
<tr>
<td>7</td>
<td>Texas A&amp;M</td>
<td>Ada</td>
<td>121</td>
</tr>
<tr>
<td>8</td>
<td>Mississippi State</td>
<td>Shadow</td>
<td>185</td>
</tr>
<tr>
<td>9</td>
<td>University of Rochester</td>
<td>BlueGene/Q</td>
<td>276</td>
</tr>
<tr>
<td>10</td>
<td>Purdue</td>
<td>Carter</td>
<td>282</td>
</tr>
</tbody>
</table>
## OUR ACADEMIC PARTNERS

<table>
<thead>
<tr>
<th>By Department</th>
<th>Cores</th>
<th>By Department</th>
<th>Cores</th>
</tr>
</thead>
<tbody>
<tr>
<td>Physics</td>
<td>9,832</td>
<td>Industrial and Physical Pharmacy</td>
<td>384</td>
</tr>
<tr>
<td>Electrical and Computer Eng.</td>
<td>9,816</td>
<td>Commercial Partners</td>
<td>304</td>
</tr>
<tr>
<td>Mechanical Engineering</td>
<td>7,008</td>
<td>Computer Science</td>
<td>280</td>
</tr>
<tr>
<td>Aeronautics and Astronautics</td>
<td>5,048</td>
<td>College of Agriculture</td>
<td>256</td>
</tr>
<tr>
<td>Aeronautics and Astronautics</td>
<td>5,048</td>
<td>Agronomy</td>
<td>240</td>
</tr>
<tr>
<td>Earth &amp; Atmospheric Sciences</td>
<td>3,632</td>
<td>Forestry and Natural Resources</td>
<td>64</td>
</tr>
<tr>
<td>Chemistry</td>
<td>1,936</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Materials Engineering</td>
<td>1,504</td>
<td>Computer and Information Tech.</td>
<td>48</td>
</tr>
<tr>
<td>Chemical Engineering</td>
<td>1,144</td>
<td>Health Sciences</td>
<td>48</td>
</tr>
<tr>
<td>Biological Sciences</td>
<td>1,104</td>
<td>Industrial Engineering</td>
<td>48</td>
</tr>
<tr>
<td>Med. Chem./Molecular Pharm</td>
<td>1,104</td>
<td>Brian Lamb School of Comm.</td>
<td>40</td>
</tr>
<tr>
<td></td>
<td></td>
<td>Animal Sciences</td>
<td>32</td>
</tr>
</tbody>
</table>

*Note: The table lists the number of academic partners for each department or core.*
MANAGEMENT, NOT MAGIC

• Develop relationship with Sponsored Programs
• Cultivate the early adopters
• Respect your project managers
• Establish operational credibility in central IT
  o Do it—take the risk
  o Do it well
• Flex the business model
• Don’t ask for money
Audience Questions and Clarifications

Costs at Purdue

• What is the annual budget for the Purdue HPC environment?
  – When Purdue started their HPC journey in 2007, Purdue started with an HPC budget of ~$2M, reallocated from other areas of the overall IT budget to permit the creation of the HPC environment.
  – In 2014, Purdue’s budget for HPC hardware is ~$4M.
Audience Questions and Clarifications

Size of the Purdue HPC Staff

• What is the size of the Purdue HPC staff?
  – Purdue has a staff of \(~(30)\) full-time equivalent staff, skilled to support the HPC environment and the research function.
  – \(~(15)\) of these individuals are Subject Matter Experts (SMEs) to assist the Purdue research community. After an initial transition period, these SMEs are expected to earn the majority of their salary from research funding in collaboration with principal investigators.
Audience Questions and Clarifications

Effectiveness of Purdue HPC Model

- Has the Purdue HPC model been effective in getting researchers to give up the computer systems in their laboratories?
  - Generally the Purdue research community is finding it simpler, easier and more cost-effective to utilize the Purdue HPC systems and services.
  - No one at Purdue who invested in the HPC Model has asked for their money back.
# HPC Comparison: Purdue and CSU

<table>
<thead>
<tr>
<th>Characteristic</th>
<th>Purdue</th>
<th>CSU</th>
</tr>
</thead>
<tbody>
<tr>
<td>HPC Cores</td>
<td>85,708</td>
<td>2,016</td>
</tr>
<tr>
<td>HPC Staff</td>
<td>(30) FTEs, of which (15) do care and feeding for the HPC and (15) are subject matter experts who assist faculty</td>
<td>(0.75) FTEs with occasional grad student</td>
</tr>
<tr>
<td>HPC Annual Funding (most recent year)</td>
<td>$4,000,000</td>
<td>$200,000</td>
</tr>
</tbody>
</table>
Summary

• Purdue’s successful “condo” model provides an opportunity for faculty to maximize their HPC capacity, taking advantage of idle CPU cycles.
• The number of faculty investing in the Purdue “condo” model continues to grow, as it is an easy and efficient way to utilize research dollars.
• Purdue’s research grants requiring HPC continues to grow; from 19% of Purdue’s research grants in 2004 to 31% of research grants in 2014.
• Staffing to support the Purdue HPC function is essential and requires individuals with research subject matter expertise to assist the research community, as well as individuals to administer and manage the HPC system.
• Purdue manages and exceeds HPC expectations by delivering on its promises through a structured, well managed program.
Peer Survey of CIOs – Research Computing Infrastructure

Pat Burns, VP for IT
Friday, Sept. 26, 2014
CSU Peers

- Iowa State University*
- Kansas State University*
- Michigan State Univ.*
- North Carolina State Univ.*
- Oklahoma State Univ.
- Oregon State Univ.
- Purdue Univ.*
- *Respondents

- Texas A & M University
- Univ. of California, Davis
- Univ. of Illinois, Urbana-Champaign
- University of Tennessee
- Virginia Polytechnic Institute & State Univ.*
- Washington State Univ.
INSTITUTIONAL CHARACTERISTICS
Appendix D – Survey of HPC at other Universities

**FTE Students**

<table>
<thead>
<tr>
<th>Institution</th>
<th>FTE Students</th>
</tr>
</thead>
<tbody>
<tr>
<td>CSU</td>
<td>24,913</td>
</tr>
<tr>
<td>Purdue</td>
<td>39,760</td>
</tr>
<tr>
<td>Virg Tech</td>
<td>31,612</td>
</tr>
<tr>
<td>Mich State</td>
<td>44,227</td>
</tr>
<tr>
<td>Iowa State</td>
<td>29,250</td>
</tr>
<tr>
<td>Kansas State</td>
<td>21,461</td>
</tr>
<tr>
<td>NC State</td>
<td>30,531</td>
</tr>
</tbody>
</table>
SURVEY RESPONSES
HPC Cores

<table>
<thead>
<tr>
<th>University</th>
<th>Cores</th>
</tr>
</thead>
<tbody>
<tr>
<td>CSU</td>
<td>2,016</td>
</tr>
<tr>
<td>Purdue</td>
<td>85,708</td>
</tr>
<tr>
<td>Virginia Tech</td>
<td>10,064</td>
</tr>
<tr>
<td>Michigan State</td>
<td>7,793</td>
</tr>
<tr>
<td>Iowa State</td>
<td>7,896</td>
</tr>
<tr>
<td>Kansas State</td>
<td>2,500</td>
</tr>
<tr>
<td>North Carolina State</td>
<td>8,600</td>
</tr>
</tbody>
</table>
Appendix D – Survey of HPC at other Universities

University HPC Funding

|$0| $500,000| $1,000,000| $1,500,000| $2,000,000| $2,500,000| $3,000,000| $3,500,000| $4,000,000| $4,500,000| $5,000,000

|$90,000| $4,500,000| $2,000,000| $2,000,000| $500,000| $160,000| $650,000

CSU | Purdue | Virg Tech | Mich State | Iowa State | Kansas State | NC State

11/30/2014
Draw

• Your own conclusions
ANY QUESTIONS?
Research computing at CSU

Tony Rappe

59 respondents to survey

Heterogeneous community

There is HPC Activities in all 8 colleges

Computing being done by Professional staff as well as grad students & post-docs

Users need fast processing, or large memory, or large disk (or 2 out of 3)

Application programs being used are homegrown, or open source, or commercial
Research computing at CSU

Majority of computation at CSU (by # of people or grant funding) is in support of experimental programs
Computation a critical part of a project, not the project

There is a significant computing developmental presence across the University (new methods, new algorithms)

Active 53 funding (from VPR database)
Computing, modeling, simulation, bioinformatics...*$78M
(not an exhaustive list)
For reference:
Solar, biofuels, methane, wind, powerhouse... $41M
Tuberculosis $46M
Total CSU $1.1B

*Projects that used model in a different context were excluded, e.g. mouse model
### Research Computing Application areas from the survey include:

<table>
<thead>
<tr>
<th>Statistics</th>
<th>Robotics</th>
</tr>
</thead>
<tbody>
<tr>
<td>- large datasets</td>
<td>Machine Learning</td>
</tr>
<tr>
<td>- large number of datasets</td>
<td>- Exercise science</td>
</tr>
<tr>
<td>Simulation</td>
<td>- Atmospheric science</td>
</tr>
<tr>
<td>- greenhouse gas emissions</td>
<td>- Biomedical engineering</td>
</tr>
<tr>
<td>- financial modeling</td>
<td>Distributed Computing and Big Data</td>
</tr>
<tr>
<td>- large-scale models in ECE</td>
<td>- Atmospheric Science</td>
</tr>
<tr>
<td>- large scale network</td>
<td>- Epidemiology</td>
</tr>
<tr>
<td>- molecular (bio, nano, polymer)</td>
<td>- Healthcare</td>
</tr>
<tr>
<td>- MCNPX Monte Carlo simulations</td>
<td>Smart Grid research</td>
</tr>
<tr>
<td>- resource management for HPC systems</td>
<td>Power systems engineering</td>
</tr>
<tr>
<td>- data center energy and thermal properties</td>
<td>Computational Electromagnetics</td>
</tr>
<tr>
<td>Atmospheric, fire, and ecological sciences</td>
<td>Civil Engineering (ordinary &amp; partial differential equations)</td>
</tr>
<tr>
<td>Ecosystem modeling</td>
<td>Bioinformatics</td>
</tr>
<tr>
<td>Geosciences</td>
<td>Genomics</td>
</tr>
<tr>
<td>Sequential Image Capture and Processing</td>
<td>(short-reads analysis, sequence analysis, etc.)</td>
</tr>
<tr>
<td>GIS analysis</td>
<td>Transcriptomics</td>
</tr>
<tr>
<td>Electronic structure (small molecule, bio, solids)</td>
<td>Proteomics</td>
</tr>
<tr>
<td>Computational Biology</td>
<td>Metabolomics</td>
</tr>
<tr>
<td>Math</td>
<td>Population genetic evaluation</td>
</tr>
<tr>
<td>Physics</td>
<td>Structural RNA, RNA-RNA interaction prediction</td>
</tr>
<tr>
<td></td>
<td>Protein structure determination</td>
</tr>
</tbody>
</table>
Needs/usage

Disk (TB up to PBs)

Processors
fast serial,
single node-multicore,
Fast interconnect up to 1000s of cores,
GPUs, accelerators

Ram (16 GB up to TB)

Cray
2,016 CPU cores
2.5 TB RAM (32 GB/node)
32 TB disk

Based on survey (hardware that people use)
applications tend to need/use
large memory (TB) Perhaps due to non-linearity
or large disk (PB) of pricing with speed
or fast parallel (1000s of cores/GPUs)

Most applications don’t need to max out in all three dimensions
Applications programs

Roll your own

Open Source

Commercial

open source > commercial > roll you own (based on # of apps)

Hardware needs generally dictated by software “vendor”
a number of applications take advantage of parallel processing but many can not, yet
Computers

Individual/group
20%/60%

Department/college
30%/30%

Cray/National resource
50%/10%

Based on number of cores
Based on number of active users

Work is getting done, grants are being funded, but almost all respondents reported that they need more resources
Support needs

Heterogeneous User base

Professional staff & Faculty
- busy doing their day job & need help in small bites
- so they reported needing consulting & scripting help (python, matlab)

Grad students and post-docs
- have a large learning curve they are users & developers
- so they need courses (discipline-specific & computing), consulting & scripting (python, matlab)

Personal aside:
If programming assistance were available, perhaps:
- scripts would progress to applications
- serial would progress to parallel

Perhaps making CSU researchers more competitive for funding
Current Courses that involve computation
(from a search of the CSU catalog)

ANEQ 575 Computational Biology in Animal Breeding.
BC 441 3D Molecular Models for Biochemistry.
CIVE542 Water Quality Modeling.
CIVE556 Seepage and Earth Dams.
CIVE607 Computational Fluid Dynamics.
CIVE631 Computational Methods in Subsurface Systems.
CS475 Parallel Programming
CS570 Advanced Computer Architecture.
CS575 Parallel Processing.
GRAD511 High Performance Computing and Visualization.
MECH650 Computational Materials from First Principles.
NB650 Computer Analysis of Neuronal Proteins.
SOCR731 Plant Breeding Data Management.
Bioinformatics Courses that involve computing
(from a search of the CSU catalog)

BSPM 576/MIP 576  Bioinformatics.
Technical computing across platforms using bioinformatics tools in molecular analyses.

CS 425 Introduction to Bioinformatics Algorithms.
Algorithms for analysis of large scale biological data.

CS 548/STAT 548  Bioinformatics Algorithms.
Computational methods for analysis of DNA/protein sequences and other biological data.

CS 646 04(3-2-0). Machine Learning in Bioinformatics.
Recent research on the supplications of machine learning in bioinformatics.
Summary

Work is getting done, grants are being funded, but more resources are needed for PIs to remain competitive.

Majority of computation at CSU is in support of experimental programs.

A critical part of a project, not the project.

There is a significant computational developmental presence across the University (that can be tapped through GSAs (GSAs are graduate service assistants, like a TA, they perform work not directly related to their research; examples include managing computing systems, synthesizing materials for screening, assembling a screening database).

Hardware needs generally dictated by software “vendor”

a number of applications can take advantage of parallel processing but many can not, yet.

Applications tend to need/use

- large memory (TB)
- or large disk (PB)
- or fast parallel (1000s of cores/GPUs)

Support needed

- Courses (discipline-specific & computing)
- Consulting
- Scripting (python, matlab)
My personal observations:

We need a heterogeneous environment modeled after campus usage/need with
a) large RAM subsystem, perhaps shared memory, (several nodes)
b) GPU-rich subsystem
c) subsystem with large (cheap) disk
d) subsystem with fast disk (SSD)
e) subsystem with large number of nodes with fast interconnect
f) distributed nodes & fast communication to (pre)process where data is being generated

Over time users could/would add nodes to the subsystem type(s) that they need

Need sophisticated queuing system and a larger support staff

HPC Support staff should include GSAs in parallel programming and discipline-specific computing (eg. bioinformatics, statistics)

A lot of work going on at CSU, very grassroots
Central leverage could help funding success.
Grants tend to be "modular".
For example, in chemistry one can ask for $450K (not going to get much more), you can either buy hardware or pay people.
It's better for CSU if you pay people (hardware has no overhead)
Cloud Computing
Rick Casey

Remote sites
- Hundreds of available remote computing sites
- Amazon, DIAG, Google, HP, Microsoft, etc. etc.

Pricing models
- Some free sites & some fee-based sites
- Subscriptions, reservations, spot price, on-demand, packages, discounts
- Many charge for:
  - CPU & GPU cores
  - RAM
  - Disk space
  - File I/O
  - Internet file transfers
- By geographic location (more remote -> higher fees)
Cloud Computing

File transfers
- Globus (fast) – 1 TB / 10 hrs., but need infrastructure at local & remote sites plus fast network connections
- Internet (slow) – 1 TB / 7 days
- May have to download results immediately; when instances terminate, all files, system configurations, etc. are lost

Tech support
- Varies considerably across sites
- May have full support, limited support, or no support
- Quality varies from good to poor
- Responsiveness varies from immediate to very long waits

Account application process
- Varies across sites
- Forms: may be simple or complex
- Grants: may require full blown grant process
- Varies from no wait time up to several months review process

Job management
- Have to learn batch queueing systems (PBS, SGE, LSF, Slurm, etc.)
- Most sites require Linux command line, unfamiliar to many

Training
- May need training for each remote site
Amazon Cloud Case Study

Dept. of Biology postdoctoral student
- Three experiments total
- Needs bioinformatics data analysis

Specs for single experiment
- 72 data files
- 1 job per data file, so 72 jobs total
- 48 CPU-hours per job, so 3,456 CPU-hours total
- Used Oklahoma State Univ. cluster (CSU PI had existing collaborations at OSU)
- 12-core server
- 128 GB RAM
- 2 GB disk per output file, so 144 GB total

Considered using Amazon Cloud service
- Use Amazon calculators to estimate costs
- Match OSU cluster specs to Amazon cluster specs (very similar but not identical)
- Next slide shows cost estimate for single experiment
- $11,854 per experiment
- $35,564 for three experiments
- Note: CSU could purchase entire cluster for $35K
Amazon Cloud Case Study

Amazon cost estimate calculator

### Compute: Amazon EC2 Instances:

<table>
<thead>
<tr>
<th>Description</th>
<th>Instances</th>
<th>Usage</th>
<th>Type</th>
<th>Billing Option</th>
<th>Monthly Cost</th>
</tr>
</thead>
<tbody>
<tr>
<td>Amazon cost</td>
<td>72</td>
<td>48 Hours/Month</td>
<td>Linux on r3.8xlarge</td>
<td>On-Demand (No Co)</td>
<td>$ 10782.72</td>
</tr>
</tbody>
</table>

### Storage: Amazon EBS Volumes:

<table>
<thead>
<tr>
<th>Description</th>
<th>Volumes</th>
<th>Volume Type</th>
<th>Storage</th>
<th>IOPS</th>
<th>Snapshot Storage</th>
</tr>
</thead>
</table>

### Elastic IP:

- Number of Additional Elastic IPs: 0
- Elastic IP Non-attached Time: 0 Hours/Month
- Number of Elastic IP Remaps: 0 Per Month

### Data Transfer:

- Inter-Region Data Transfer Out: 0 GB/Month
- Data Transfer Out: 150 GB/Month
- Data Transfer In: 0 GB/Month
- VPC Peering Data Transfer: 0 GB/Month
- Intra-Region Data Transfer: 0 GB/Month
- Public IP/Elastic IP Data Transfer: 0 GB/Month

### Elastic Load Balancing:

- Number of Elastic LBs: 0
- Total Data Processed by all ELBs: 0 GB/Month
Summary

- Many available cloud service providers
- Free or fee-based services
- Wide variety of price models
- Costs can be prohibitive at well-known sites
- Account process varies: fast & free to slow & full blown grant process
- File transfer rates can be a serious bottleneck
- Tech support varies by site; some sites offer no support
ISTeC Research Computing Open Forum: Using NSF or National Laboratory Resources for High Performance Computing

Bhavesh Khemka
Off-campus Federal HPC Resources Available

- federal ("free") HPC resource providers
  - NSF
    - XSEDE program
    - Blue Waters program
  - government laboratories
  - domain specific resources
    - Pathogen Portal
    - DIAG (Data Intensive Academic Grid)
- gaining access to NSF machines
  - applying to grants that award HPC time
- gaining access to HPC resources of government labs
  - by having collaborative projects with them
  - applying to grants that award HPC time
NSF Resources – XSEDE Program – Startup Allocation

• *startup* allocations – usually for experimenting with XSEDE platforms, application development, etc.
• total startup allocation across all resources cannot exceed 200,000 service units (SUs)
  ▲ SU is defined as the use of one core for one hour
• application needs: title, abstract, keywords, PI contact information, field of science, CV of PI, XSEDE resources requested, grants that support the research
• quick turn-around time for application
• awards are for a year
NSF Resources – XSEDE Program – Research Allocation

- research allocations – needs formal request documents and CVs of PIs/Co-PIs
- when applying, should attach paper(s) that use results obtained from a startup allocation
- justify the allocation requested with results (obtained from a startup allocation)
- submission periods are available 4 times a year
- approved allocations begin in 3 months
- awards are for a year
Additional Information About XSEDE Program

- startup allocations are easy to obtain and have very low turnaround times
- XSEDE does not have any constraints on the source of funding for the project that is requesting HPC time
- once you obtain an allocation, their service is great
- unofficially ‘allocations help desk’ said ~75% of research allocation applicants get awarded some fraction of their request (requests are usually 3-5 times higher than available hours)
- when submitting request, need to mention how well the target application scales with the resources
  - this information is used to decide how much allocation an applicant is awarded
NSF Resources – Blue Waters Program

- at least 80% of the Blue Waters system is available to researchers through an NSF application
- NSF applications open annually and award time for a year
- “Proposers must show a compelling science or engineering challenge that will require petascale computing resources.”
- “Problem should effectively exploit the petascale computing capabilities offered by Blue Waters.”
- to put in perspective:
  even just 1 petaflop is equivalent to ~53x ISTeC Cray (ISTeC Cray has a peak performance of 19 teraflops)
- unofficially ‘help desk’ said the acceptance rate for these applications “in one of the past solicitations was around 60%”
Access to Titan at Oak Ridge National Laboratory

- three different programs in which one can apply
  - INCITE (once a year)
    - “focus on projects that use a large fractions of the system or require unique architectural infrastructure that cannot be performed anywhere else”
  - ALCC – ASCR (Advanced Scientific Computing Research) Leadership Computing Challenge (once a year)
    - “high-risk, high-payoff simulations in areas directly related to the DOE mission”
  - Director’s Discretion (anytime)
    - “short-duration projects” (usually INCITE and ALCC scaling experiments and testing)

- allocations are for a year and require quarterly reports and a close-out report
- when asked about acceptance rates for different allocations they said that information is not available for us
Additional Feedback from Users

- for domain specific resources like DIAG, a user said that very little technical support or help was provided.
- regarding using national laboratory resources, a user said that even if one was inside the National Renewable Energy Laboratory (NREL), it would be hard to get time on its HPC. For outsiders, it is next to impossible.
Main Concerns Using Federal Resources

• problem type and/or size must match compute center’s interests
  ▲ usually hard for small to medium sized applications
• need to submit an application (usually) a few months in advance and getting compute time awarded is competitive
  ▲ notification of the result of the application usually comes in about 3-4 months after application
• different centers have different compute systems and so learning can be an issue
  ▲ especially for researchers who run applications and store results in machines from different centers
• allocations are for a year at most and need to reapply
• moving data back and forth can be time-consuming
Thank You

Questions?

Feedback?

Your experience with federal HPC resources?
HPC Training and Consulting – Ray Browning

- Training
  - Technical support
  - Training
    - Weekly tutorials on selected topic
    - Graduate Student Forums
      - Bootcamps – getting started
      - One-One help
    - Meetup groups
    - Online materials

- Consulting
  - Software development
  - Performance optimization
  - Data management
Possible HPC Model – Statistics/Bioinformatics Lab

Service/Consulting Arm

- Graybill Statistics Lab
  - Existing successful structure can be expanded.
  - Provides a framework for growth.

- Current director is retiring
  - Opportunity for change in leadership and expansion of scope.

- Combination of institutional support, a fee-for-service model, and collaborative science.
  - User fees for services with deliverables (e.g. full service data analysis)
  - Consulting/education continue to freely accessible.

- Physical space provided by CNS and administrative support provided by Department of Statistics.

Director (TBD)
Special Faculty Appointment
Bioinformatics Focus

Statistics Consultants:
- Phil Turk, Ph.D.
- Ann Hess, Ph.D.
- TBD, Ph.D.

Bioinformatics Analyst(s) (TBD)
- GTAs

Regional Resources
UCD/CCTSI

GTAs

Slide from Jessica Prenni
Questions to consider (discussion included):

- Relative importance of training/consulting to HPC
  - Training important to ~30% of open forum attendees
  - Increased resources: need for training may increase
- What training/services are necessary
  - Graduate classes specific to hardware (Grad 510 and 511 mentioned as good for Cray)
  - Faculty training via boot camps or workshops
  - Online tutorials for those wanted to get started
- How would fee for service be structured
  - Some debate as to whether HPC service should be free
  - System admin support via CSU with specific project support from extramural funding (as consultants)
  - Support for Stats lab model as template
- Staffing needs
  - GTA’s a great first line of contact
  - More system staff essential (3/4 FTE is not enough)
    - Can offer system and application support
Appendix I:
Poster for Research Computing Open Forum

Want Better Research Faster?
How Can CSU Make High-Performance Computing Work for You?

ISTeC
Research Computing Open Forum
Friday, September 26
1pm - 3pm
Morgan Library Event Hall
(dessert and beverages will be available)

Objective: To gather feedback from CSU researchers in an effort to provide the high-performance computing equipment, services, education, and consulting needed to enhance their research

Agenda: (presentation minutes/audience feedback and discussion minutes)
2. Welcome - Pat Burns, VP Information Technology (5/5)
3. Brief Overview of ISTeC Cray - Rick Casey, ACNS/IDRC (5/5)
4. Summary of Purdue CIO HPC Approach - Scott Novogratz, CVMBS (5/5)
5. Results of Survey of HPC at Other Universities - Pat Burns, VPIT (5/5)
6. Results of Survey of HPC Needs at CSU - Tony Rappe, Chemistry (10/10)
7. Using Cloud Computing - Rick Casey, ACNS/IDRC (5/5)
8. Using NSF or National Lab Machines - Bhavesh Khemka, Elec. & Computer Eng. (5/5)
9. Model for CSU HPC Consulting - Ray Browning, Biomedical Eng. (5/5)
10. Additional feedback and discussion (20 minutes)

ISTeC (Information Science and Technology Center) is a university-wide organization for promoting, facilitating, and enhancing CSU's research, education, and outreach activities pertaining to the design and innovative application of computer, communication, and information systems. For more information please see ISTeC.Colostate.edu