Understanding the ACI Role

- Data Management & Curation
- Support & Training
- Vision & Coordination
- Community Building
- Computing Services
- Campus Infrastructure
ACI Vision for Research Computing at UW Madison

● **Shared Solutions for Shared Success**
  ○ Leverage shared resources while ensuring community access
  ○ Reduce duplication of effort while providing professional redundancy
  ○ Provide guidance and advice while training a new generation of scientists

● **Enable a step change in computing for each participant**
Vision & Coordination: ACI Committee

- Katrina Forest
- Trina McMahon
- Edgar Spalding
- Richard Townsend
- Dave Vanness
- Jim Walker
- Paul Wilson (Faculty Director)
- Representatives of:
  - CIO, Grad School, WID CCT
Computing Services - CHTC

- Substantial capacity upgrade funded by campus
- ~726,000 cpu-hours/day (average)
  - 8 colleges
  - 42 departments
  - 168 projects
  - 725 users
- Highlights
  - Equivalent to ~\(\frac{1}{3}\) of total national NSF resource!!
  - 87% of total is HTC
  - 10% from Open Science Grid
  - 3% from idle DoIT managed machines
Computing Services - CHTC

CHTC 2015-2015 Usage - L&S (176M)

- Physics: 52.4%
- Economics: 19.9%
- Statistics: 7.6%
- Computer Sciences: 5.6%
- Chemistry: 5.6%
- Mathematics: 7.6%
- Biology: 5.6%
- Astronomy: 5.6%
- Zoology: 5.6%
- Atmospheric Sciences: 5.6%
- Botany: 5.6%
- Geoscience: 5.6%
- Other: 5.6%
Computing Services - CHTC

CHTC 2014-2015 Usage - CALS (25M)

- Biochemistry: 60.8%
- Genetics: 29.5%
- Animal Sciences: 6.2%
- Entomology
- Bacteriology
- Other
Computing Services - CHTC

CHTC 2015-2015 Usage - SMPH (12M)

- 67.5%
- 15.2%
- 6.8%
- 5.3%

Biostatistics and Medical Informatics
Medical Physics
Psychiatry
Oncology
Medicine
Neurology
Pathology and Laboratory Medicine
Other
Computing Services - CHTC

CHTC 2014-2015 HPC Usage - by Dept (26M)

- Materials Science and Engineering: 45%
- Chemistry: 17.7%
- Chemical and Biological Engineering: 10.9%
- Astronomy: 8.6%
- Engineering Physics: 7.4%
- Mechanical Engineering: 6.4%
- Civil and Environmental Engineering: 6.4%
- Physics: 0%
● Collaborating on facilitation

● Shared storage
  ○ Attractive for modest sizes
  ○ Challenging at large scale

● Virtual machines for research applications
  ○ CHTC operating system images available for researchers

● Ongoing conversations about research business model
Support & Training - Facilitation

- Critical to ACI success
  - Nexus of information about researcher needs and expectations
- 2013: First Research Computing Facilitator (RCF) hired in CHTC
- 2014: ACI-REF* - NSF grant to develop concept of facilitation
- 2014: Math/Botany experiment with departmental RCF
- 2014: Additional RCF under ACI-REF program
- 2015: Morgridge Institute adds RCF
- 2015: Establish community of facilitators

*ACI-REF: Advanced Cyberinfrastructure Research and Education Facilitator
Support & Training - ACI-REF

● Joint project with 6 campuses
  ○ Clemson, Harvard, Utah, USC, Hawaii

● Hierarchical network of facilitation experts
  ○ Defining best practices
  ○ Sharing specific experiences
  ○ Developing training material

● National leadership
  ○ Many campuses seeking to join
  ○ Establishing a consortium model
  ○ Focus on campus-based computing and substantial campus commitments
Support & Training

● Three workshops per year
  ○ 2 general workshops + 1 targeted workshop
    ■ Waisman/Davidson group
    ■ Social Sciences
  ○ ~40 students per workshop
● Growing pool of instructors & helpers
  ○ 5 “Certified” instructors
● Preparing for first “Data Carpentry” workshop
  January 2016
Community Building

- Research System Administrators Group
  - Many research sysadmins are alone
  - Provides local network and community of practice

- Facilitators Group
  - Will expand from explicit facilitators to include *de facto* facilitators

- Ad-hoc research communities
  - COMSOL users
  - Markov chain Monte Carlo
  - The Hacker Within
  - Molecular Microbial Ecology and Evolution (MoMiEE)
Data Management & Curation

- Biggest emerging gap
  - Unique challenges

- Beginning collaboration & engagement with
  - Research Data Services
  - Electronic Lab Notebooks
  - Campus Computing Infrastructure

- Facilitators as first line of contact
Campus Infrastructure

- Ongoing improvements of network
  - Some funded by NSF grant (CC-NIE)
- Examples of sustained network traffic near 100Gb/s
  - 9/14/15: 90 Gb/s for 10-20 minutes on a 20 Gb/s background
I just wanted to write a short note about how excellent our experience with the new HPC cluster has been. Overall it has met and surpassed all our expectations for speed, stability, and ease of use, including informed and timely technical support. A further unexpected benefit has been the ability to rapidly and easily purchase new equipment. This process used to take me about 6 months, with significant personal and student time invested. The ACI has made us dramatically more efficient and nimble in our equipment purchases. Many thanks for all the excellent work!
–Dane Morgan, Material Sciences & Engineering

The computational demands of my group’s Bayesian statistical models are daunting under normal circumstances and are particularly demanding when dealing with the hundreds of thousands of responses from international large-scale educational surveys we use. The Center for High Throughput Computing, and particularly the extraordinary assistance of Lauren Michael, has enabled my group to easily carry out our research, which would otherwise be almost impossible. It is not an exaggeration to say that the success of our group is due, in large part, to the resources of the Center for High Throughput Computing. - David Kaplan, Chair of Educational Psychology

Lauren Michael has been extremely helpful in getting my post-doc up to speed on the use of high-throughput computation. Lauren’s value to the overall enterprise is hard to overestimate. Putting someone so knowledgeable and so capable of explaining procedures in simple but powerful terms greatly enhances the effective power and utility of the millions invested in the hardware. For me, the appearance of high-throughput and high-performance computation facilities on campus - with no cost, at least for now - has been the most important development to facilitate scientific research since the appearance of the UW Biotechnology Center and the computerization of central library resources.
- Tom Givnish, Botany
Next Steps

● Institutionalize ACI in Research Computing Officer
  ○ Leadership of strategic campus vision
● Engage with broader set of service partners
  ○ PI’s have expressed interest in:
    ■ Storage!!!
    ■ Social media
  ○ Discuss model for shared services
● Develop new communities
  ○ Software licenses
  ○ Methods & Algorithms
Questions?

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