UAB Research Computing

Resources and Activities

Research Computing Day
September 13, 2012

UAB IT Research Computing

UAB INFORMATION TECHNOLOGY

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Engaged professional staff collaborate with investigators to maximize the research impact

Research Computing System

The Research Computing System is designed to provide services to researchers in three core areas

- **Data Analysis and Simulation**

  Using the High Performance Computing (HPC) fabric we call Cheaha for analyzing data and running simulations. Many applications are already available or you can install your own

- **Data Storage and Sharing**

  Supporting storage solutions and the trusted exchange of information using virtual data containers to spark new ideas (available beginning October 2012)

- **Application Development**

  Providing virtual machines and web-hosted development tools empowering you to serve others with your research
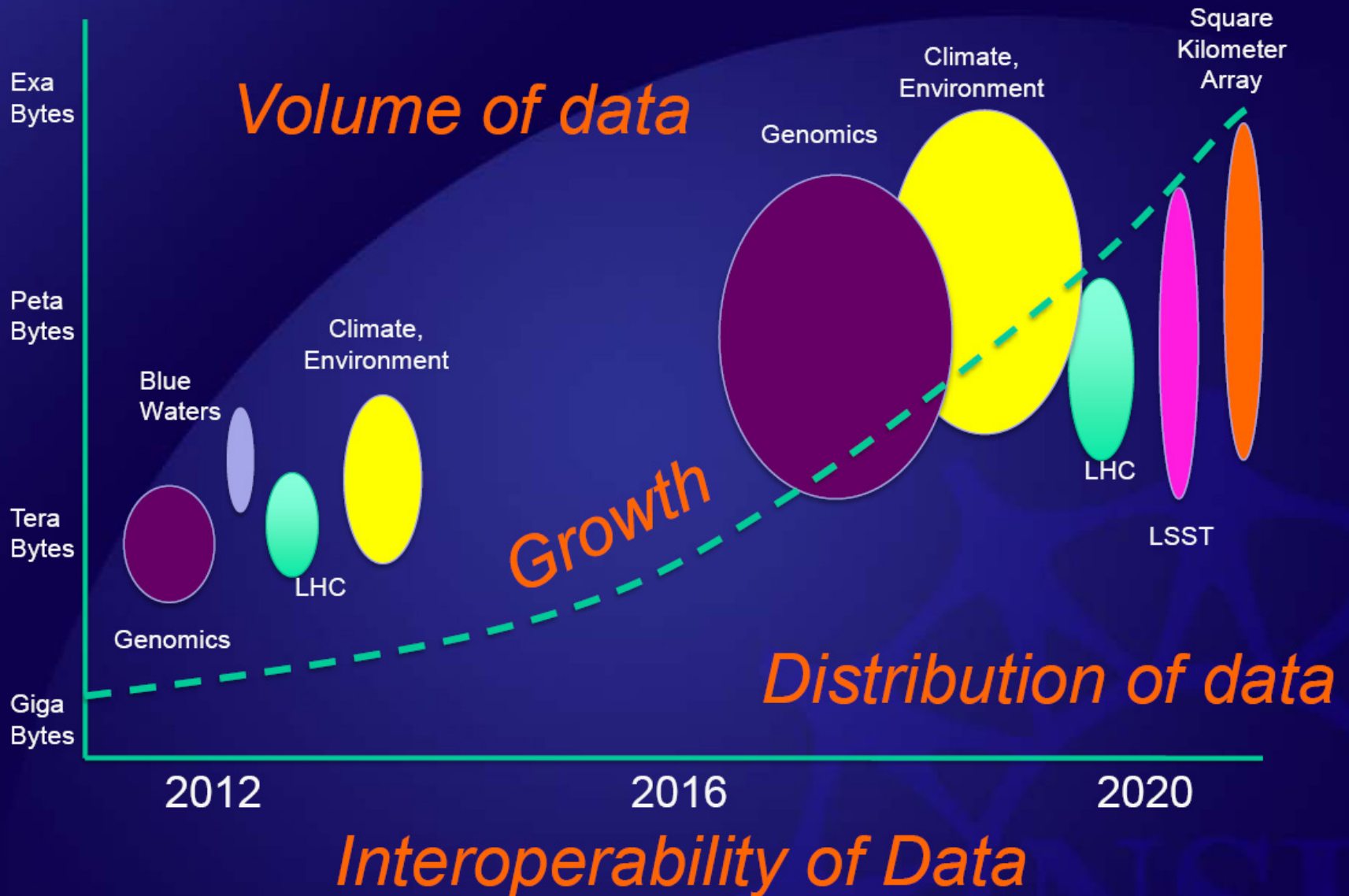
UAB Research Computing System

- Operated by UAB IT Research Computing Group
- 868 cores, three hardware generations, one SGE scheduler
- ~9Tflops compute power, 180TB High performance storage
- **Research Storage – bringing ½ Petabyte on-line over next few months**
- Virtual Machine fabric with OpenNebula

https://docs.uabgrid.uab.edu/wiki/Cheaha

Data Challenges

10
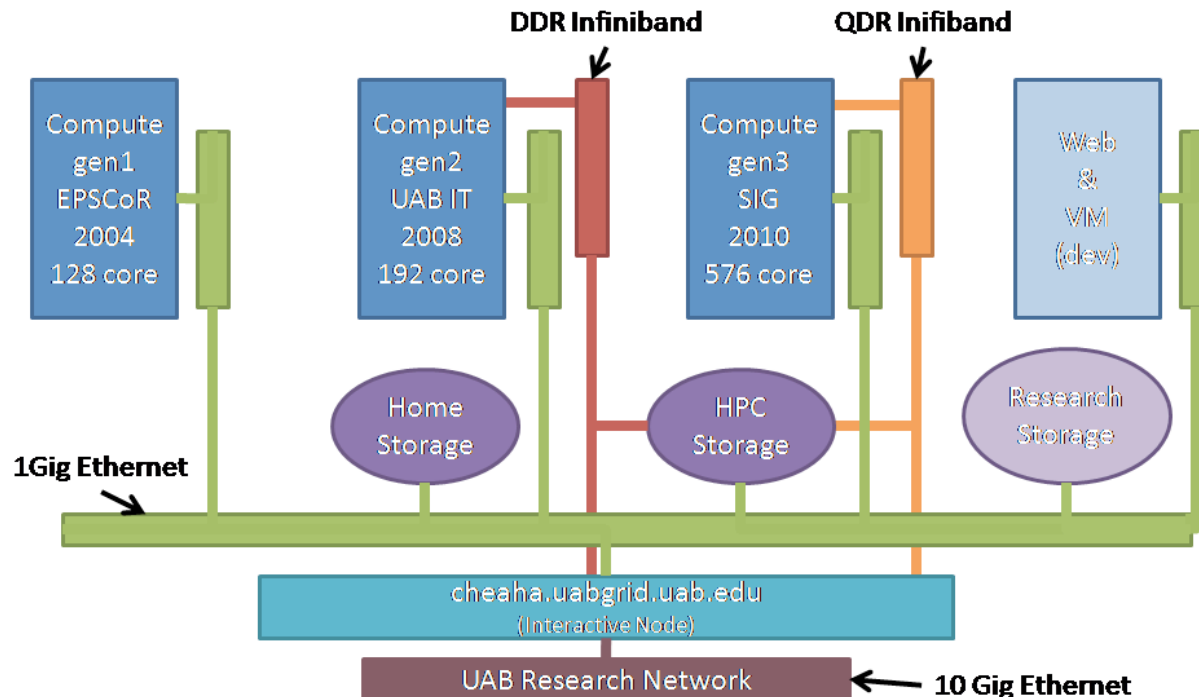
Storage Cloud-scape

Other Clouds

Campus Cloud

Other Clouds
- Commercial price schedules
- Not Close to UAB HPC
- Features dictated by service provider
- Eg.
  - Dropbox, SugarSync, Box.net, AmazonS3, Rackspace, *Cloud

Campus Cloud
- < Commercial Cost
- Close to UAB HPC
- Fully customizable

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Research Storage Project

- Fall 2011:
  - Announce intent to expand storage capacity for research use, including a goal of the "first Terabyte for free"
- Spring 2012 and Summer 2012:
  - Pilot a storage architecture with Dell Inc.
    - Includes storage and capacity to build storage-oriented applications
  - Explore use cases for research storage
    - Desktop integration – same view of files on cluster from desktop
    - Virtual containers – storage is virtualized for use in applications
    - Backup to storage – eg. build a Timecapsule for Macs
    - Group storage – dedicate storage for use storage for
    - Secure storage – TrueCrypt containers across platforms
    - Mobile access – iFiles on the iPhone
  - Acquire 420TB storage from Dell Inc.
- Fall 2012
  - Begin roll out of new storage (beginning in October)
  - First TeraByte for Free
  - Offer storage cost model both incremental and condo
  - Initial features
    - Cluster access
    - Campus access (desktop integration via CIFS)
   - Mobile access (via standard apps)

UAB & DELL

Research Storage Cost Models

- Campus Cloud Storage (raw storage):
  - 1 TB – free for researchers as announced on Sept 15, 2011 (no backup)
  - >1 TB- Cost: $150/TB/Yr
  - Condo model: $12,000 for 36TB Raw for 3Yrs
- Hosted Internet2 Net+ services with box.net
  - Data synchronization solution for all platforms
  - Special discussion at end of presentation

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Computing Use and Scalability

Cheaha Utilization

Compute Hours per Month by Group

Legend: 1. SSG 2. CCSB 3. SoE–ME 4. CBSE 6. Other Groups 5. SoE
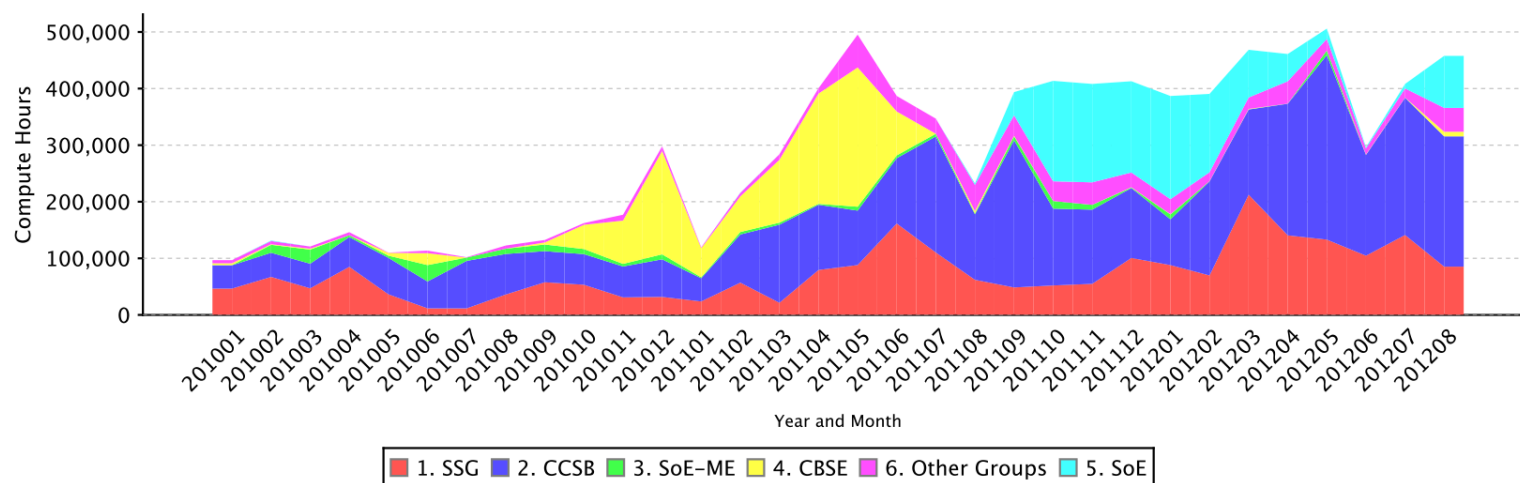
Application Scaling Focus Areas

- Structural Biology
  - NAMD 2011
  - Autodock 2012
- Neurology
  - DTI image processing 2012

- Genetics
  - Galaxy 2011 (on going)

Structural Biology Scaling 2012 High-Throughput Molecular Docking

- Virtual Screening with Autodock
- UAB Condor Pilot
    https://docs.uabgrid.uab.edu/wiki/UAB_Condor_Pilot
- Summary
    - Computing on spare cycle campus condor pool and OSG is comparable to UAB HPC capacity

- Project Partners
    UAB IT Research Computing
    Department of Computer and Information Science
    UAB IT Desktop Computing
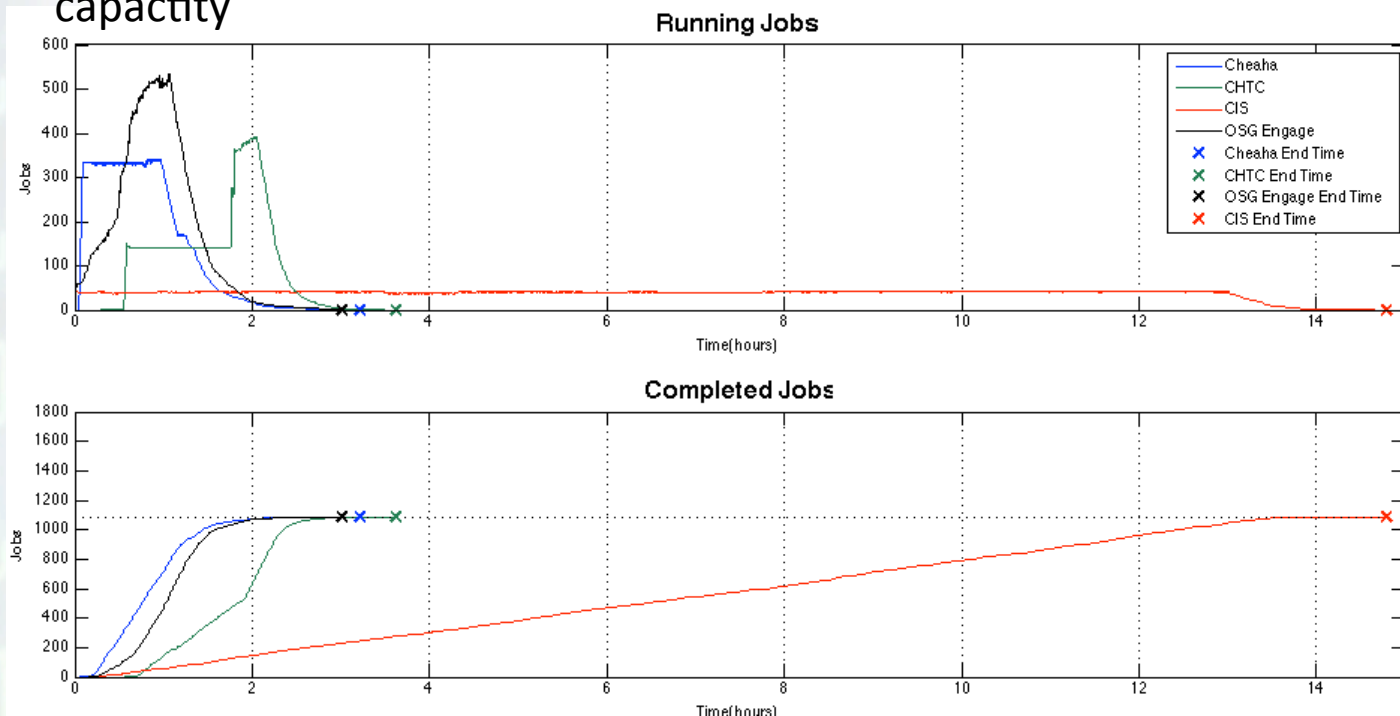
Application Development Preview
Virtual Machines!

What's Motivating Us?

- Research Reproducibility

- Pattern Recognition

    - Applications

    - Computers

    - Networks

- Researcher Autonomy

Goals into 2013

- Build out storage services
    - Eventually bake in new features like redundancy, NSF4, AFP, and on and on
- Open virtualization fabric for general use
- Document operations to grow trust
- Build Community
    - hpc-announce and hpc-users lists
- Number one challenge is scaling effort!

Special Discussion

Research Storage Services and Cost

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  - Data synchronization solution for all platforms
  - Targeting rate of $2.00/GB/Yr

Box.net

- Hosted Internet2 Net+ box.net service
- Targeted Rate $2.00/GB/Year
- InCommon(BlazerID) based user accounts
- Security Compliance
- Account Administration by UAB Research Computing
- Features: Online workspace, file sharing, mobile access, file commenting, group discussions, online documentation, updates, version history, user management, security controls, easy-to-use, box sync
- http://www.internet2.edu/netplus/box/