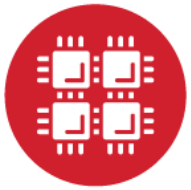

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Statewide Users Group

John Herbert, SUG Vice Chair

Associate Professor, Chemistry, Ohio State University

Bale Theater

Nov. 8, 2013

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Daniel Lacks, Professor, Chemical Engineering
Case Western Reserve University

Molecular Simulation of Interfacial Properties

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Pankaj Shah, Executive Director
Ohio Supercomputer Center & OARnet

Executive Update

2013 Focus Areas for OSC and OARnet

Ohio Supercomputer Center

- Strategic hires
- Funding opportunities and business model development
- Faculty-joint appointments!
- IntelSim - Beyond NDEMC (National Digital Engineering and Manufacturing Consortium)
- Big data management
- Research compute and storage infrastructure
- Campus outreach, regional alliances

OARnet

- Federation and Identity management
- Applications/Net+ services
- Business models and new pricing schema
- Succession planning
- Strategic hires
- Data centers
- State of Ohio transformation project/process
- Fiber IRUs

Factors for Continued OSC Growth

- To be competitive for National Science Foundation high performance computing grants, we need to be prepared to support the Extreme Science and Engineering Discovery Environment (XSEDE)
- Needs:
  - Meet XSEDE Level 1 software and services baseline, which will require 2 FTEs to comply
  - Demonstrate progress towards meeting these capabilities
  - Need a principal investigator with strong NSF connections and national HPC reputation

Strategic Hires

- Interim Director of Supercomputing
  - Dave Hudak
- Doug Johnson
  - Additional duties
- Need to hire 2 additional FTEs, to comply with XSEDE Level 1 software and services baseline
- Research & Innovation Center director position posted
- Joint appointment for Rajiv Ramnath
  - Jumpstart AweSim program

OSC Financial Update

Fiscal Year 2014

	Ohio Supercomputer Center		
	FY13 Actual	FY14 Budget	Variance
Sources of Revenue			
User Fees	828,077	230,000	(598,077)
Grant/Contracts	2,067,961	3,250,960	1,182,999
Grant/Contracts - BTOP	2,612,235	0	(2,612,235)
Other Funding	0	0	0
Regents Funding (Higher Ed Subsidy)	3,347,418	3,747,412	399,994
K12 Funding	0	0	0
OARnet Operating/Reserve Transfers	168	0	(168)
Total Revenue	**8,855,859**	**7,228,372**	**(1,627,487)**
Operating Expenses			
Personnel/Benefits	3,349,205	3,981,129	631,924
SOCC Power	770,000	385,000	(385,000)
Purchased Services	1,165,741	961,567	(204,174)
Equipment Maintenance	194,422	100,000	(94,422)
Equipment	22,091	10,000	(12,091)
Equipment – BTOP	2,612,235	0	(2,612,235)
Other Operating Expenses	489,267	397,829	(91,438)
Indirect Costs	324,724	670,833	346,109
Total Operating Expenses	**8,927,685**	**6,506,358**	**(2,421,327)**
Net Income (Loss)	**(71,827)**	**722,014**	**793,840**

Capital Proposal Planning

RFI Issued Oct. 11; Due Dec. 2

- Major growth in compute and storage demand
  - Higher Education
    - Health and biosciences
    - Energy
    - Food production
    - Materials
  - Manufacturing
    - Modeling and simulation
  - Technology
    - AweSim

Capital Proposal Planning

- Multiple infrastructure projects to support larger scales
  - Infrastructure servers
  - Storage servers
  - SOCC remediation
- Goal 1: Compute cluster proposal
  - 0.5 to 1 PF
  - Deployed early 2015
- Goal 2: Storage expansion proposal
  - 4 PB spinning disk, 10+ PB tape

Detailed Proposal Items

- User-facing hardware and software
  - Compute cluster
  - Project storage upgrades
  - LTO6 tape library upgrade
  - Software capital purchases/upgrades
- Non-user facing hardware and software
  - SOCC UPS/PDU upgrades
  - Cooling infrastructure
- Infrastructure
  - Other, broader upgrades
    - Interface lab/BALE upgrades
    - Fishbowl/showroom
    - Conference room improvements
  - Staff system upgrades
  - Furniture, work environment

Additional Areas of Interest

- System upgrade/long term options
- Novel procurement options
- Cloud resources bundled with purchase
- Partnership opportunities
  - Workforce development
  - Collaborative development
  - Research

Proposed:
Ohio Research and Commercialization Portal

What

- Feasibility study for web-based, searchable database of faculty expertise, research facilities, and intellectual property across Ohio academic research institutions

Why

- Improve ability to create connections between industry need, faculty expertise and interest to accelerate economic growth in Ohio
- Improve possibility of securing investment capital

Deliverables

- Feasibility study to determine current availability of information at each institution
- Determine incentives for university/industry participation
- Recommend solutions for portal development, implementation, and maintenance

Ohio Supercomputer Center

An OH·TECH Consortium Member

Christopher Hadad

Allocations Committee Update

Projects awarded between meetings (1)

- Standard Requests (10,000 RUs)
  - Feng Qin, Computer Science and Engineering, OSU
  - Lungfei Lee, Economics, OSU
  - Bharat Bhushan, Mechanical and Aero Engineering, OSU
  - Janet Box-Steffensmeier, Political Science, OSU,
  - Mark P Foster, Biochemistry Administration, OSU
  - Richard A Miller, Civil and Environmental Engineering, UCN
- Classroom Requests (5,000 RUs)
  - Sherwin Singer, Chemistry, OSU
  - P. Sadayappan, Computer Science and Engineering, OSU
  - Chris DeFraia, Biology, KYC
  - Massimo Olivucci, Chemistry, BGS
- Total of 80,000 RUs

Projects awarded between meetings (2a)

- Startup Requests (5,000 RUs each) – total: 190,000 RUs
  1. Anita Mattson, Chemistry and Biochemistry, OSU
  2. Yungui Huang, Center for Quantitative and Computational Biology, Nationwide
  3. Jiankui Yuan, Radiation Oncology, CWR
  4. Caroline Wagner, John Glenn School, OSU
  5. Yunseok Kang, Injury Biomechanics Research Lab, OSU
  6. Timothy Haab, AEDE, OSU
  7. Seung Hyun Kim, Mechanical and Aero Engineering, OSU
  8. Joshua Gross, Biological Sciences, UCN
  9. Hongxing Liu, Geography, UCN
  10. Andrew Paluch, Chemical, Paper, and Biomedical Engineering, MIU
  11. Amit Sharma, Physics, WSU
  12. Yalin Dong, Mechanical Engineering, UAK

  (to be continued)

Projects awarded between meetings (2b)

- Startup Requests (5,000 RUs each) – total: 190,000 Rus
  13. Ian Krajbich, Psychology, OSU
  14. Julia Thomas, Economics. OSU
  15. Nikolai Priezjev, Mechanical and Materials Engineering, WSU
  16. Bo Li, Mechanical and Aerospace Engineering, CWR
  17. Sanford Shew, Director of Research Computing Services, OSU
  18. Katrina Cornish, Bioemergent Materials, OSU
  19. Kelly Wrighton, Microbiology, OSU
  20. Guofen Yu, Physical Sciences, Findlay
  21. Alok Sutradhar, Plastic Surgery/Mechanical Engineering, OSU
  22. Byounghoon Seok, Economics, OSU
  23. Matthew Kahle, Mathematics, OSU
  24. Daniel Buccholz, Biological Sciences, UCN
  25. Minjeong Jeon, Psychology, OSU

  (to be continued)

Projects awarded between meetings (2c)

- Startup Requests (5,000 RUs each) – total: 190,000 Rus
  26. Rouzbeh Amini, Biomedical Engineering, UAK
  27. Rebecca Willits, Biomedical Engineering, UAK
  28. Xiang Li, Physics, CLS
  29. George Qin, Engineering and Computer Science, CED
  30. Steven Higgins, Chemistry, WSU
  31. Cynthia Timmers, James Cancer Center, OSU
  32. Forrest Sheng Bao, Electrical and Computer Engineering, UAK
  33. Liza Comita, EEOB, OSU
  34. Chi-Chih Chen, ESL/Electrical and Computer Engineering, OSU
  35. Len Brillson, Physics, OSU
  36. Murali Sundaram, Mechanical Engineering, UCN
  37. Sean Crowe, Libraries, UCN
  38. Mark Turner, Aerospace Engineering, UCN

Major (7) Requests – 30,000 RUs each

- Major Requests
  1. Shaurya Prakash, Mechanical and Aero Engineering, OSU
  2. David McComb, Materials Science and Engineering, OSU
  3. CK Shum, Earth Sciences, OSU
  4. Alexander Tarnovsky, Chemistry, BGS
  5. Anna Gudmundsdottir, Chemistry, UCN
  6. Wanjian Yin, Physics and Astronomy, UTL (*tabled*)
  7. Barry Dunietz, Chemistry, KSU (*tabled*)

Discovery (5) Requests

1. Purnima Kumar, Dentistry, OSU, 100,000 (*tabled*)
2. Sandip Mazumder, Mechanical and Aero Engineering, OSU, 200,000
3. Giorgio Rizzoni, CAR (Mechanical Engineering), OSU, 36,900
4. David McComb, Materials Science and Engineering, OSU, 100,000 (*tabled*)
5. Sameek Roychowdhury, Medical Oncology, OSU, 60,000(*tabled*)

Total Awards for Allocation Meeting

- Startup (5,000 RUs): 38 requests, **190,000**
- Classroom (5,000 RUs): 4 requests, **20,000**
- Standard (10,000 RUs): 6 requests, **60,000**
- Major (30,000 RUs): 5 requests, **150,000**
- Discovery requests: **236,900**

- Total of **656,900** RUs

- Discussed HPC models for research groups (condo)
- How to facilitate biomedical and bioinformatic researchers

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An OH·TECH Consortium Member

Alan Chalker, Ph.D.

Director of AweSim

AweSim Update

FY13 Non-Academic Project Usage

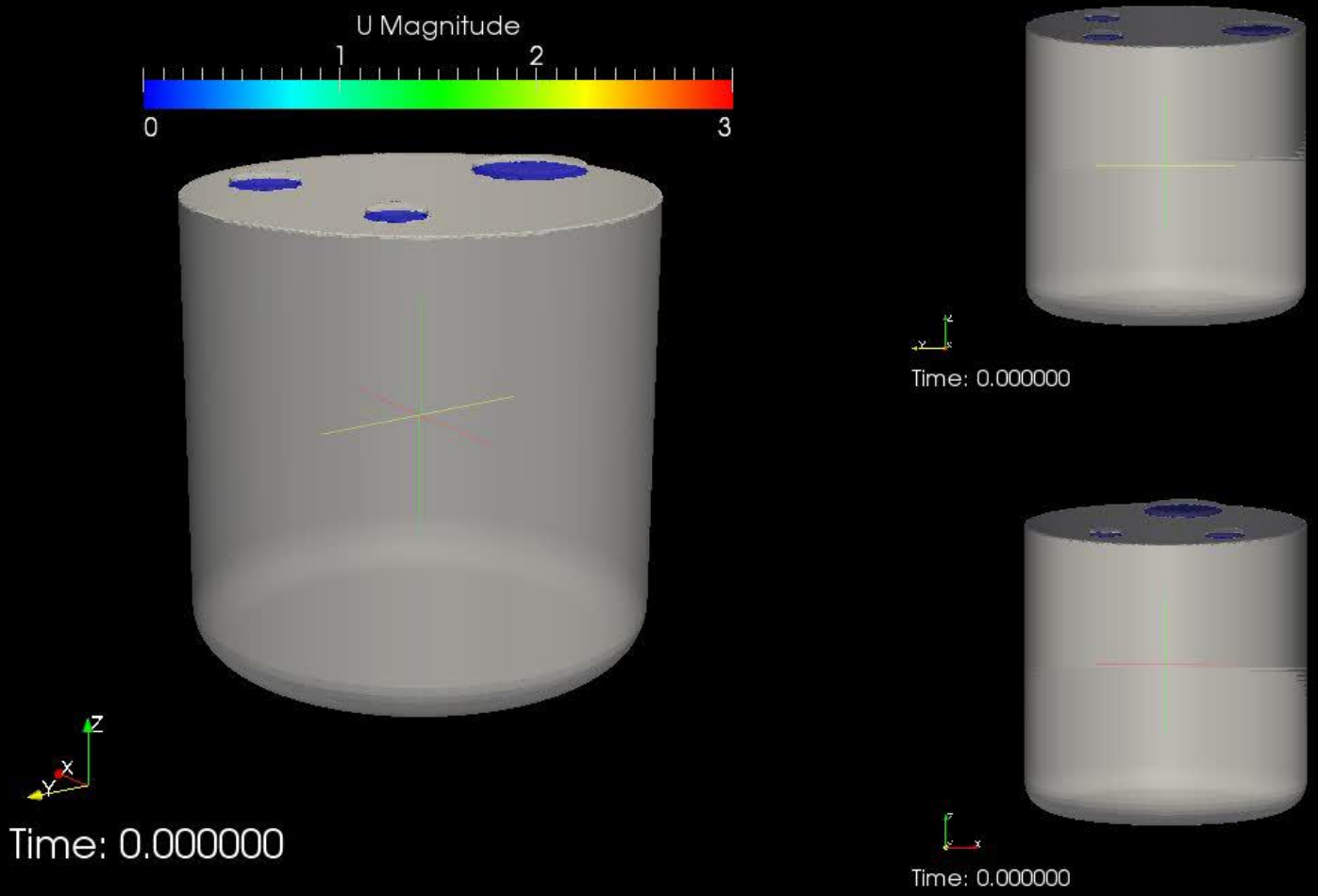
- NDEMC
  - 10 active projects
  - ~1M CPU hours used
- Commercial Clients
  - 9 active clients
  - ~8.4M CPU hours used
- Other Projects
  - Includes Truck Add-on and Fan Sim portals
  - 4 active projects
  - ~2.2M CPU hours used

1M CPU hours is equivalent to using about 115 CPUs *nonstop* for the entire year.

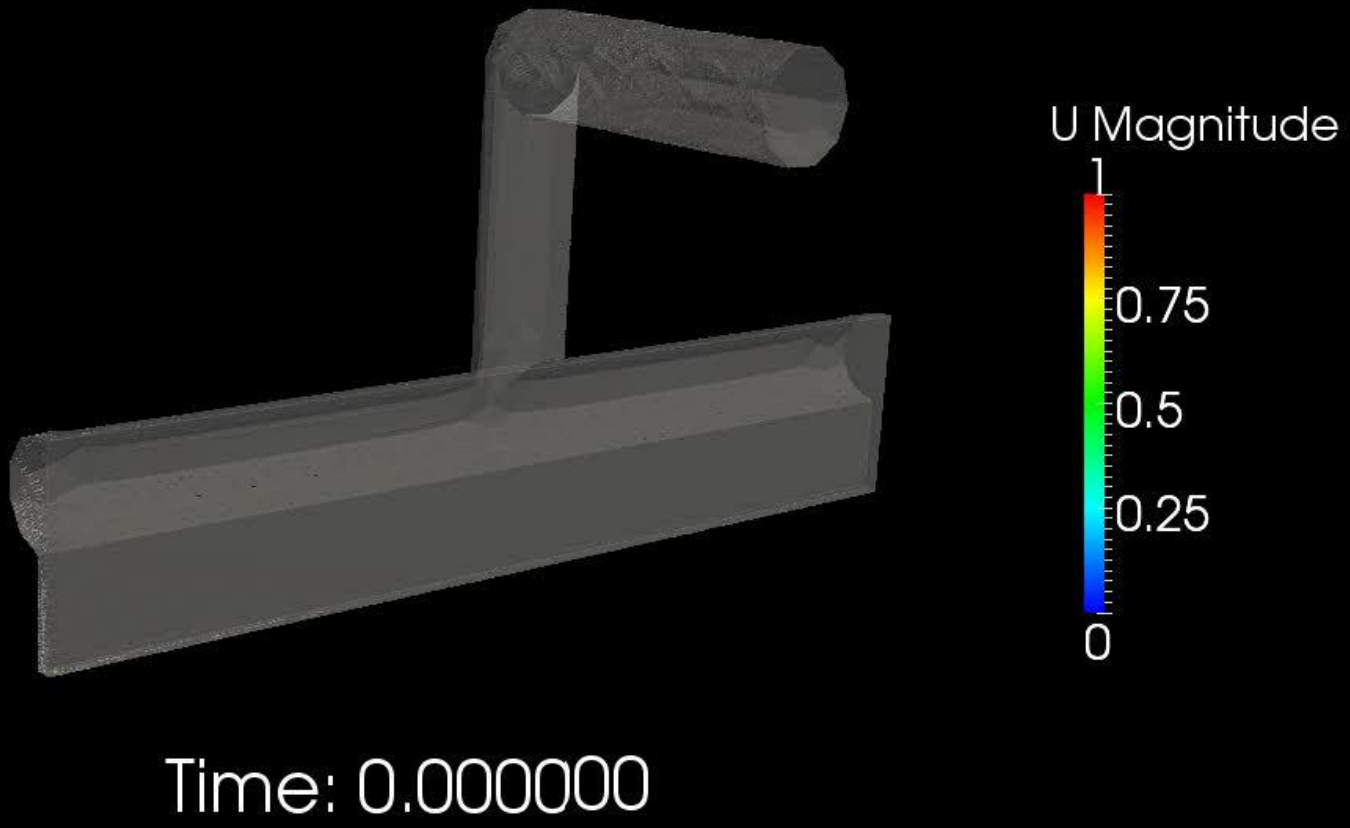
AWESIM

Virtual Designs. Real Benefits.

Example App: Container Fill Sim



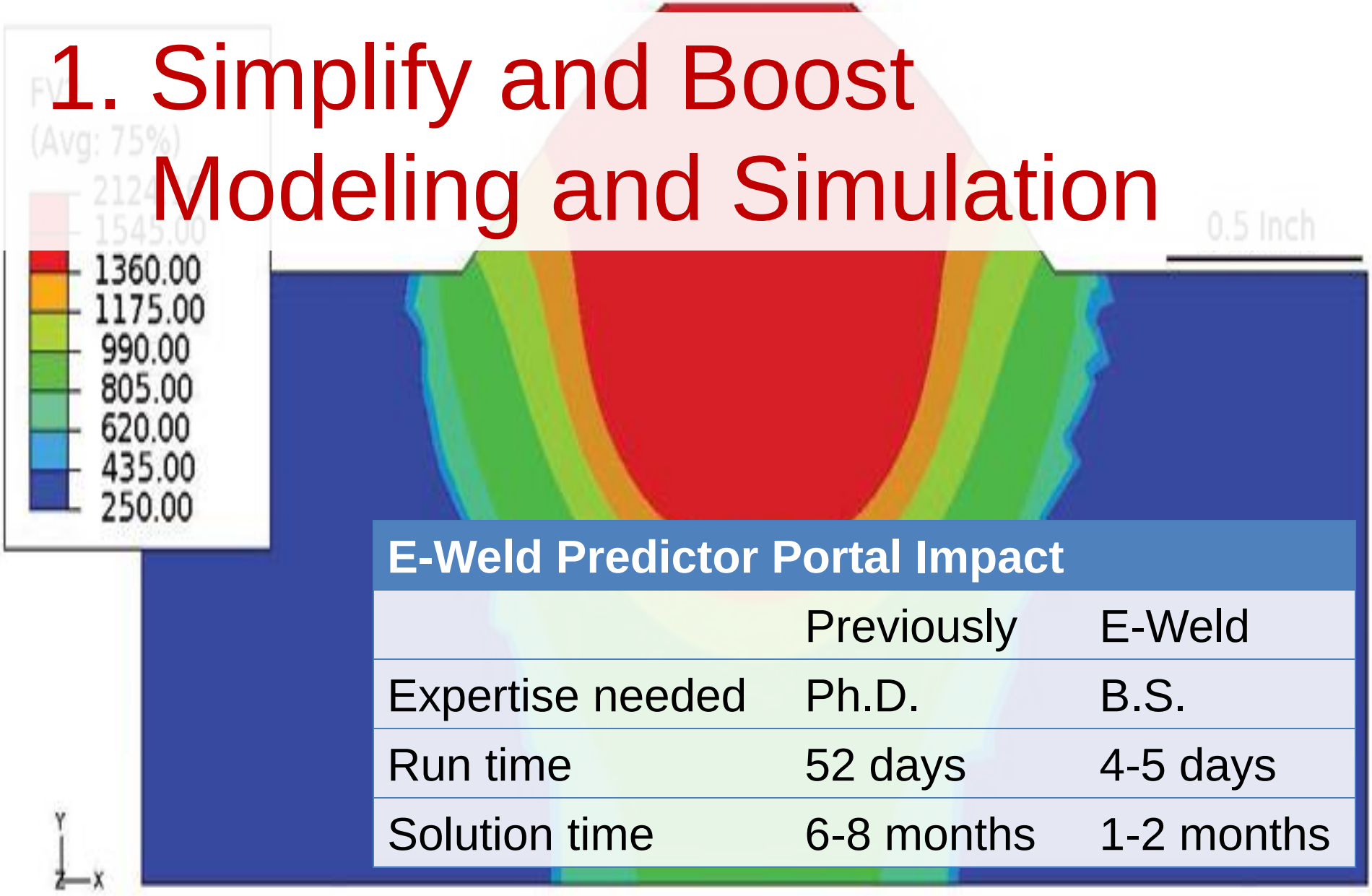
Example App: Manifold Flow



Three Reasons to Care About AWESIM

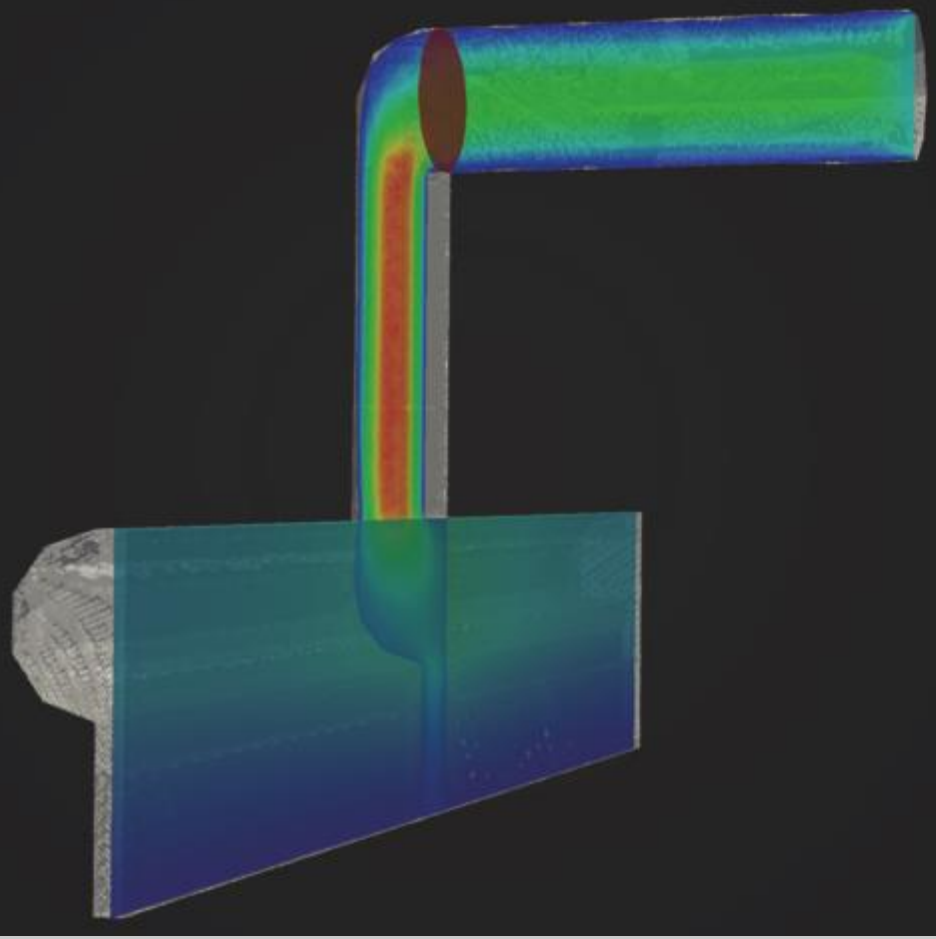
AweSim is going to change the way companies compete, through adoption of simulation-driven design.

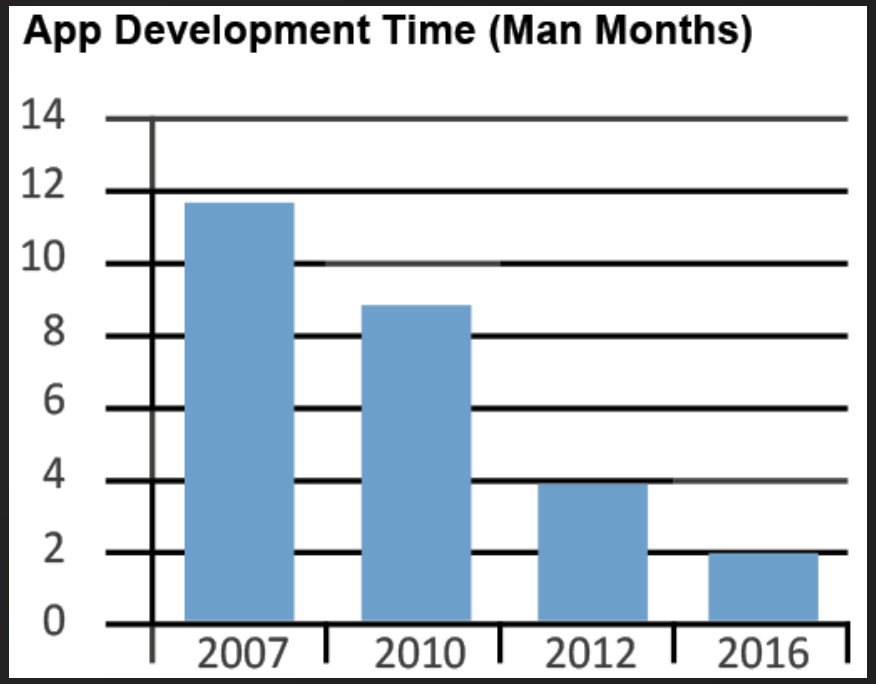
1. Simplify and Boost Modeling and Simulation



E-Weld Predictor Portal Impact		
	Previously	E-Weld
Expertise needed	Ph.D.	B.S.
Run time	52 days	4-5 days
Solution time	6-8 months	1-2 months

2. Make better use of computational expertise





3. Opportunity to create your manufacturing apps

- Processing of advanced aerospace materials
- Thermal processing for food sterilization
- Virtual wind tunnel
- Structural classics explorer
- Virtual test rig

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An OH·TECH Consortium Member

Dave Hudak, Ph.D.

Senior Research Scientist

Research Update

Agenda

- Research initiatives
- Proposal status
- National collaborations

Research Initiatives

- OSU Discovery Themes in data analytics
  - Discovery Themes is a 10-year program to expand faculty
  - First area is data analytics
  - OSC partnered with 12 (or more) research teams to propose common analytics infrastructure
- Intel Parallel Computing Center
  - Modernizing applications to increase parallelism and scalability
  - Talking to OSC users to identify candidate applications
  - Any interested collaborators should contact Dave Hudak, Karen Tomko or Brian Guilfoos

OH-TECH Proposals Pending

Funding Opportunity	Submit Date
Air Force Research Laboratory, AFRL/RX, Materials and Manufacturing Directorate BAA-RQKM-2013-0005, AFRL Research Collaboration Program **"Radio Frequency Signal Processing for Layered Sensing"**	07/26/13
Department of Energy – under AltaSim Technologies – DE-FOA-0000969, SBIR Phase I **"Design of Large Scale Electronic Circuits using Cloud Based Computational Analysis"**	10/18/13
Department of Energy – under AltaSim Technologies – DE-FOA-0000969, SBIR Phase I **"Optimization of Heat Treatment Procedures"**	10/18/13
Department of Energy – under AltaSim Technologies – DE-FOA-0000969, SBIR Phase I **"Development of Additive Manufacturing Process Technology"**	10/18/13
Department of Commerce – NIST 2013-NIST-AMTECH-01, Advanced Manufacturing Technology Consortia **"Establishing the AweSim Consortium: Developing a Technology and Market Roadmap for Virtual Design Apps Bring Real Competitive Advantage to Advanced Manufacturing"**	11/01/13
Department of Commerce – NIST 2013-NIST-AMTECH-01 – under University of Tennessee-Knoxville Advanced Manufacturing Technology Consortia (AMTech) **"Proposal on Consortium for Development and Deployment of High Performance Computational End Stations for Advanced Manufacturing (CESAM) for SMEs"**	11/01/13
National Science Foundation – NSF 13-585, CISE Research Infrastructure (CRI) **"II-New: Research Infrastructure for Energy-aware High Performance Computing (HPC) and Data Analytics on Heterogeneous Systems"**	11/04/13
National Science Foundation – NSF 13-585 – under Bowling Green State University; CISE Research Infrastructure (CRI) **"II-New: Accelerator-based Heterogeneous Computing Infrastructure for Data-driven and Information-driven Applications"**	11/04/13

OH-TECH Proposals Awarded

as of 09/03/13

Funding Opportunity	OH-TECH Award Amount
Ohio Department of Transportation; Partnered Research Exploration Program 2014 **"Linking Land Use & Travel in Ohio-Incorporating Vehicle Choice & Decline Components"**	$65,565
National Science Foundation – under University of Illinois NCSA NSF Blue Waters Project **"Blue Waters Community Outreach Shared Education Materials / Blue Waters Community Outreach Graduate Fellowship Program"**	$332,866
National Science Foundation **"SC13, SC14, Little Fe Workshop"**	$49,996
Department of Health and Human Services – CDC – NIOSH – under University of Louisville Occupational Safety and Health Research **"Home Healthcare Hazard Training through Virtual Simulation"**	$215,896
Ohio State Library Board LSTA **"Project II-2-13 The OSU Libraries Connect Ohio Resource Sharing Project"**	$900,000
Ohio State Library Board LSTA **"Project 11-1-13 The OSU Libraries Connect Ohio Resource Sharing Project"**	$700,000
Sao Paulo Research Foundation (FAPESP) Brazil and The Ohio State University OSU Partnership Call for Research Proposals 2013 **"Building a Digital Bridge for Research Collaboration between Ohio State Univeristy and Sao Paulo Campuses"**	$10,000
Educause **"Scaffold to the Stars" Supplemental Funding**	$12,347

National Collaborations

- Computational Science Education
  - Computational Science minor approved for Arts and Sciences at Ohio State
- XSEDE Activities
  - Dave Hudak Level 3 manager for industrial relations
    - Completing Industrial Challenge Program
  - XSEDE'14 Conference in Atlanta, GA
    - Karen Tomko leading the student program
    - Steve Gordon chair of Education and Outreach program
  - XSEDE online course in parallel computing in Spring semester
    - Contact Steve Gordon for details

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Doug Johnson

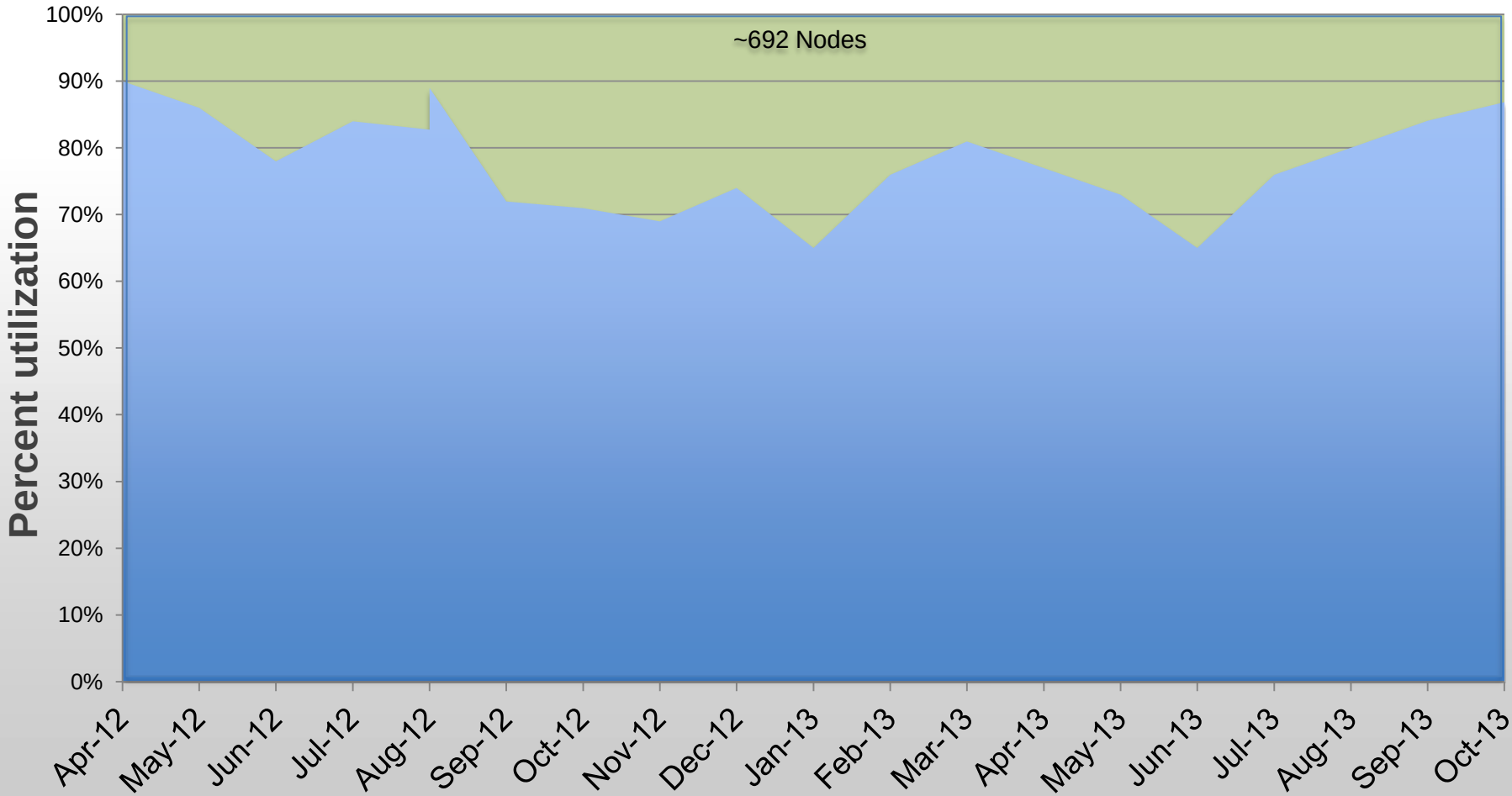
HPC Systems and Operations Update

Outline

- System and Storage Utilization
- Activities
- Upcoming
  - Hardware upgrades

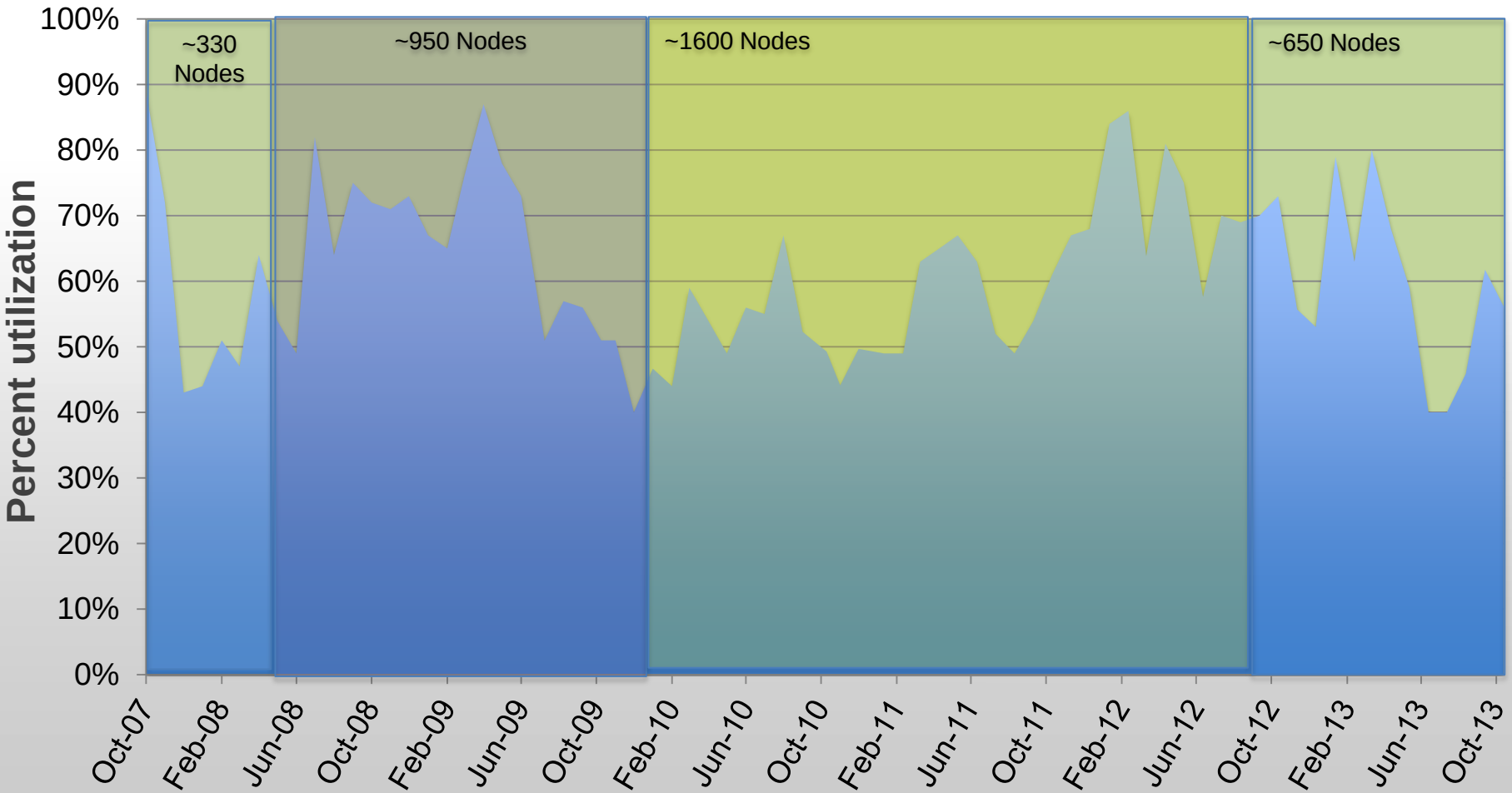
Oakley Lifetime Utilization

85% Average for August-October, 2013



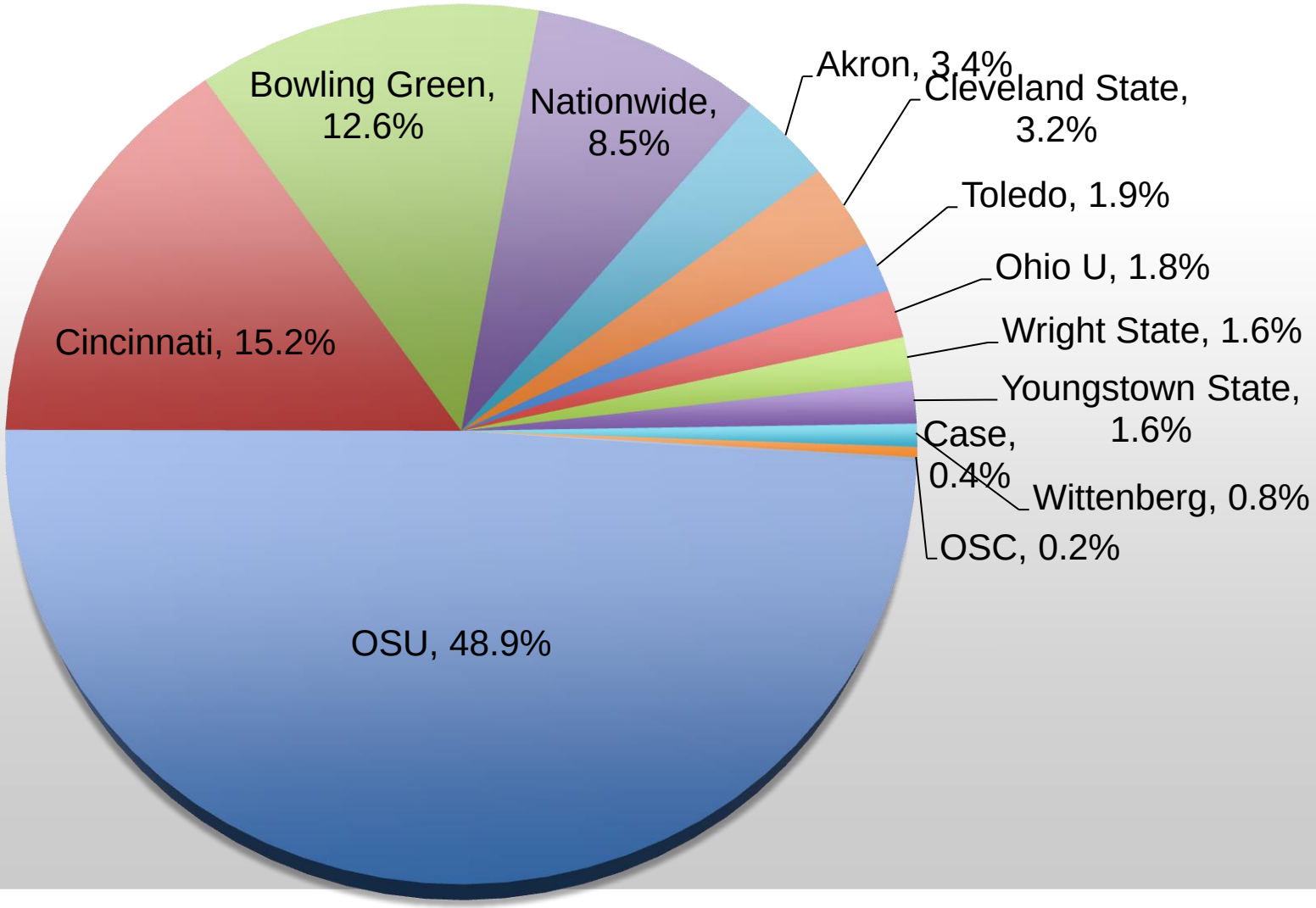
Glenn Lifetime Utilization

55% Average for August –October, 2013



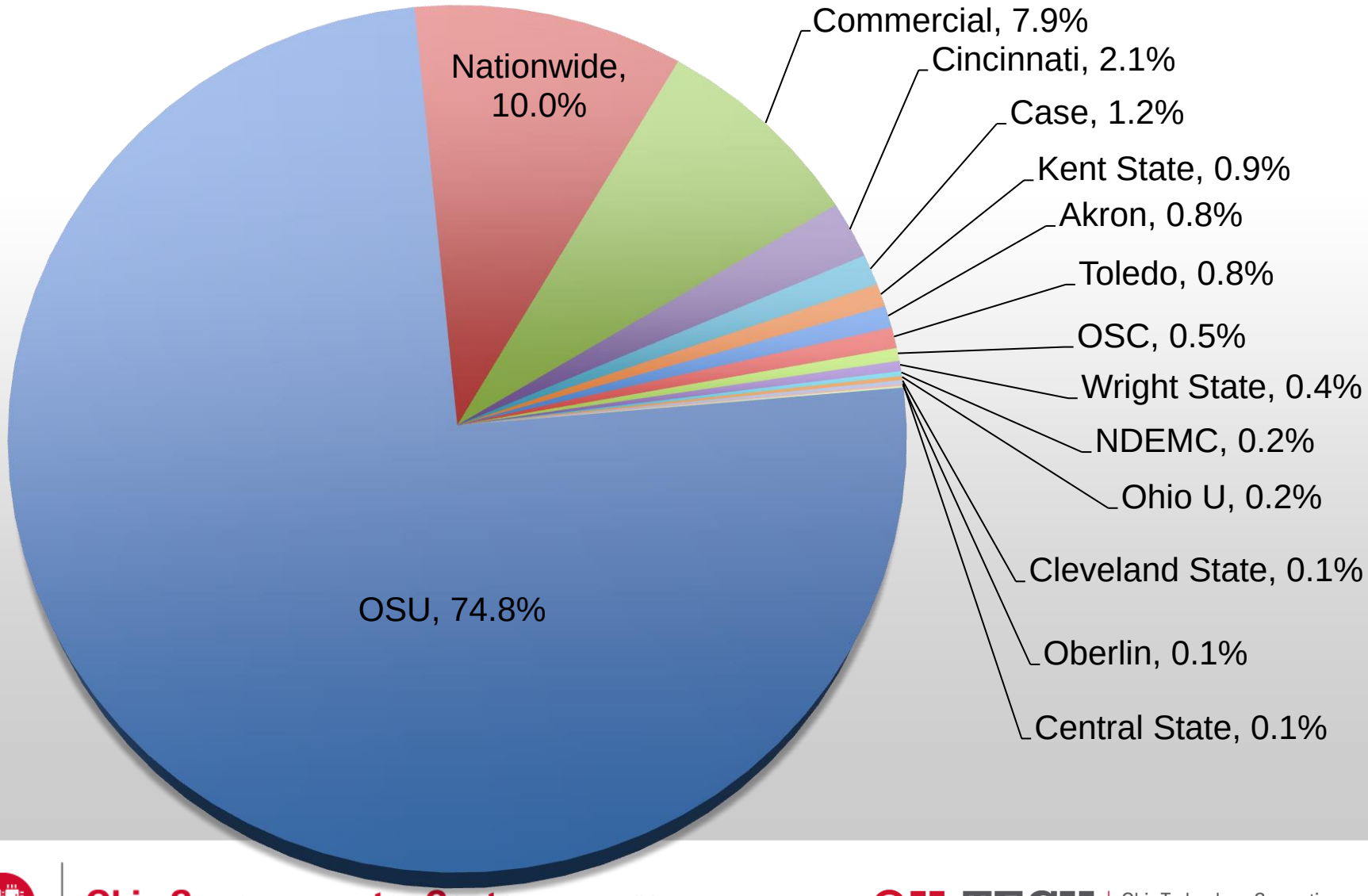
Percentage of Total Utilization By Institution - Glenn

August to October, 2013

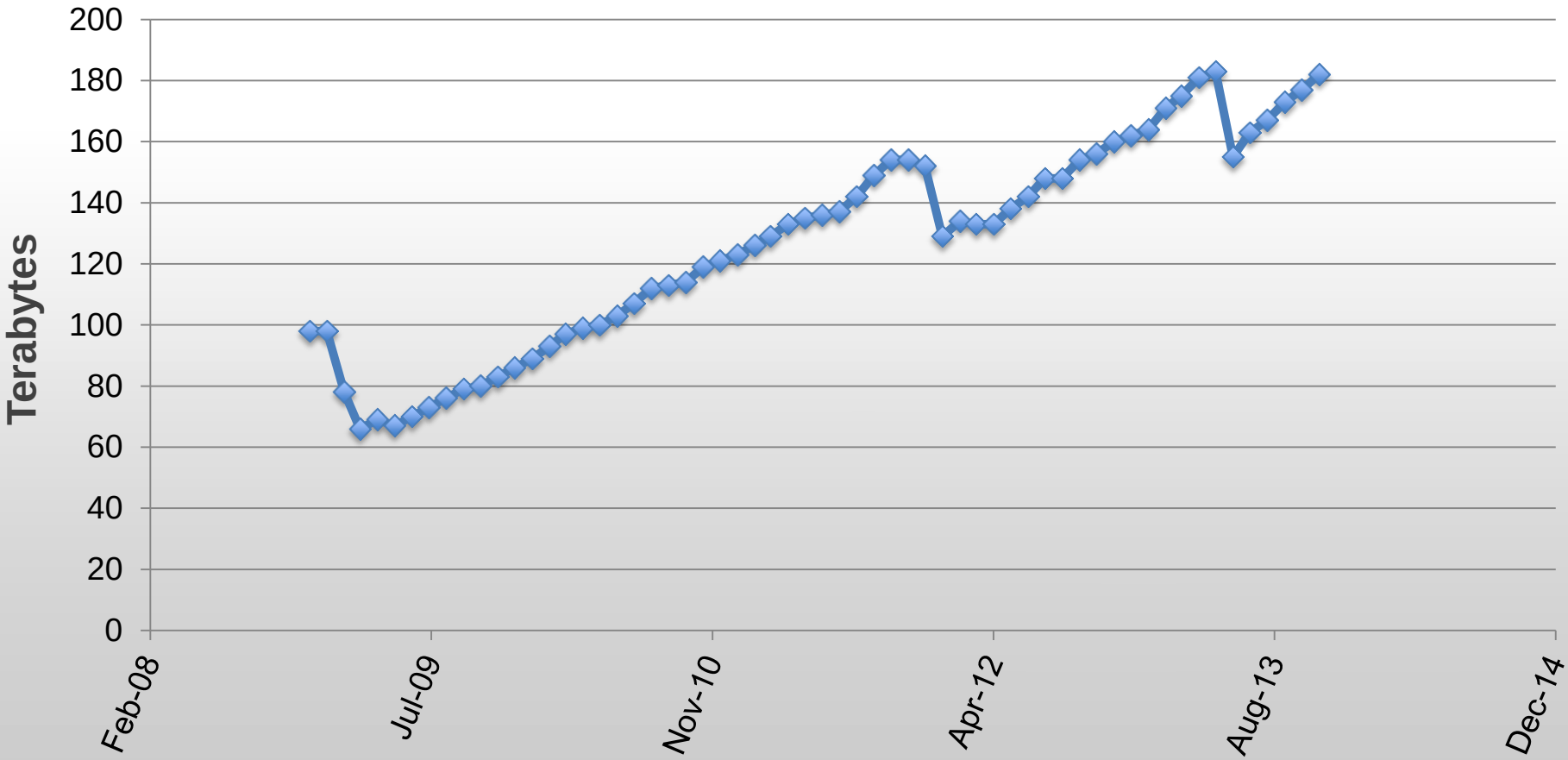


Percentage of Total Utilization By Institution - Oakley

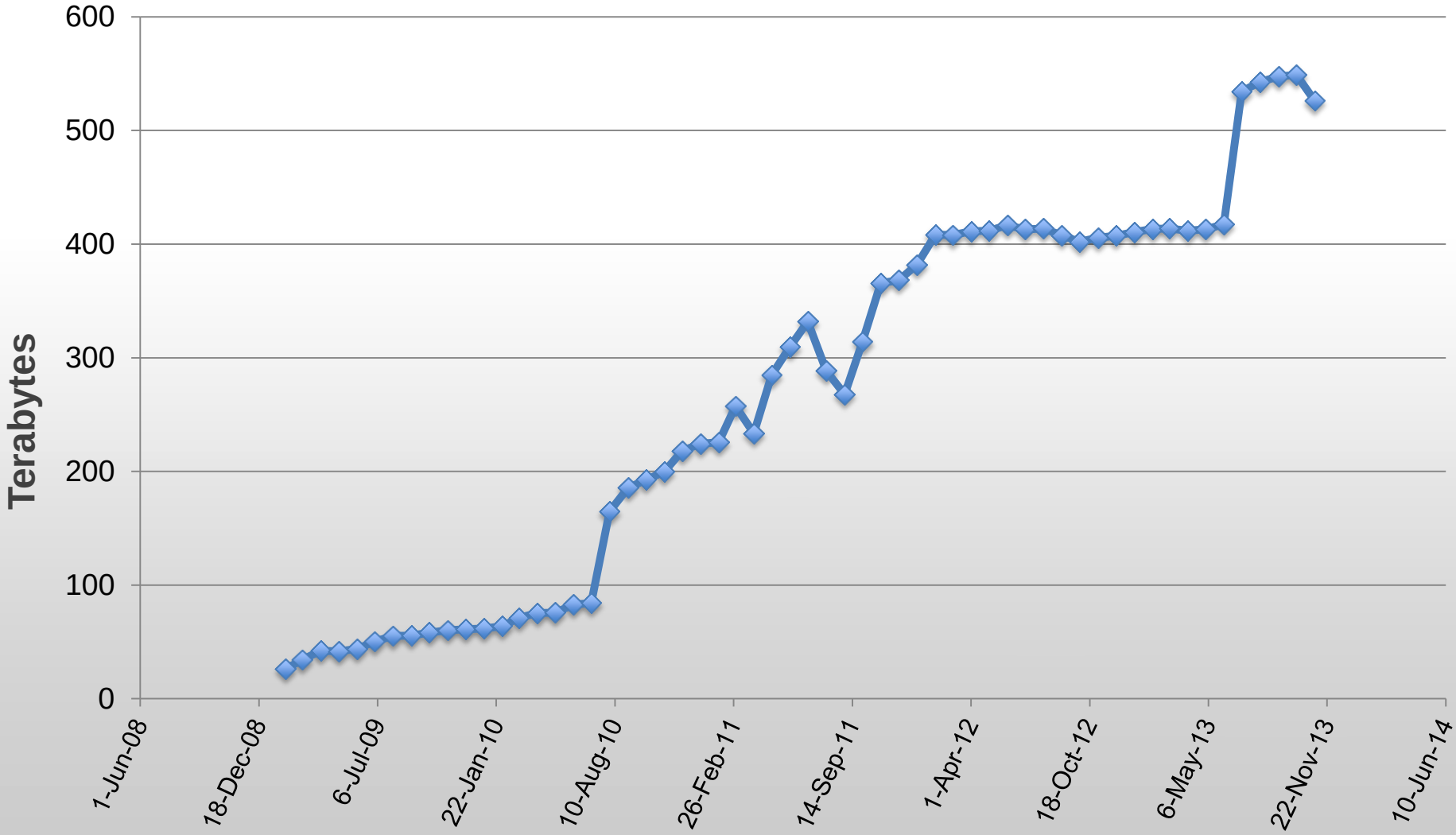
August to October, 2013



Home Directory Usage Trends (300 TB Total)



Project Storage Usage Trends (~1 PB Total)



Activities

- Downtime for SOCC power changes on Sept. 29
- Move OSC to different UPS and generator
- Provides a growth path
  - ~70 KVA available with existing infrastructure
  - ~200 KVA additional with minimal additions
- Kernel upgrade
- Ethernet switch firmware upgrades

Activities (cont.)

- Network Changes
  - Glenn node connectivity to home directory servers upgraded to 10Gb Ethernet
  - VM servers upgraded to 10Gb Ethernet
- GPFS Migration Preparation
  - Testing new servers
  - Reconfiguration of backups
  - Server GPFS software upgrade
- Start revamp of Nagios monitoring framework

Activities (cont.)

- Finished beta test of IBM LTFS-EE
  - Will want to consider for future
- Ruby cluster
  - Efforts to make this a multi-user system still ongoing
- Open Science Grid (OSG) services
- Lin Li presentation at Central Ohio Tivoli User Group Meeting
  - “Implement IBM GPFS with TSM on Linux Platform”
- RFI

Upcoming

- OSC software infrastructure improvements
- SSO and Grid services
- SC13
- HIPAA data support at OSC
- Ruby Cluster
- Project file system migration to GPFS
- Cut-over to new Nagios server
- Host systems for SimCenter for OSU College of Engineering

Hardware Upgrades

- Home directories
- Network, Ethernet and Infiniband
- Tape library drives and media
- Lustre servers
- VM servers
- Infrastructure servers

Ohio Supercomputer Center

An OH·TECH Consortium Member

Brian Guilfoos, Science & Technology Support Manager

User Support, Education and Training

Agenda

- 2014 annual allocations, available hours
- ARMSTRONG replacement plan
- Results of Lustre policy enforcement (+ a reminder)
- Memory containers, job epilogue
- Strategies for dealing with backed-up queues
- Ticket summary
- System Utilization notes
- Training
- Comprehensive upcoming event calendar

Please ask questions as we go! Lots of material today!

2014 Allocations

Total RU allocated in the last 12 months	8,302,316
Annual Allocations	1,230,000
Total RU used in the last 12 months	8,373,901
% of allocations unused	64%*
Total Future Commit – unused allocations from the last 12 months	4,493,512*
Total Future Commit	11,759,547*
% of future commit from the last 12 months	38%*

Annual CPU Hours Available (Glenn)	46,673,280
Annual CPU Hours Available (Oakley)	72,743,040
Total CPU Hours	119,416,320
Total RU Available	11,941,632
RUs Available to Allocate (10% holdback for director's discretion)	10,747,469
RUs Available per month	895,622

ARMSTRONG replacement

- Phase I
  - Institute a new site with password, shell, and email change capability
- Phase II
  - Migrate PI functions of ARMSTRONG to the new site
  - Upgrade some additional user applications (eg, allocations) to the new site.
- No timeline currently, but Phase I has been marked as “high priority” by OH-TECH project management

Lustre Data Expiration

- Lustre data policy:
  - Files untouched for 180 days will be removed
  - Removal will occur once a week
  - In the event of full file system, we will delete the oldest files first until the file system is usable again
- Eventually: 1 million file count quota per user
  - Reminder: Lustre performs best with big files!
- Voluntary compliance made a tremendous difference – thank you!
- Purge policy in place, has dramatically improved the situation on the filesystem.
- **REMINDER: NO FILES ARE BACKED UP ON LUSTRE**
  - Filesystem is scratch space. Data loss is always a possibility

Fractional Node Charging for Serial Jobs - Oakley

- Technical solution in testing
- Limits users to a maximum of 4GB/core* (Oakley STANDARD NODE)
- Memory requests in batch scripts will now be limits
- Two phase rollout
  - Better diagnostic information at the end of jobs (Done!)
  - Memory enforcement & charging changes – two examples that both request ¼ of a node:
    - nodes=1:ppn=3
      - Implicit limit of 12 GB of RAM
    - nodes=1:ppn=1,mem=12GB
      - Will be assigned 1 core, 12 GB of RAM
      - Will be charged for 3 cores (12GB/(4GB/core))
- Parallel jobs unaffected (already charged for all cores)

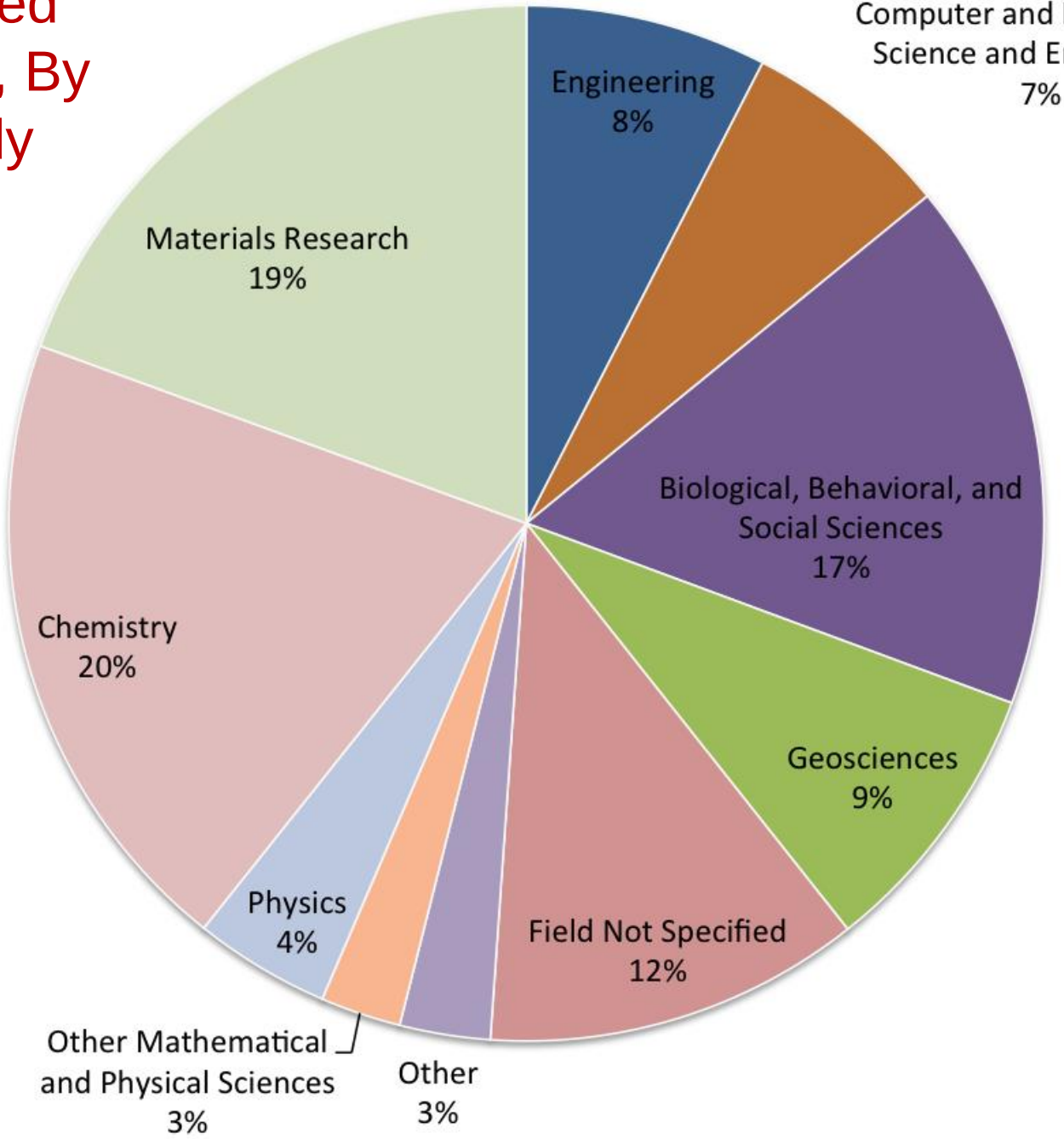
Congestion on Oakley

- System perpetually full
- We do not anticipate this changing significantly, despite the occasional lulls. “The New Normal”
- Size jobs appropriately
  - If your walltime is predictable, make requests with a reasonable safety factor – let the scheduler attempt to backfill your jobs.
  - Don’t request significantly more cores/memory than your job requires
- Can you run on Glenn?
  - Less busy
  - Contact OSC Help if required software is missing

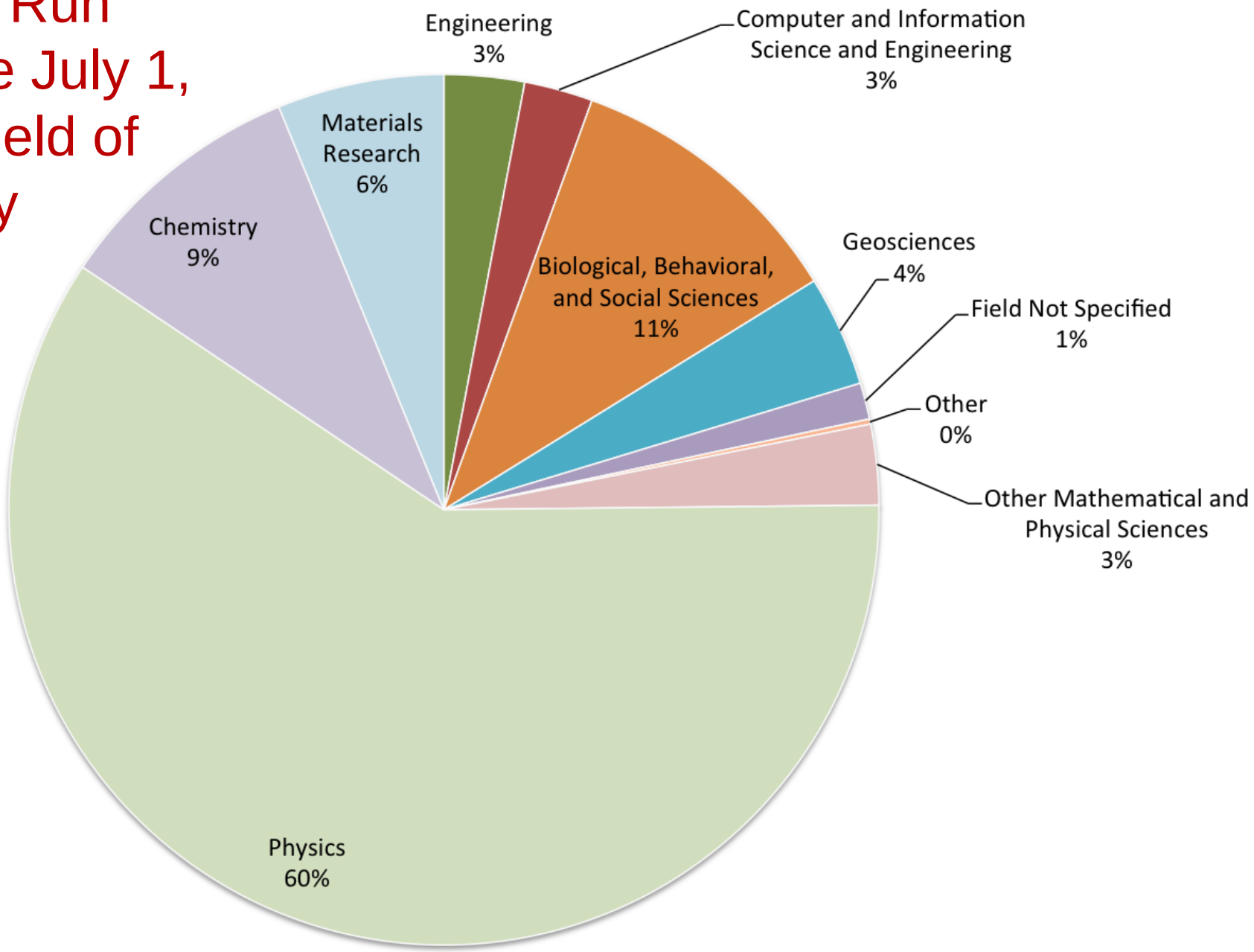
Incidents

- 141 new tickets in the last 120 days
  - 40 in “High Performance Computing”
  - 70 in “Statewide Software Licensing”
  - Remainder scattered across other categories
- 103 closed or resolved
- 16 active
- 22 waiting

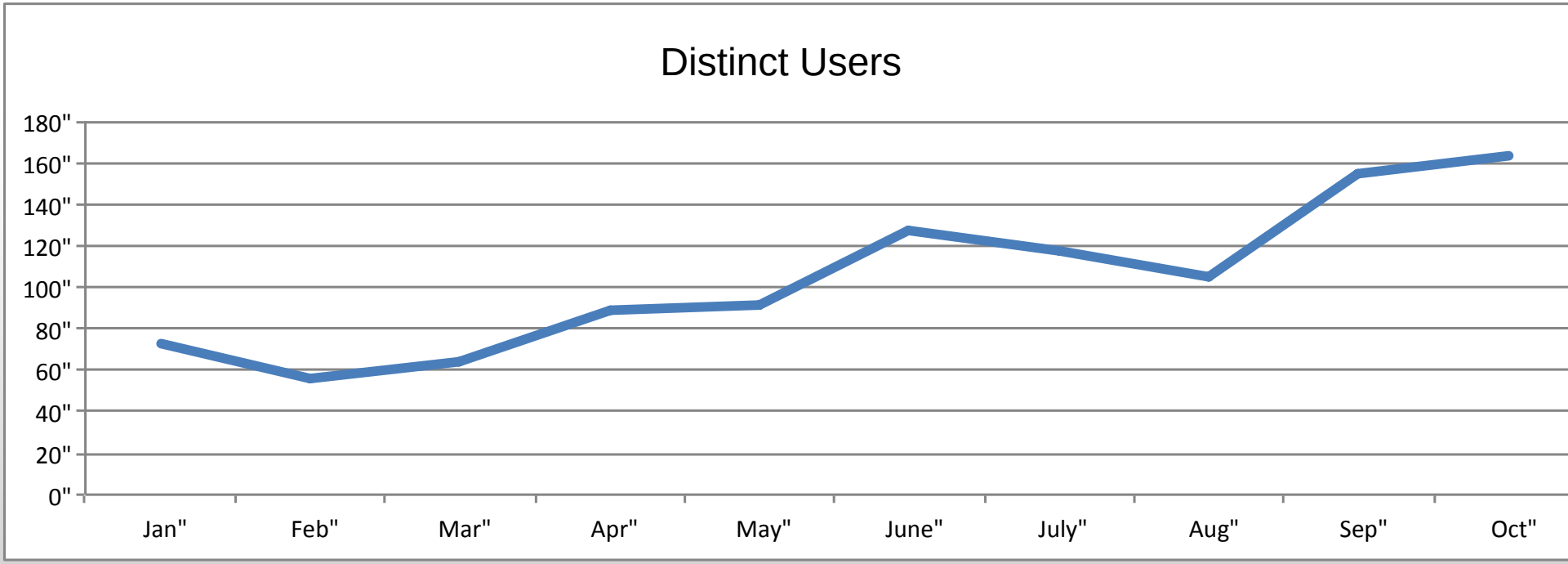
RU Consumed Since July 1, By Field of Study



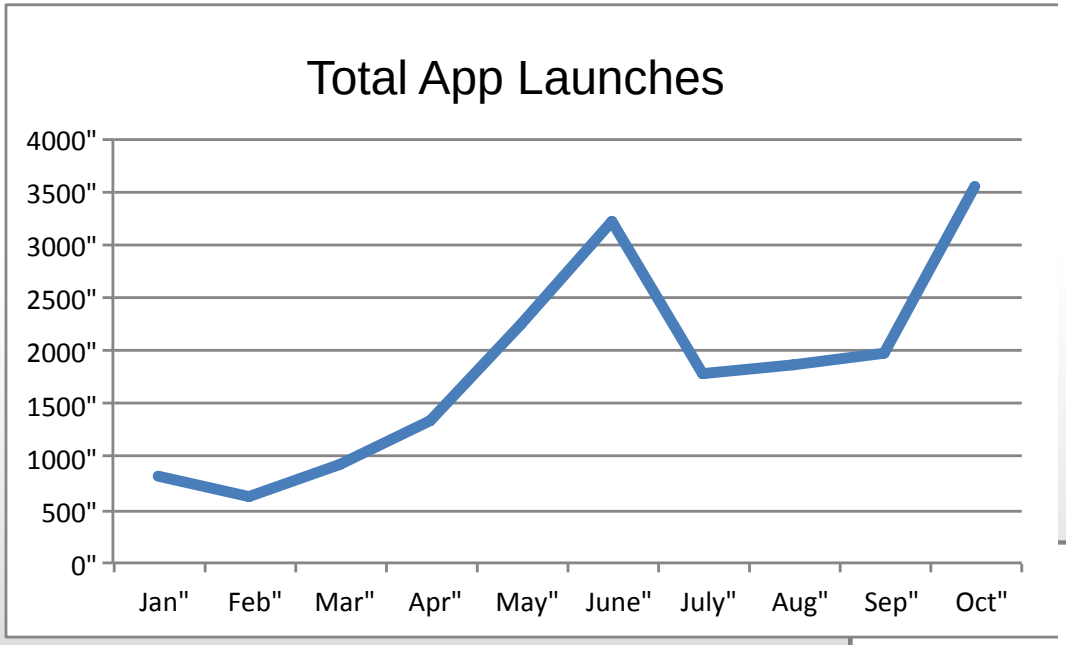
Jobs Run Since July 1, By Field of Study

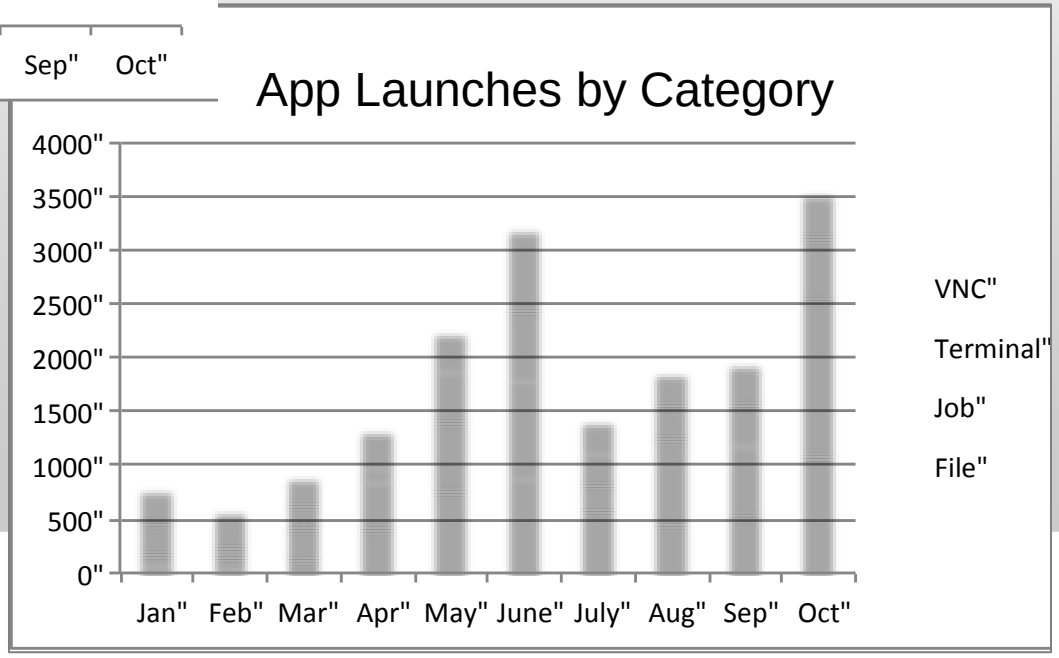


OnDemand Usage



OnDemand Usage





Training

- Intro to OSC @ UC on October 8th was a great success
- Partnering with PSC to offer remote XSEDE training (tentative, and NOT CONFIRMED dates)
  - MPI, Dec. 3-4
  - Big Data (Hadoop & SPARQL), Feb. 4
- Video training for OnDemand
  - In production
  - To be posted on osc.edu in the OnDemand documentation
- Planning “skills classes” for first semester 2014
  - Please contact us if you have specific requests

Upcoming Events Calendar

- November 11 – Veteran's Day (OSC closed)
- November 18-22 – Supercomputing 13, Denver
- November 28-29 – Thanksgiving Holiday (OSC closed)
- December 3-4 – XSEDE HPC Workshop (BALE)
- December 12 – OSC/OARnet Advisory Board
- December 24-25 – Christmas Holiday (OSC closed)
- February 4 – XSEDE HPC Workshop (BALE)
- March 6 – Statewide User Group Meeting

Stay Up to Date!

- www.osc.edu/supercomputing
  - Entry point for all documentation
  - Current “Known Issues” listed at the bottom of the page
- osc.edu/n
  - System notices (downtimes, etc)
- osc.edu/e
  - Upcoming events (training, etc)
- Follow us on Twitter for push notices
  - www.twitter.com/HPCNotices
- For help, contact OSC Help
  - oschelp@osc.edu

Ohio Supercomputer Center

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Karen Tomko

XSEDE Update

XSEDE Overview

www.xsede.org

XSEDE

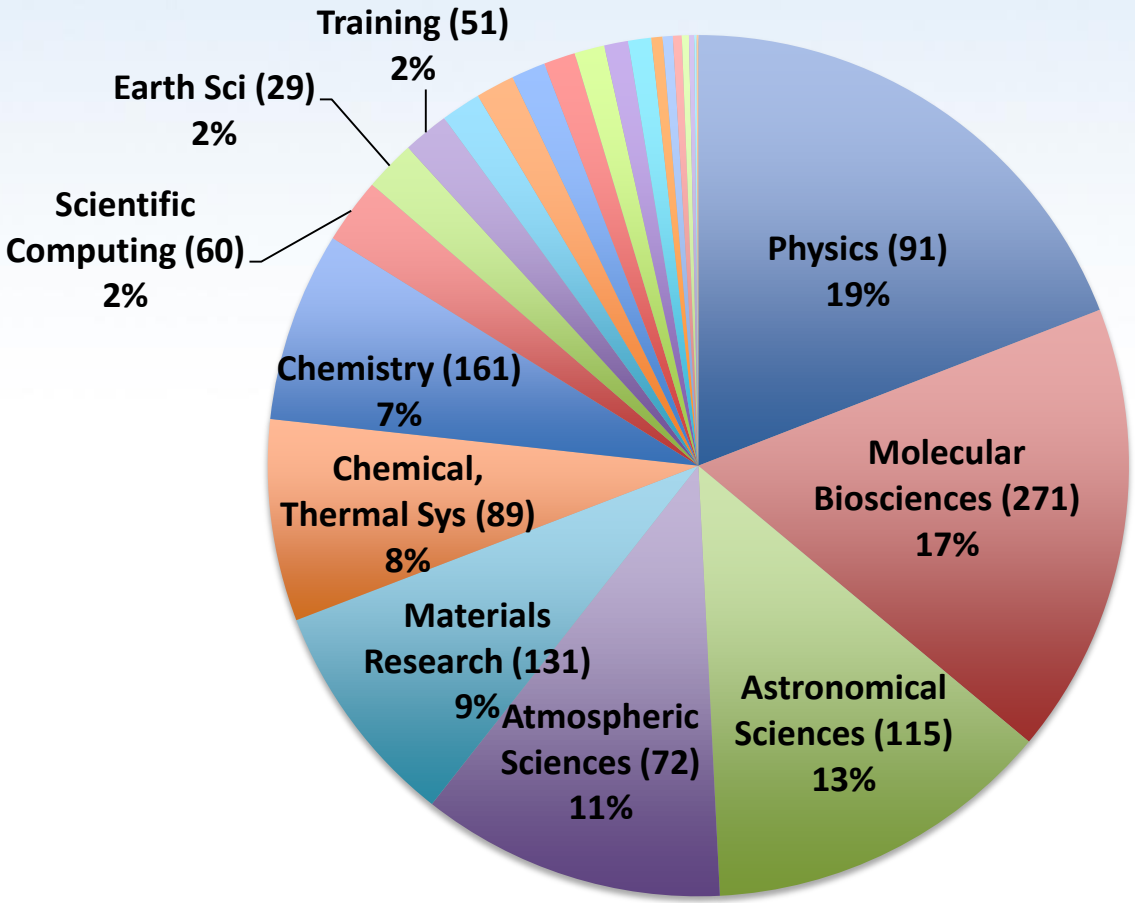
Extreme Science and Engineering Discovery Environment

17-Jul-12

What is XSEDE

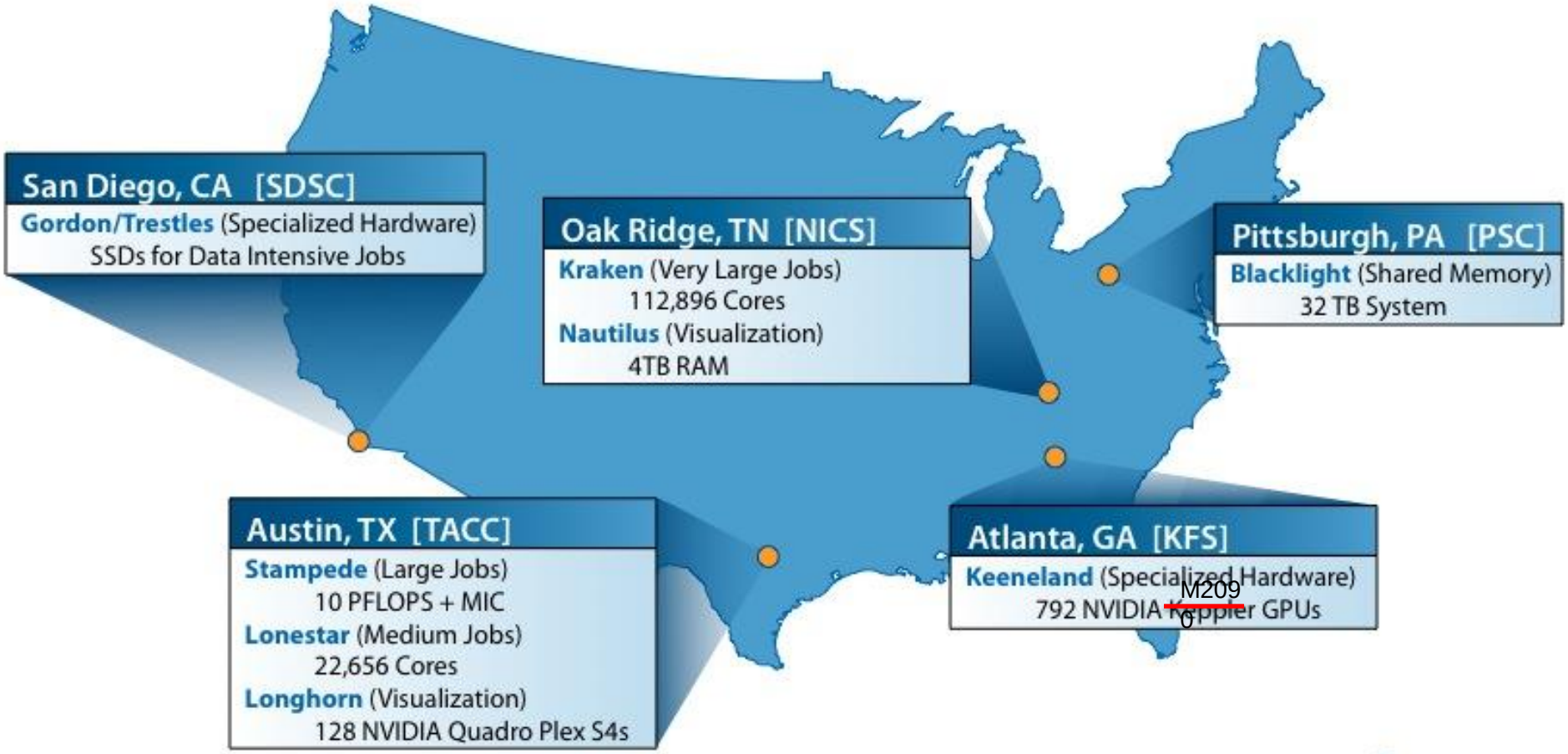
- Extreme Science and Engineering Discovery Environment.
- Supports 16 supercomputers, high-end visualization and data analysis resources nationally.
- 5-year, $121M project funded by NSF. It replaces the NSF TeraGrid project.

Who Uses XSEDE?



- >2 billion cpu-hours allocated
- 1400 allocations
- 350 institutions
- 32 research domains

XSEDE Computing Resources



CONTACT: HELP@XSEDE.ORG

Data Storage and Transfer

- SDSC Gordon
  - SSD system with fast storage
- NCSA Mass Storage System
  - http://www.ncsa.illinois.edu/UserInfo/Data/MSS
- NICS HPSS
  - http://www.nics.utk.edu/computing-resources/hpss/
- Easy data transfer
  - In-browser SFTP or SCP clients through Portal SSH
- Standard data transfer
  - SCP to move data in/out of XSEDE systems
    - Requires SSH key setup
  - Rsync to move data in
- High performance data transfer
  - Globus Online: https://www.globusonline.org/

Types of Allocations

- Campus Champion
  - Get your feet wet with XSEDE
  - < 10k cpu-hours
  - 2 day lead time
- Start-Up
  - Benchmark and gain experience with resources
  - 200k cpu-hours
  - 2 week lead time
- Education
  - Class and workshop support
  - Short term (1 week to 6 months)
- XSEDE Research Allocation (XRAC)
  - Up to 10M cpu-hours
  - 10 page request, 4 month lead time

https://www.xsede.org/how-to-get-an-allocation

Other Resources

- Science Gateways
- Extended Support
- Open Science Grid
- FutureGrid
- Blue Waters (NCSA)
- Titan (ORNL/NICS)
- ALCF (Argonne)
- Hopper (NERSC)

Support Resources

- Local Campus Champion
  - That's me!
  - Karen Tomko, ktomko@osc.edu
- Centralized XSEDE help
  - help@xsede.org
- Extended one-on-one help (ECSS):
  - https://www.xsede.org/ecss
- Training
  - http://www.xsede.org/training


Our reach will forever
exceed our grasp, but,
in stretching our horizon,
we forever improve our world.
XSEDE
Extreme Science and Engineering
Discovery Environment

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Rick Prairie

Software Committee

Call for Participation

- When
  - Software committee meets prior to SUG meetings
  - Discussion via email between meetings
- What
  - Decisions on which software packages are purchased for academic use, respond to new software requests
  - Would like domain science working groups to help build software portfolios for their science field
- How to get involved
  - Send email to ktomko@osc.edu to volunteer or suggest a working group

Software Items for Review

- MolPro
  - Requested by Amit Sharma, WSU
  - Scott Brozell had done some initial testing of an evaluation version
  - Faster than some existing packages for test case, good parallel scaling
  - Cost is $5600 for a 1 year non-commercial site license (parallel execution)
- XFdtd from Remcom Software
  - Invoice for renewal of support received, $1575
  - OSC split the cost of initial purchase with researcher
  - No use outside of group
  - Renewal invoice forwarded to researcher
- VASP
  - Licensed per Research Group
  - Investigating site level install
  - Process for license confirmation to be put in place
  - Groups with license for 4.6 will not be given access to 5.X versions

Renewals – Calendar Year 2013

Software	Expiration (2013)	License Term (years)	Projected Cost	Renewal Started
MATLAB DCS	March 1	1	$3,750	Completed
CSD	April 1	1	$1,500	Completed
COMSOL	June 15	1	$3,695	Completed
OSU MATLAB	September 30	1	$21,503	Completed
LS-Dyna	December 27	1	$500	Completed
Gaussian	December 31	1	$12,000	Payment in progress

Renewals – Calendar Year 2014

Software	Expiration (2014)	License Term (years)	Projected Cost	Renewal Started
MATLAB DCS	April 1	1	$3,750	No
CSD	April 1	1	$1,575	Quote Received

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John Heimaster

Hardware Committee

Questions

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