XSEDE

Extreme Science and Engineering Discovery Environment

XSEDE Overview, Training Focus

Midwest Big Data Hub Meeting
March 9 – 10, 2018

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XSEDE Overview

XSEDE:

- Is an NSF-funded virtual organization
- Integrates and coordinates the sharing of advanced digital services (e.g. supercomputers, visualization, data analysis resources)
- Serves researchers nationally to support science
- Provides users with seamless integration to NSF's high-performance computing and data resources

https://www.xsede.org/about/what-we-do

XSEDE Resources

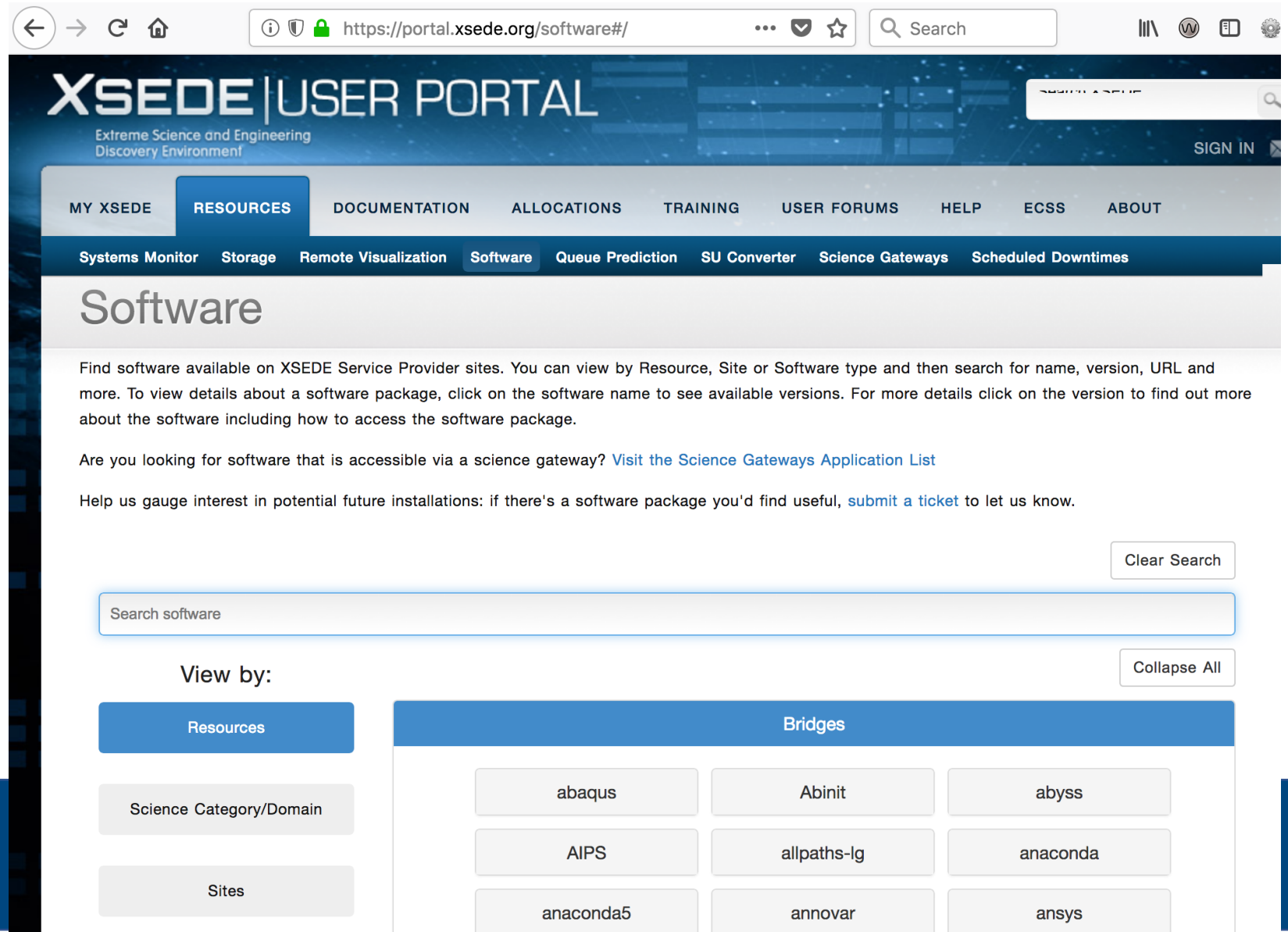
Resources include

- Multi-core high performance computing (HPC)
- Many-core HPC
- Distributed high-throughput computing (HTC)
- Visualization
- Data analysis
- Large-memory
- Data storage
- Cloud

https://www.xsede.org/ecosystem/resources

Resource	Org	Type
HP/NVIDIA Interactive Visualization and Data Analytics System (Maverick)	TACC	vis
IU/TACC (Jetstream)	TACC	compute
IU/TACC Storage (Jetstream Storage)	UT Austin	storage
LSU Cluster (superMIC)	LSU CCT	compute
Open Science Grid (OSG)	OSG	compute
PSC Bridges GPU (Bridges GPU)	PSC	compute
PSC Large Memory Nodes (Bridges Large)	PSC	compute
PSC Regular Memory (Bridges)	PSC	compute
PSC Storage (Bridges Pylon)	PSC	storage
SDSC Comet GPU Nodes (Comet GPU)	SDSC	compute
SDSC Dell Cluster with Intel Haswell Processors (Comet)	SDSC	compute
SDSC Medium-term disk storage (Data Oasis)	SDSC	storage
Stanford University GPU Cluster (XStream)	Stanford U	compute
TACC Data Analytics System (Wrangler)	TACC	compute
TACC Dell/Intel Knights Landing, Skylake System (Stampede2)	UT Austin	compute
TACC Long-term Storage (Wrangler Storage)	TACC	storage
TACC Long-term tape Archival Storage (Ranch)	TACC	storage

Software on XSEDE Resources



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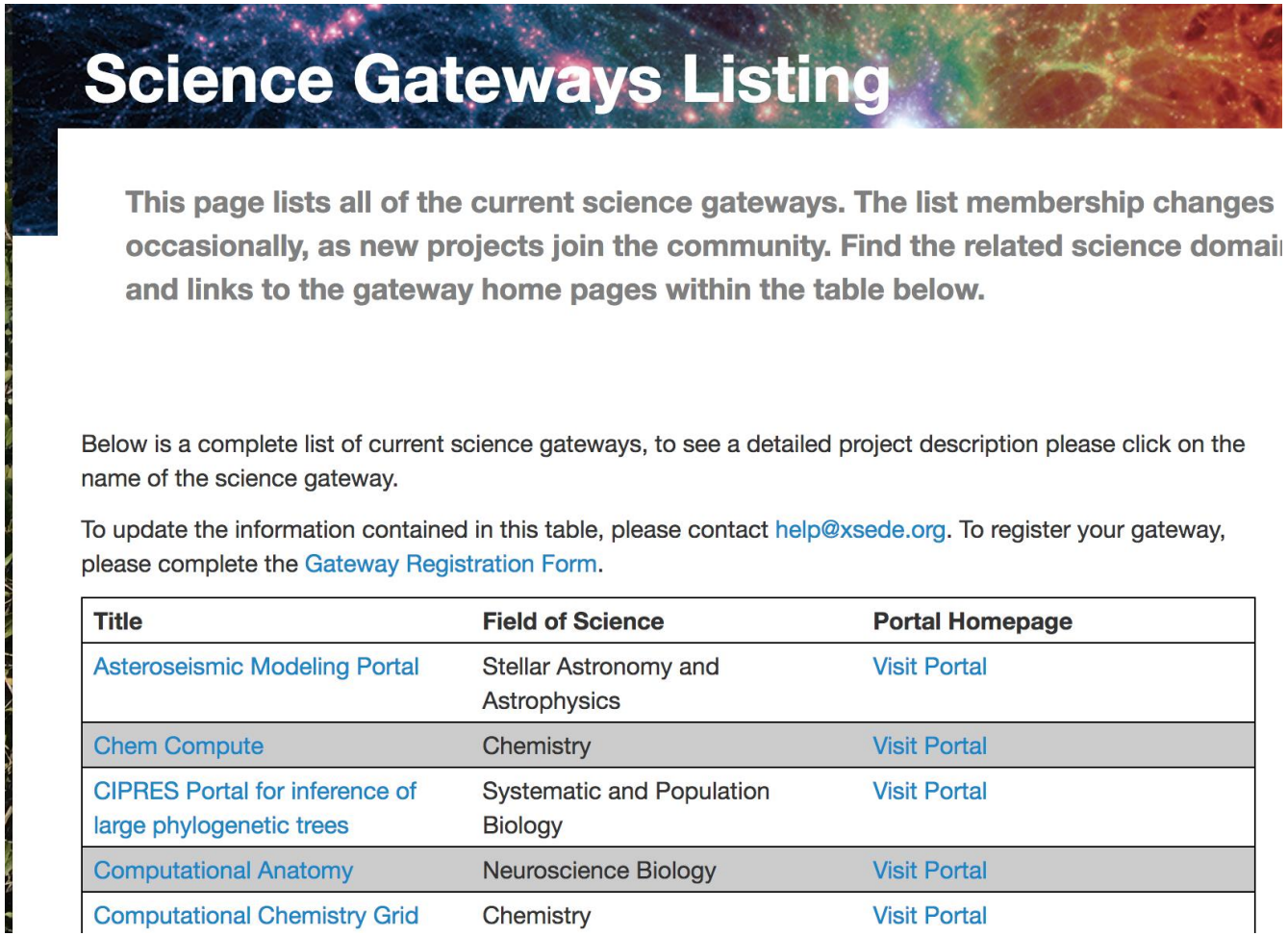
Science Gateways

https://www.xsede.org/ecosystem/science-gateways



Science Gateways Listing

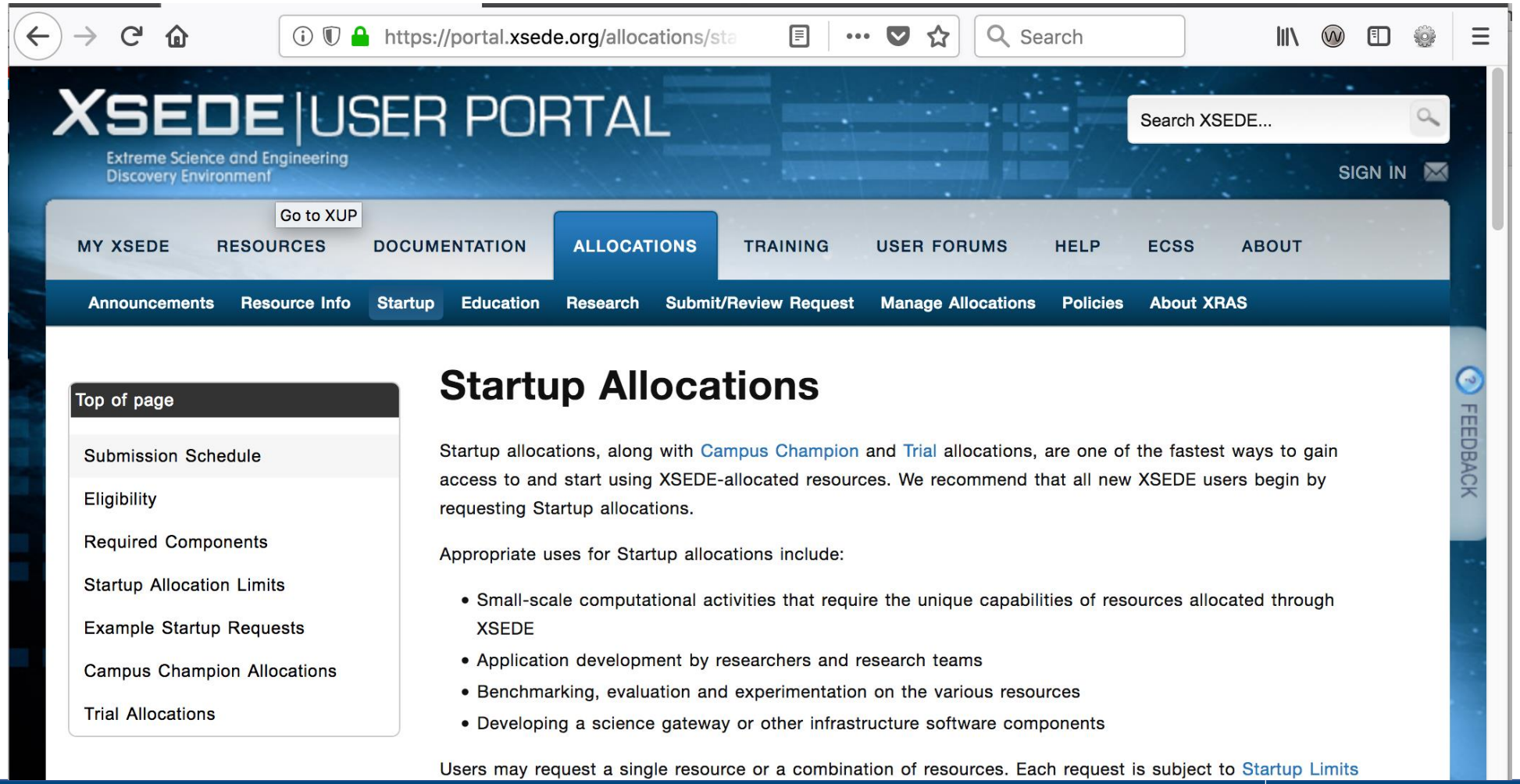
This page lists all of the current science gateways. The list membership changes occasionally, as new projects join the community. Find the related science domai and links to the gateway home pages within the table below.

Below is a complete list of current science gateways, to see a detailed project description please click on the name of the science gateway.

To update the information contained in this table, please contact help@xsede.org. To register your gateway, please complete the Gateway Registration Form.

Title	Field of Science	Portal Homepage
Asteroseismic Modeling Portal	Stellar Astronomy and Astrophysics	Visit Portal
Chem Compute	Chemistry	Visit Portal
CIPRES Portal for inference of large phylogenetic trees	Systematic and Population Biology	Visit Portal
Computational Anatomy	Neuroscience Biology	Visit Portal
Computational Chemistry Grid	Chemistry	Visit Portal

XSEDE Allocations



Serve your community & help XSEDE via XRAC

XSEDE Resource Allocations Committee (XRAC)

XSEDE Resource Allocations Service

Who

About 40 computational experts from academia, research labs, and industry

What

Review large-scale requests to use XSEDE-allocated resources
No more than 10 requests per meeting

Why

Serve the community, see how the system works
help ensure NSF resource portfolio used efficiently

Where

Meetings held at seasonally advantageous locations around the country

When

Four meetings per year, you're asked to attend at least three
First week of March, June, December, and week before Labor Day

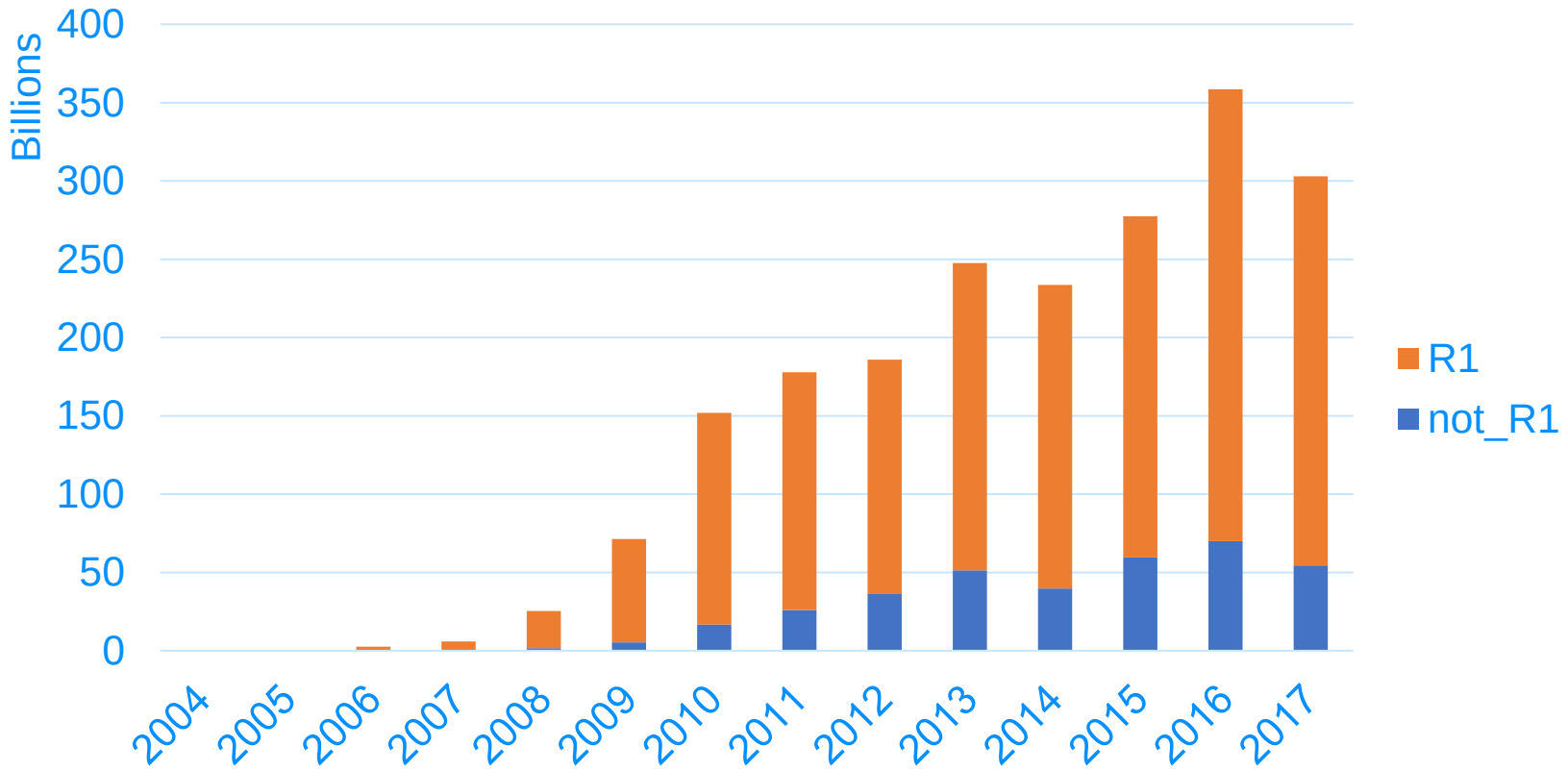
How

All travel expenses paid by XSEDE • All-electronic submission and review system
Meetings start Sunday evening and end Monday afternoon

Interested? Contact
Ken Hackworth • hackworth@psc.edu

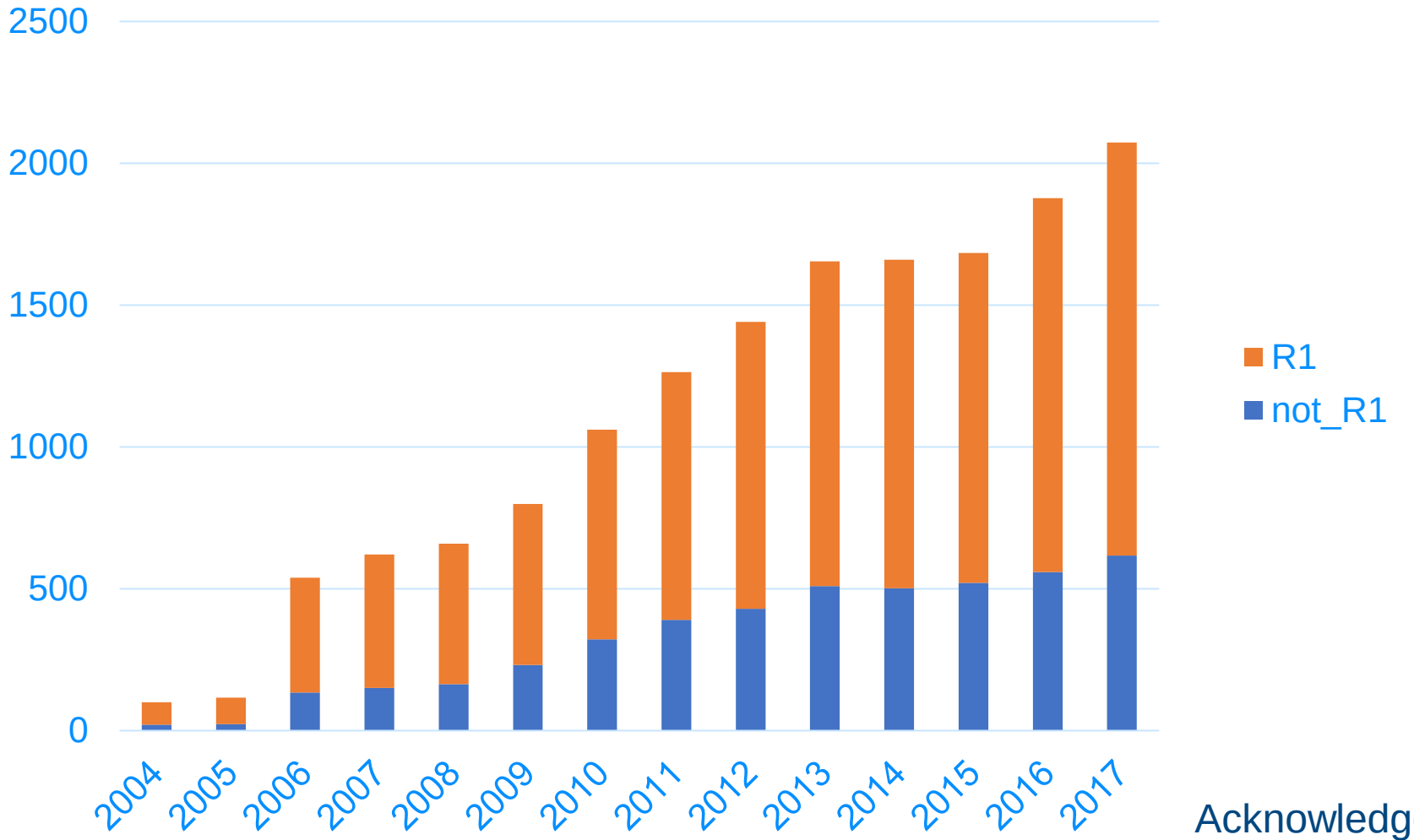
For more on XSEDE
www.xsede.org • portal.xsede.org

Usage by R1s and non-R1s, in Normalized Units



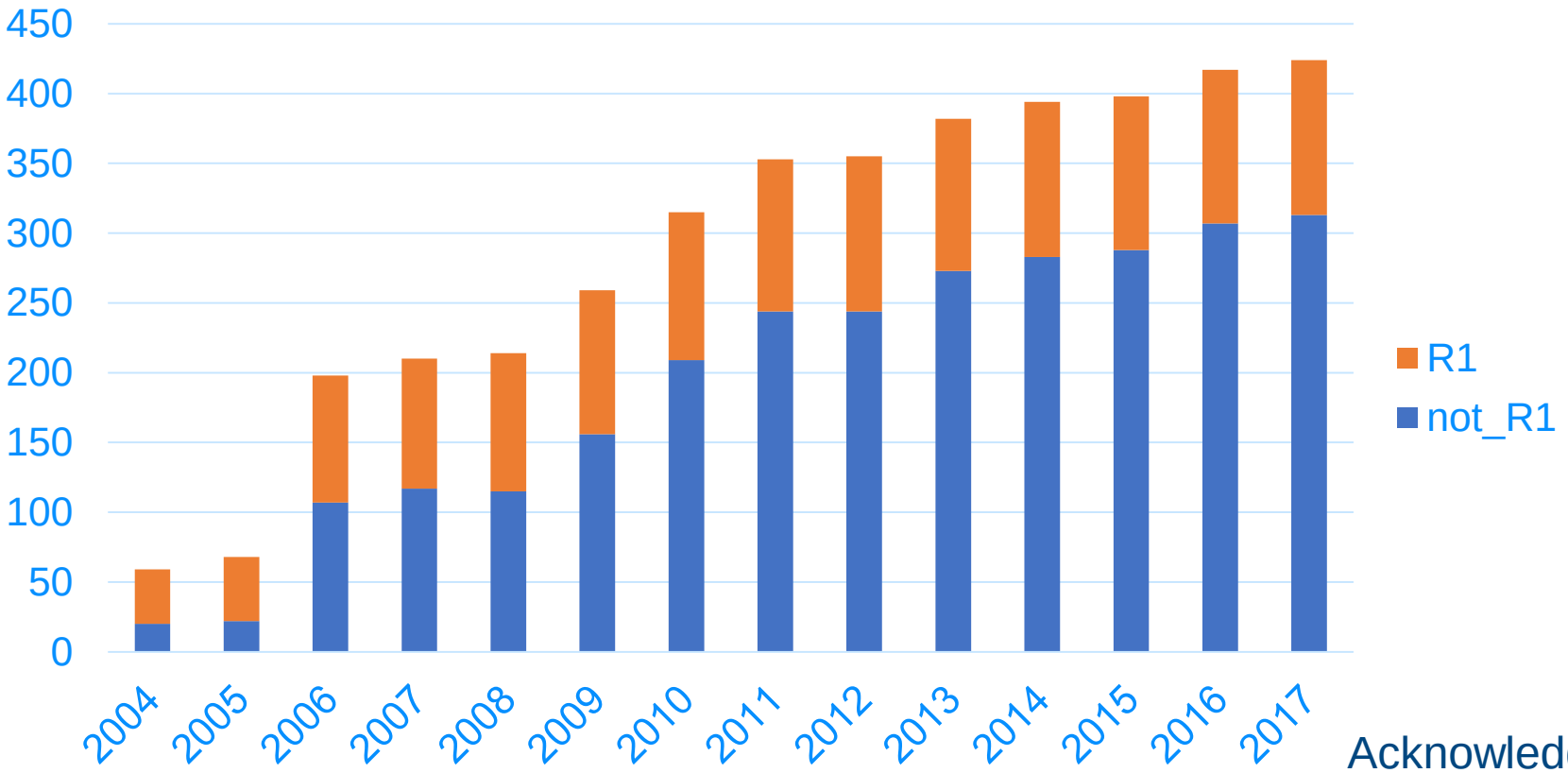
Acknowledgement: Dave Hart

Allocated PIs from R1s and non-R1s



Acknowledgement: Dave Hart

Number of R1 & non-R1 Institutions Represented in Allocations



Acknowledgement: Dave Hart

XSEDE Programs and Activities

Provides the expertise to ensure that researchers can make the most of the supercomputers and tools, including:

- Extended Collaborative Support Service (ECSS) – team experts with researchers
- XSEDE Cyberinfrastructure Integration (XCI) - provides an advanced hardware and software architecture that allows for individualized user experiences
- XSEDE User Portal web interface allows users to monitor and access XSEDE resources, manage jobs on those resources, report issues, and analyze and visualize results.
- Coordinated allocations of NSF's high-end resources and digital services, through the XSEDE Resource Allocation Service (RAS) team.
- A powerful and extensible network, maintained by the XSEDE Operations team, with fast connections to the XSEDE Service Providers
- Training, Education, and Outreach through the Community Engagement & Enrichment (CEE) team that expand participation in XSEDE-based projects, curriculum development, and traditional training opportunities.
- Advanced support for novel and innovative projects.
- A fellowship program that brings Campus Champions to work closely with XSEDE advanced user support staff.

https://www.xsede.org/about/what-we-do

XSEDE Training

Training is available in a variety of formats, including multicast, webinars, online training, and in person workshops. Suggestions for new topics are encouraged via the feedback form. For more information, see:

- XSEDE Training Overview for a summary guide of materials available
- XSEDE Training Course Catalog including listings across formats and sites
- Course Calendar with registration for upcoming training courses
- Online Training on materials relevant to XSEDE users
- Badges are available
- Roadmaps are in development

Training materials focus on systems and software supported by the XSEDE Service Providers, covering programming principles and techniques for using resources and services. Training classes are offered in high performance computing, visualization, data management, distributed and grid computing, science gateways, and more.

XSEDE Monthly Workshop Series

- Rotating (Nuts and Bolts) Topics
  - MPI, OpenMP, OpenACC, Big Data, Summer Boot Camp
- Up to 25 satellite sites per session
  - Sites are spread geographically and include MSIs and National Labs
- Register VIA XSEDE Portal:
  - https://portal.xsede.org/course-calendar
- To Become a Satellite Site or Questions Contact:
  - Tom Maiden – tmaiden@psc.edu

Acknowledgement: Tom Maiden

XSEDE Monthly Workshop: Big Data

Day 1		Day 2
11:00	Welcome	Machine Learning: Recommender System with Spark
11:25	Intro to Big Data	
12:00	Hadoop	
12:30	Intro to Spark	
1:00	Lunch	Lunch
2:00	Spark	Deep Learning with Tensorflow
3:30	Spark Exercises	
4:30	Spark	Bridges: A Big Data Platform
5:00	Adjourn	Adjourn

Acknowledgement: Tom Maiden

XSEDE Training Providers

This group	Offers	On	To	Approx
Training	Async online modules	Many HPC topics	Everyone	Ongoing
Training, SP	Webcast	Getting started	Everyone	Quarterly
Training	Multicast live training	HPC Topics	Satellite sites	Monthly
Broadening Participation	On-site training	HPC and XSEDE	Underrepresented institutions	Quarterly (academic year focus)
ECSS ESTEO	Webcast and live training	New resources, new capabilities	XSEDE Staff	Annual series
ECSS ESTEO	All formats	Many HPC topics	Everyone	Ongoing
Service Providers	On-site and webcast	Local resource	Everyone	
ECSS, SPs	Webcast	Varied	Campus Champions	Quarterly

Events and registrations: https://portal.xsede.org/course-calendar

ESTEO

- Mentor Campus Champion Fellows
- Deliver live training events especially in collaboration with CEE Broadening Participation
- Orchestrate ECSS internal staff training seminars
  https://www.xsede.org/documents/10165/1589367/RDMA_Spark_Hadoop.pdf
- Respond to requests for service
  http://www.calendar.gatech.edu/event/595496
- Review training modules, Retire training modules
- Support Meetings and BOFS
- Mentoring
- Review Education Allocation Proposals
- Support Campus Champions
- Manage US Participation in International HPC Summer School

Acknowledgement: Jay Alameda

Education

https://www.xsede.org/community-engagement/educator-programs

Curriculum and Educator Programs

XSEDE pursues innovation and collaboration in computational science education.

Campus Visits

XSEDE campus visits emphasize the need for
education and offer guidance concerning cou

Campus visits bring together faculty, students
discuss the importance of having a workforce

Participating in Collaborative Online Courses

XSEDE sponsors full-semester online courses taught through collaborations with faculty at participating institutions.

The XSEDE courses consist of recorded lectures that can be watched by students independently or in their own local classrooms. Each lecture comes with built-in quizzes that are used as part of the grading for the course. In addition, several computer exercises are typically available that students can run on XSEDE computational resources to gain practical experience and have credit for the work recorded in their class grade.

The capstone assignment for a course often is a final project supervised by the local faculty members.

The first of these courses is Applications of Parallel Computers, taught by Jim Demmel at the University of California, Berkeley. View the course content.

How Faculty Can Participate

If you are a faculty member interested in collaborating with XSEDE in this program, you will need to create a course in your own academic schedule that your local students can register for and receive credit. You and your students will then use the online materials and XSEDE resources to complete the course.

Local faculty who participate in the program meet periodically with the XSEDE instructors and staff to discuss schedules, suggestions for course improvement, and any questions related to operations. The local faculties are responsible for assigning final grades to all of their own students.

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CEE: Broadening Participation Program

Expand awareness of XSEDE

- Campus Visits
- Conference Exhibiting
- Papers
- News

Identify programs and researchers who can benefit from XSEDE services

- Conference Exhibiting
- Campus Visits
- Training Events
- Consulting

Enable institutions and faculty to use advanced computing to increase their research productivity

- Build and Maintain a Thriving Peer Support Community
- Deliver training mapped to needs
- Connect researchers with XSEDE services and expertise

Create scalable and sustainable models and best practices

- Enhance curriculum
- Foster productive campus champions
- Create connections to the CI Ecosystem

Acknowledgement: Linda Akli

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Cyberinfrastructure Resource Integration

- Software toolkits, consulting services, provider coordination
  - Cluster distribution, scientific software, XSEDE-like environment
  - Site visits to help install
  - Information and support for joining the XSEDE federation
- Impacts
  - 7 clusters and more than 700 TeraFLOPS of computing on CRI software
  - New data analytics program supported at Bentley University, short video at http://bit.ly/xsede-ba

Acknowledgement: Rich Knepper

Campus Champions

The Campus Champions Program is a group of 400+ Champions at 200+ US colleges, universities, and other research-focused institutions, whose role is to **help researchers at their institutions to use research computing**, especially (but not exclusively) large scale and high end computing.

The Campus Champions started as a way to drive users to XSEDE TeraGrid machines, but over time we've become a **national community of practice in research computing facilitation**.

What is a Campus Champion?

A Campus Champion is an **employee of, or affiliated with, a college or university (or other institution engaged in research)**, whose role includes helping their institution's researchers, educators and scholars (faculty, postdocs, graduate students, undergraduates, and professionals) with their computing-intensive and data-intensive research, education, scholarship and/or creative activity, including but not limited to helping them to use advanced digital capabilities to improve, grow and/or accelerate these achievements.

Who are the Campus Champions?

https://www.xsede.org/community-engagement/campus-champions/current

https://www.hpc.msstate.edu/publications/docs/2017/01/1517907816979.pdf

Acknowledgement: Marisa Brazil

Questions?

Final comments:

- Student programs at PEARC: https://www.pearc18.pearc.org/student-program
- Many opportunities announced through the XUP; sign up for an account at portal.xsede.org

Acknowledgements:

- On individual slides
- www.xsede.org
- portal.xsede.org