Overview of XSEDE and Introduction to XSEDE 2.0 and Beyond

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XSEDE
Extreme Science and Engineering Discovery Environment

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- Please cite as: Towns, John Towns, John. *Overview of XSEDE and Introduction to XSEDE 2.0 and Beyond,* May 2015, [http://www.slideshare.net/jtownsil/overview-of-xsede-and-introduction-to-xsede-20-and-beyond]
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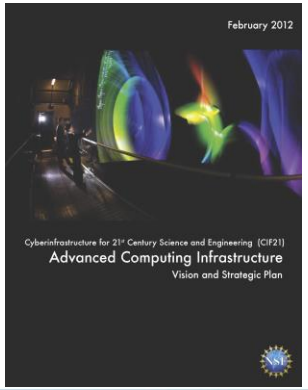
XSEDE in Context

- XSEDE is an award made under the eXtreme Digital solicitation
  - TeraGrid Phase III: eXtreme Digital Resources for Science and Engineering (XD), NSF 08-571
- Consistent with NSF's vision and strategy statements

NSF's Strategic Planning Documents

- *Investing in Science, Engineering, and Education for the Nation's Future - National Science Foundation Strategic Plan for 2014-2018*
  - www.nsf.gov/pubs/2014/nsf14043/nsf14043.pdf
  - Vision: *A Nation that creates and exploits new concepts in science and engineering and provides global leadership in research and education.*
- *Cyberinfrastructure Framework for 21st Century Science and Engineering*
  - www.nsf.gov/cif21
- NSF's *Advanced Computing Infrastructure: Vision and Strategic Plan*
  - www.nsf.gov/pubs/2012/nsf12051/nsf12051.pdf



XSEDE – accelerating scientific discovery

XSEDE's Vision:

a world of digitally-enabled scholars, researchers, and engineers participating in multidisciplinary collaborations while seamlessly accessing computing resources and sharing data to tackle society's grand challenges.

XSEDE's Mission:

to substantially enhance the productivity of a growing community of scholars, researchers, and engineers through access to advanced digital services that support open research;

and to coordinate and add significant value to the leading cyberinfrastructure resources funded by the NSF and other agencies.

Strategic Goal #1:

Deepen and Extend Use

XSEDE will:

a. *deepen the use—make more effective use*—of the advanced digital services ecosystem by existing scholars, researchers, and engineers, and

b. *extend the use* to new communities.

c. We will *contribute to preparation—workforce development*—of the current and next generation of scholars, researchers, and engineers in the use of advanced digital services via training, education, and outreach; and

d. we will *raise the general awareness of the value of advanced digital services*.

Strategic Goal #2:

Advance the Ecosystem

Exploiting its internal efforts and drawing on those of others, XSEDE will advance the broader ecosystem of advanced digital services by:

a. *creating an open and evolving e-infrastructure*, and
b. *enhancing the array of technical expertise and support services* offered

Strategic Goal #3:

Sustain the Ecosystem

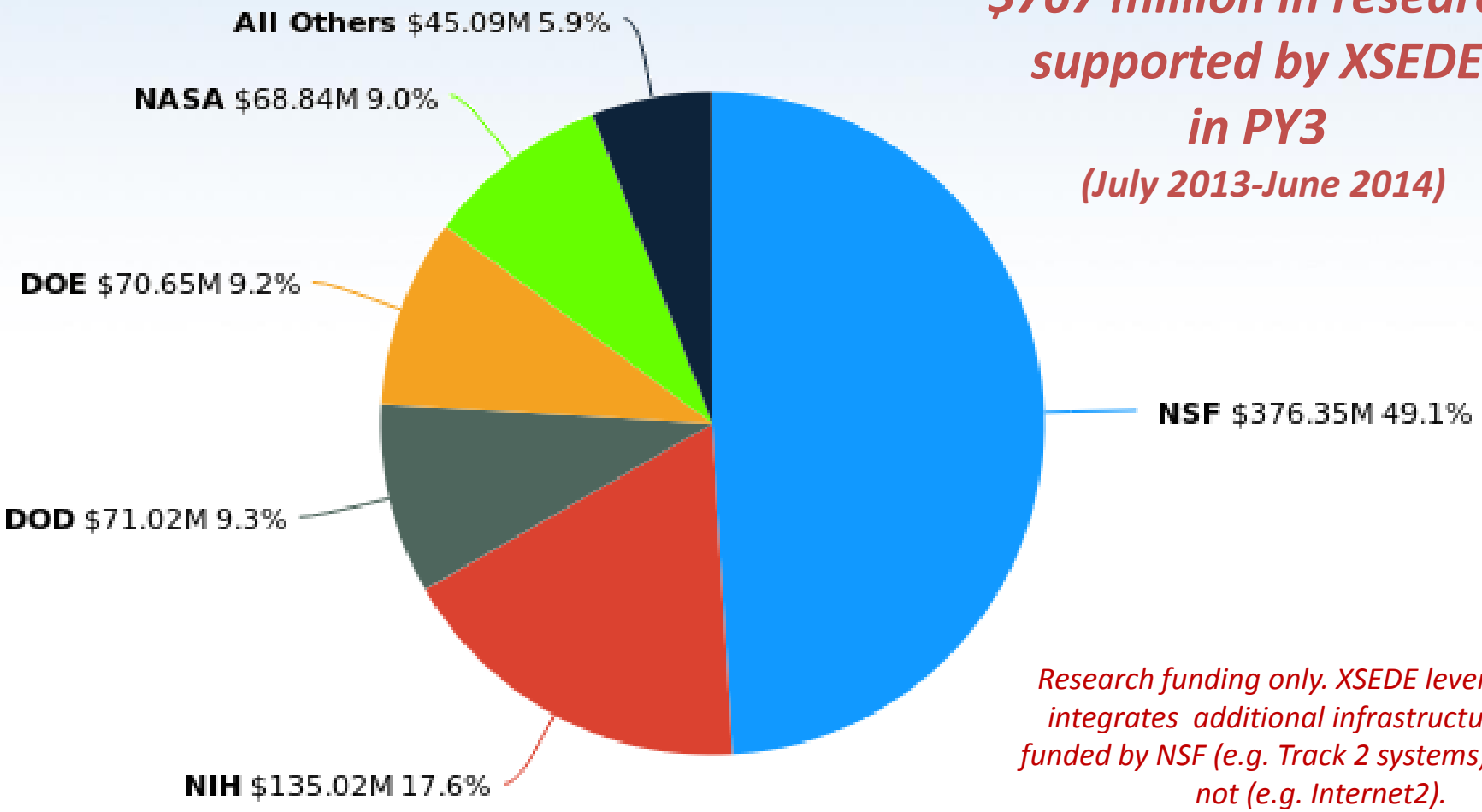
XSEDE will sustain the advanced digital services ecosystem by:

a. *assuring and maintaining a reliable, efficient, and secure infrastructure*, and
b. *providing excellent user support services*
c. XSEDE will further *operate an effective, productive, and*
d. *innovative virtual organization*

XSEDE Factoids: high-order bits

- 5 year, US$121M project
  - plus US$9M, 5 year Technology Investigation Service
    - separate award from NSF
  - option for additional 5 years of funding upon major review after PY3
- No funding for major hardware
  - coordinate, support and create a national/international cyberinfrastructure
  - coordinate allocations, support, training and documentation for >$100M of concurrent project awards from NSF
- ~112 FTE /~250 individuals funded across 20 partner institutions
  - this requires solid partnering!

Total Research Funding Supported by XSEDE in Program Year 3



$767 million in research supported by XSEDE in PY3

(July 2013-June 2014)

Research funding only. XSEDE leverages and integrates additional infrastructure, some funded by NSF (e.g. Track 2 systems) and some not (e.g. Internet2).

What is XSEDE?

- An ecosystem of advanced digital services accelerating scientific discovery
  - support a growing portfolio of resources and services
    - advanced computing, high-end visualization, data analysis, and other resources and services
    - interoperability with other infrastructures
- A virtual organization (partnership!) providing
  - dynamic distributed infrastructure
  - support services and technical expertise to enable researchers engineers and scholars
    - addressing the most important and challenging problems facing the nation and world
- More than just a project funded by the National Science Foundation
  - XSEDE is a path-finding experiment in how to develop, deploy and support e-science infrastructure

XSEDE's Distinguishing Characteristics: *Governance*

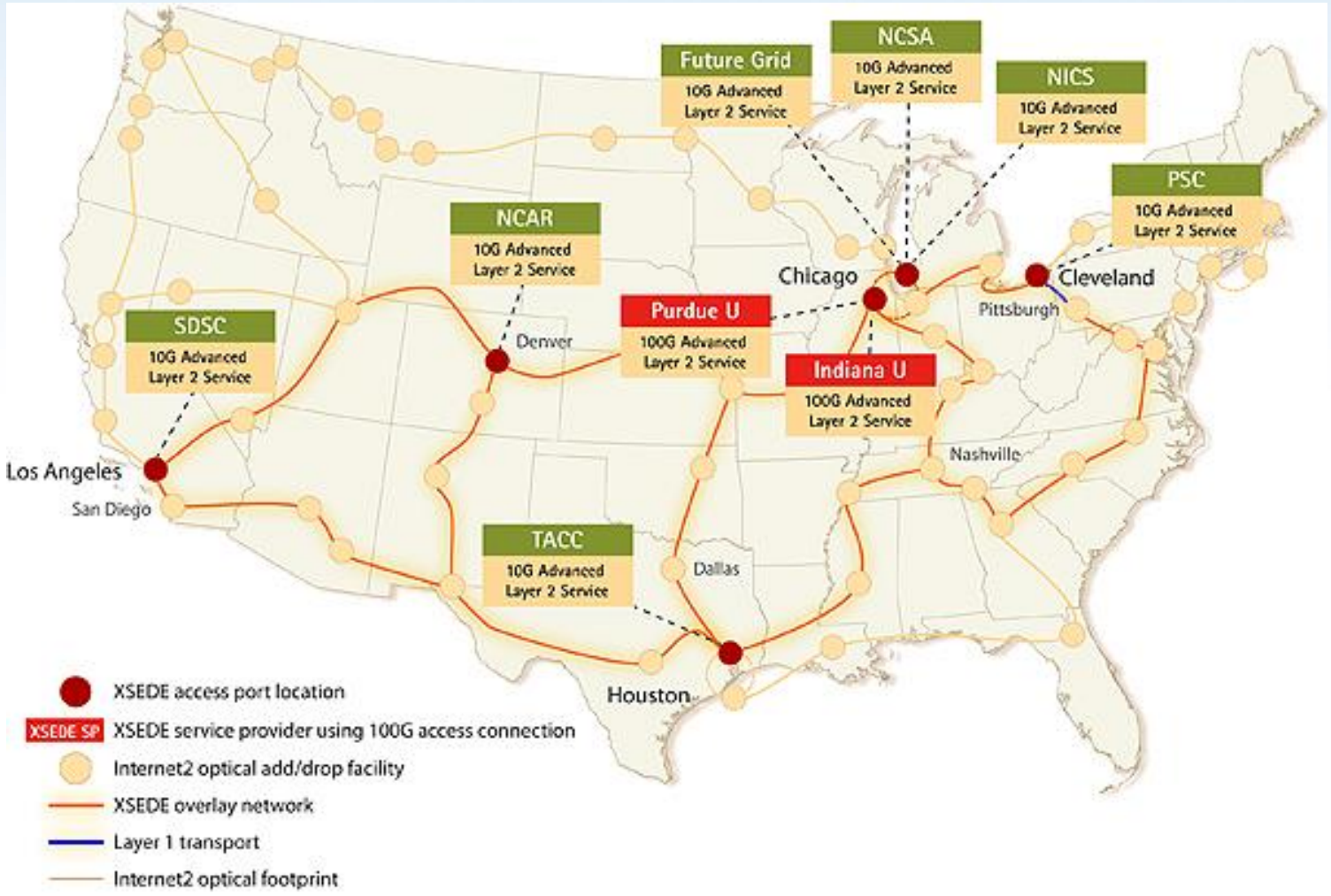
- World-class leadership
  - partnership led by NCSA, NICS, PSC, TACC and SDSC
    - CI centers with deep experience
  - partners who strongly complement these CI centers with expertise in science, engineering, technology and education

XSEDE offers efficient and effective integrated access to a variety of resources

- Leading-edge distributed memory systems
- Very large shared memory systems
- High throughput systems, including Open Science Grid (OSG)
- Visualization engines
- Accelerators like GPUs and Xeon PHIs

Many scientific problems have components that call for use of more than one architecture.

XSEDEnet – Using Internet2's AL2S Service



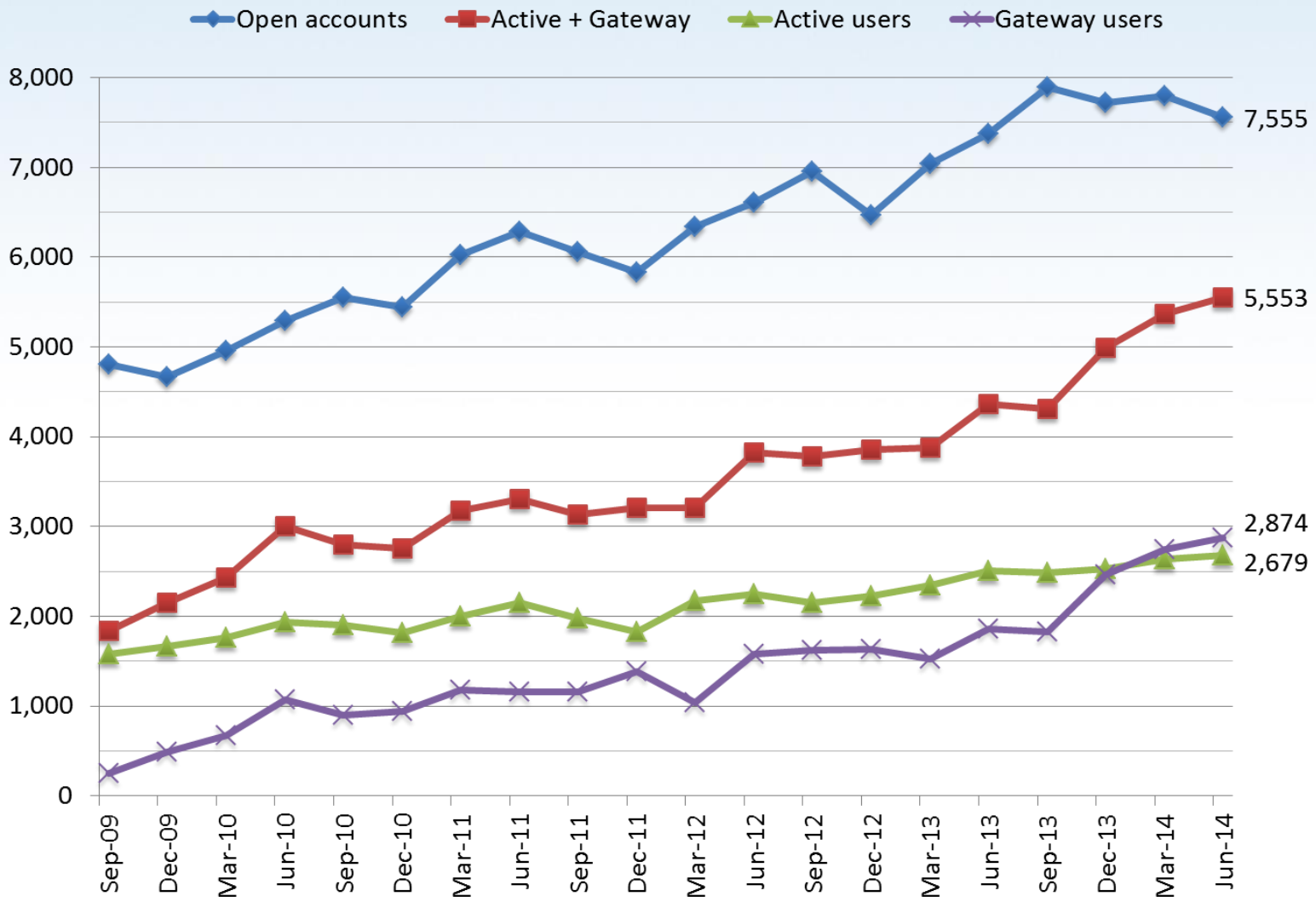
What do you mean by “Advanced Digital Services?”

- Often use the terms “resources” and “services”
  - these should be interpreted very broadly
  - most are likely not operated by XSEDE
- Examples of resources
  - compute engines: HPC, HTC (high throughput computing), campus, departmental, research group, project, …
  - data: simulation output, input files, instrument data, repositories, public databases, private databases, …
  - instruments: telescopes, beam lines, sensor nets, shake tables, microscopes, …
  - infrastructure: local networks, wide-area networks, …
- Examples of services
  - collaboration: wikis, forums, telepresence, …
  - data: data transport, data management, sharing, curation, provenance, …
  - access/used: authentication, authorization, accounting, …
  - coordination: meta-queuing, …
  - support: helpdesk, consulting, ECSS, training, …
  - And many more: education, outreach, community building, …

Direct interactions with the Community

- Facilitate broad range of ground-breaking research
  - provided in-depth support contributing to improved user productivity
  - supported over 14,000 publications to date
- Seamlessly integrate and retire resources
  - transition users smoothly
- Pursue new disciplinary areas
  - increasing the diversity of disciplines utilizing advanced digital services
- Campus Champions continue to reach new heights
  - over 240 Champions at more then 185 institutions
  - expanding program: Regional, Student, and Domain Champions

XSEDE Computational User Census



Services Provided to the Community

- The XSEDE User Portal as the place for users to go to get information and support
  - a single location for their needs
  - create a single account that gives you access to all XSEDE resources: over 18,000 accounts!
- Over 90,000 training registrations in past year!
  - HPCU and CI-Tutor, as well as center trainings, have been used in universities around the country to prepare students to use the nation's pre-eminent computational resources
- Field and route over 10,000 tickets annually

Diverse ECSS Expertise Possible Because of Scale

- ***Fields of expertise***: astrophysics, bioinformatics**,** CFD, chemistry, computer science, climate modeling, engineering, **genomics**, hydrology, **humanities , machine learning,** molecular dynamics, **phylogenetics**, physics, seismology, **statistics**.
- ***Technologies:*** clusters, large shared memory systems, **MICs, GPUs**
- ***Languages:*** C, C++,Fortran, MPI, OpenMP, **Java, JavaScript,** shell programming, CUDA, OpenACC, **Python, R, MATLAB**

- ***Techniques***: benchmarking, **cloud computing**, Condor, **data mining, databases,** FFTs, finite element methods, grid generation, grid middleware**,** Lattice Boltzmann methods, libraries, linear algebra, Monte Carlo methods, parallel debugging, parallel I/O, petascale computing, scheduling, science gateways, visualization, **workflows**

XSEDE had Major Review in September 2014

- From original cooperative agreement:
  - *"At approximately the 36th month NSF will engage in a comprehensive external review of the XSEDE project to determine whether it is appropriate to renew funding for an additional 60 months or consider issuing a new solicitation and proceeding with a full recompetition."*
- Review held in September 2014; panel said:
  - *"positive impact on science"*
  - *has "provided the user community with capabilities for seamlessly utilizing systems operated by multiple service providers"*
  - *an "impressive milestone" being achieved*
  - *"growing evidence (of) successfully coordinating outreach … and … participation by underrepresented groups."*

XSEDE Invited to Submit Renewal Proposal

- Letter received from NSF inviting a renewal proposal
  - non-competitive submission
  - will be reviewed as rigorously as a competitive proposal
- Some parameters for the proposal submission:
  - $100-$120M
    - first round funding totaled ~$130M
  - 5 years of operations, July 2016 – July 2021
  - page limit of 30 pages
  - no option for renewal
  - due June 15, 2015
    - *we are at T - 4.5 weeks and counting*

Priorities for PY6-PY10: Extended Collaborative Support Service

- Continue to provide excellent support to the research community via ECSS
  - this effort must continue to evolve as needs and technologies evolve
  - support for data analysis and visualization (including analytics)
    - support for sensitive data
  - support for executing applications in virtual machines and containers

Priorities for PY6-PY10: Community Infrastructure

- Continue to evolve the XSEDE infrastructure
  - must provide support for and integration of "Track 2" resource
- Expose this architecture to the broader community
  - facilitate integration of broad range of services
    - provide discoverability
  - become the "connector of services" to support the research enterprise

Priorities for PY6-PY10: Toward "Sustainability"

- Developing services on offer to others: providing basic cyberinfrastructure services
  - expose services developed and put in place to operate the XSEDE environment
  - where necessary customize/extend for needs of other projects
  - charge incremental costs for operating/supporting services for other projects
- Objective is not to make money!
  - provides mechanism for other NSF project investments to leverage the XSEDE investment
  - can lead to significant cost saving across NSF CI investments
  - others can leverage this too: projects, institutions, regional consortia, …
- Pilot under way: NCAR with XRAS
  - will use XRAS to support allocation of NCAR resources
  - expressions of interest from some campuses

Collaborations with Blue Waters

- Identifying opportunities for leverage
  - pursuing use of XRAS to support non-PRAC allocations of Blue Waters
  - Consider integration of PRAC and XRAC processes?
- Looking for other opportunities
  - What does the community see as most important to consider?

Meet me in St. Louis!

Save the date!

XSEDE15 WILL TAKE PLACE IN ST. LOUIS, JULY 26-30, 2015.

Thanks to you, XSEDE has become an established ecosystem of HPC resources. Help us take the next step.

The annual XSEDE conference brings together the extended community of individuals interested in advancing research cyberinfrastructure and integrated digital services for the benefit of science and society.

XSEDE

Extreme Science and Engineering Discovery Environment

xsede.org/xsede15 | #XSEDE15

Questions?


Our reach will forever
exceed our grasp, but,
in stretching our horizon,
we forever improve our world.
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