8 July 2019

XSEDE Overview

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XSEDE

Extreme Science and Engineering Discovery Environment



Supported by OAC 15-48562.

Motivation for XSEDE:

- Scientific advancement across multiple disciplines requires a variety of resources and services
- XSEDE is about increased productivity of the community and providing expanded capabilities
 - leads to more science
 - is sometimes the difference between a feasible project and an impractical one
 - lowers barriers to adoption
- XSEDE provides a *comprehensive eScience infrastructure* composed of expertly managed and evolving advanced *heterogeneous digital resources and services* integrated into a general-purpose infrastructure



XSEDE – accelerating scientific discovery

- XSEDE's Vision: a world of digitally enabled scholars, researchers, and engineers participating in multidisciplinary collaborations while seamlessly accessing advanced computing resources and sharing data to tackle society's grand challenges.
- XSEDE's Mission: to enhance the productivity of a growing community of scholars, researchers, and engineers through access to advanced digital services that support open research by coordinating and adding value to the leading cyberinfrastructure resources funded by the NSF and other agencies.



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XSEDE Factoids: high order bits

- 5 year, US\$110M project
 - pursuing additional funding via independent proposals
 - initial 5 year award: \$121M project + ~\$4.6M in supplements
 - plus \$9M, 5 year Technology Investigation Service
- No funding for major hardware
 - coordination, support and creating a national/international cyberinfrastructure
 - coordinate allocations, support, training and documentation for >\$100M of concurrent project awards from NSF
- ~90 FTE /~180 individuals funded across 19 partner institutions in 4 time zones
 - this requires solid partnering!



Vision/Mission: Enable Realizing Best Science





XSEDE's Distinguishing Characteristics: World-class Leadership Partnership led by:

Partners who strongly complement these CI centers with expertise in science, engineering, technology and education

NESA VPSC TAGE SDSC









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)
- Support for VM's and containers and HPC Cloud
- Visualization engines
- Accelerators like GPUs and Xeon PHIs
- Extensive library of research applications

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



Significant Contributions to Community by XSEDE: Supporting the Community

- Over 9,200 researchers used allocated resources in RY3 (up from ~8,500 in RY2)
 - over 6,000 of these were grad/undergrad students
- More than 13,000 verified publications supported to date (since start of XSEDE 1.0)
 - >2,500 new in RY3
 - ~300,000 citations; i10-index > 6,400
- Over 16,800 active users of XSEDE User Portal in RY3
 - nearly 7,300 of these were not associated with an allocation (up from ~2,600 in RY2!)
- More than 930 requests for major compute allocations reviewed in RY3
 - over 1,100 requests for startup and educational allocations
- Over 16,000 service requests addressed in RY3
 - approaching 50,000 service requests addressed to date in XSEDE 2.0
- Completed 47 ECSS projects that assisted computational research teams with an average productivity gain of 13.5 months in RY3
 - 142 projects completed during XSEDE 2.0 thus far



XSEDE User Portal: THE User Site portal.xsede.org

- XSEDE User Portal (XUP) is designed to be the only site a user needs to use XSEDE
- XUP presents information relevant to users
 - user info is easier to find
 - XUP also provides dynamic data about XSEDE systems
 - capabilities to manage usage, files, data
- As a user you can
 - request an allocation, and manage allocations
 - sign up for training
 - request help
 - manage files and data, and much more!
- Portal provides single sign-on to all XSEDE resources



Current XSEDE Compute Resources

- Stampede2 @ TACC
 - 12.8 PFLOPS (PF) Dell Cluster w/ Intel Knights Landing, Skylake
- Comet @ SDSC
 - 2.1 PF cluster w/GPUs
- Bridges @ PSC
 - 1 PF w/ large memory (3 TB and 12 TB) and GPU nodes
- SuperMIC @ LSU
 - 925 TF Dell Cluster w/ GPUs and Xeon PHIs

- Jetstream @ Indiana
 - 516 TF HPC Cloud
- Open Science Grid
 - 160,000 CPU cores
- Wrangler @ TACC
 - 62 TF data analytics system

https://www.xsede.org/web/xup/resource-monitor



Current XSEDE Data and Software Resources

- Storage
 - Ranch @ TACC
 - 61 PB tape
 - Pylon @ PSC
 - 10 PB disk
 - Wrangler @ TACC
 - 10 PB disk
 - Data Oasis @ SDSC
 - 4 PB tape
 - Jetstream Storage
 - 1 PB disk

- Software: 100s of titles
 - domain software
 - chemistry, CFD, bioinformatics, physics, astronomy, biology, engineering, statistics,...
 - tools
 - middleware, visualization, scripting, performance analysis, data storage and management, ...
 - compilers and libraries
 - most languages supported, math libraries, machine learning, ...

<u>https://portal.xsede.org/software#</u>

https://www.xsede.org/web/xup/resource-monitor



ECSS is an Allocated Service

- Extended Collaborative Support Service
 - improves the productivity of the XSEDE user community through meaningful collaborations
- Expert staff can be requested for collaborations lasting months to a year
 - requests made through the XSEDE allocation system when requesting computational resources
- Typical collaborations require 20-25% staff time for one year
- Critical mass engenders success
 - ~26 FTEs (~65 individuals) for project work at 9 sites
 - +4 ECSS Affiliates (skilled volunteers)
 - advanced degrees in a variety of science and technology fields
 - some staff co-author publications or write proposals with PI team, a few are later funded by PI team





More information at: www.xsede.org



