XSEDE: An Advanced and Integrated Set of Digital Resources for Science and Engineering

Linda Akli, SURA
Assistant Director, Training, Education & Outreach & XSEDE Underrepresented Community Engagement
Outline

• Create an XSEDE User Portal Account
• Gateways
• User Services
  – Training
  – Extended Collaborative Support Service
• Learn How to Requesting Access to Resources
What is XSEDE?

• The XSEDE mission is to accelerate discovery by enhancing the productivity of researchers, engineers, and scholars by deepening and extending the use of advanced digital services.

• Scientists and Engineers around the world use XSEDE resources and services: supercomputers, high-end visualization, data analysis storage, collections of data, and help services.

• XSEDE lowers technological barriers to the access and use of computing resources. Using XSEDE, researchers can establish private, secure environments that have all the resources, services, and collaboration support they need to be productive.
XSEDE Supports a Breadth of Research

- Earthquake Science
- Molecular Dynamics
- Nanotechnology
- Plant Science
- Storm Modeling
- Epidemiology
- Particle Physics
- Economic Analysis of Phone Network Patterns
- Large Scale Video Analytics (LSVA) Decision Making Theory
- Library Collection Analysis

Three-dimensional model of major vessels and bifurcations of the human arterial tree reconstructed with gOREK from a set of computed tomography (CT), digital subtraction angiography CT and magnetic resonance angiography images.

A snapshot of an animation for water level prediction including the wind-wave signature.
Why would you use XSEDE?
XSEDE User Portal (XUP) (portal.xsede.org)

• Single point-of-entry to information about XSEDE services and utilities for using them

• Anyone can create an XUP user account and access non-project features such as receive e-news, ask a question of a consultant, or register for a training workshop.

• There are additional steps to access resources to run your code, models, simulation or access data analytics tools.
Create and login to your XUP account

1. From the XUP homepage, click CREATE ACCOUNT
2. Complete the User Account Form
3. Verify your account request
4. Select your username and password
5. Login to the XUP portal.xsede.org

Click the CREATE ACCOUNT link to access the XUP User Account Form
XSEDE Acceptable Use Policy

• Must accept the User Responsibilities Form after creating your XUP account and again at the beginning of each allocation you receive.

• Choose a strong password and protect it.

• Close SSH terminals and log out of the User Portal when you are finished with your session.

• Report Suspicious Activity: email help@xsede.org or call 1-866-907-2383 immediately, regardless of the time of day.

XSEDE Cybersecurity Tutorial
http://www.citutor.org
Your My XSEDE webpage

(1) WELCOME TO XUP
- Quick access to commonly used features.

(2) LATEST UPDATES
- Latest information specific to your user account.

(3) MY ACTIVE ALLOCATIONS
- Summary of the active projects for which you are either a PI or member.
Today, there are approximately 35 gateways using XSEDE
Gateways democratize access
(https://www.xsede.org/web/guest/gateways-listing)

• Almost anyone can investigate questions using high end resources
  – Not just those in high profile research groups
• Gateways allow anyone with a web browser to explore
• Foster new ideas, cross-disciplinary approaches
  – Encourage students to experiment
• But used in production, too
  – Significant number of papers resulting from gateways, including GridChem, nanoHUB
  – Scientists can focus on challenging science problems rather than challenging infrastructure problems
XSEDE User Services

• Technical information
  – Always available via web site and XSEDE user portal

• Training
  – Sign up for classes to learn to use XSEDE resources

• Extended Collaborative Support Services
  – Human resources to help with performance analysis, petascale optimization, efficient use of accelerators, I/O optimization, the development of community gateways and work and data flow systems

• Allocations
  – Request access to XSEDE’s systems

• Help Desk/Consultants
Update your XUP User Profile

**MY XSEDE→Profile**

- View and or change your user information (organization, address).
- Make sure your email address is correct. XSEDE staff will use it to communicate with you regarding your allocation.
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• Help Desk/Consultants
XSEDE Training

• XSEDE provides extensive training
  – Covering every major resource
  – From beginner to advanced classes
  – At locations across the country
  – Online via
    • asynchronous technologies
    • Webcasts (many with slides at HPC University)

• Web-based education credit courses
XSEDE offers training courses to teach users how to maximize their productivity and impact in using the XSEDE services. The training classes focus on systems and software supported by the XSEDE Service Providers, covering programming principles and techniques for using resources and services effectively. Training classes are offered in high performance computing, visualization, data management, distributed and grid computing, science gateways, and more.

Current and potential XSEDE users should review the XSEDE Training Course Listing and browse the current Course Calendar for a list of upcoming training courses at XSEDE Sites. XSEDE also maintains a list Online Training materials of relevance to XSEDE users. The list of online training materials will be expanded as new materials are developed; suggestions for additions can also be submitted via the feedback form.
Calendar of Training Events:

https://www.xsede.org/web/xup/course-calendar

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<tr>
<th>START DATE</th>
<th>END DATE</th>
<th>CLASS NAME</th>
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<tbody>
<tr>
<td>06/10/2015</td>
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<td>Power Up Your Research with XSEDE @ Vanderbilt University</td>
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Online Training: https://www.xsede.org/web/xup/online-training

New to XSEDE?

View the latest recordings from our training classes to learn more:

- **XSEDE New User Tutorial**
  - Recorded: April 24, 2015
  - Run time: 2:23:59
  - Marcela Madrid and Tom Maiden of PSC provide an overview of XSEDE, its services and capabilities. The second half of the presentation provides details on each of XSEDE's compute resources.

- **Writing and Submitting a Successful XSEDE Proposal**
  - Recorded: April 9, 2014
  - Run time: 1:17:16
  - This presentation details all the requirements needed for successful research allocation requests. Topics covered include Computation Methodologies, Justification for SUIs requested and many others.

For the latest training courses please view the XSEDE Course Calendar.

On Demand Training

Several online training opportunities are available for both XSEDE and the various technology areas within XSEDE. Please view the list of available training classes below:
HPC University Portal

• Training and education resources
• Computational science and education blog
• Today’s XSEDE Presentations -
  http://www.hpcuniversity.org/trainingMaterials/198/

www.hpcuniversity.org
XSEDE User Services

• Technical information
  – Always available via web site and XSEDE user portal

• Training
  – Sign up for classes to learn to use XSEDE resources

Extended Collaborative Support Services
  – Human resources to help with performance analysis, petascale optimization, efficient use of accelerators, I/O optimization, the development of community gateways and work and data flow systems

• Allocations
  – Request access to XSEDE’s systems

• Help Desk/Consultants
Extended Collaborative Support Service (https://www.xsede.org/web/guest/ecss-projects)

• **Extended Support for Research Teams (ESRT)**
  – optimize their application codes, improve their work and data flows, and increase the effectiveness of their use of XSEDE digital infrastructure.

• **Novel and Innovative Projects**
  – communities that traditionally haven’t used HPC

• **Extended Support for Community Codes**
  – researchers and community code developers to deploy, harden, and optimize software systems

• **Extended Support for Science Gateways**
XSEDE User Services

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  – Sign up for classes to learn to use XSEDE resources

• Extended Collaborative Support Services
  – Human resources to help with performance analysis, petascale optimization, efficient use of accelerators, I/O optimization, the development of community gateways and work and data flow systems

Allocations
  – Request access to XSEDE’s systems and people

• Help Desk/Consultants
The Lingo

Allocation Request Types

- Startup  Development/testing/porting/benchmarking
- Education  Classroom, Training
- Research  Program (usually funded)

- PI  Principal Investigator
- XRAS  XSEDE Resource Allocations System
- XRAC  XSEDE Resource Allocations Committee
- SU  Service Unit = 1 Core-hour

3 Types of XSEDE Projects
XSEDE Projects

An XSEDE Project is like a bank account for allocations.

- It is permanent, only one per PI.
- It holds a year’s worth of allocation (on 1 or more systems)
- PI’s request an allocation renewal each year thereafter.
- An Allocation awarded to a New Request creates an XSEDE Project.

A PI’s Computational Projects evolve over the years.

- Computational Projects begin, end and extend.
- In subsequent years successful Renewal Requests provide allocations for new Computational Projects under the same XSEDE Project. Your XSEDE Project remains the same.
- A Renewal Requests is just like New Request, but must contain a Progress Report of last year’s Computational Projects and list of publications from past year’s allocation.
“Traditional” v. Community

• XRAC proposals are accepted in four general categories of research activities
  – Single Principal Investigator
  – Large research Collaborations (e.g., MILC consortium)
  – Community Consortiums (e.g., NEES)
  – Community Services (e.g., XSEDE Gateways)

• The general requirements for proposals of all four types remain largely the same.
  – Whether requesting compute, storage, visualization, or extended collaborative support or some combination
Eligibility

- Principal investigator (PI) **must be a researcher or educator** at a U.S.-based **institution**, including federal research **labs** or **commercial organizations**, (Commercial requests must guarantee that their results are publically available, and work must be in collaboration with an open science organization.)

- A **postdoctoral researcher is eligible** to be a PI.

- A qualified advisor may apply for an allocation for his or her class; but a high school, undergraduate or graduate student **may not be a PI.**
Overview: Startup/Education Requests

portal.xsede.org → Allocations → Submit/Review Request **

- Web forms: Investigator, Resource Request, ...
- Requires only an abstract and CV
- Reviewed by a XSEDE Staff (Startup Allocations Committee)
- 2 weeks from submission to award availability
- For code devel / performance eval / small-scaling computations / classroom & training instruction
- Details:
  - Request limit: 200,000 SUs total or combination of all resources requested
  - Reviewed: within 2 weeks of submission
  - Deadlines: None
  - Awards Begin: within 2 weeks of submission
Proposal Document(s)

https://www.xsede.org/web/xup/allocation-policies**

- CV(s) required for all requests.
- Abstract for startup/education request (in forms, or as a PDF document)
- Proposal “Main Document” for Research request (renewals/supplements)

Key to a successful review:
- Adhere to page limits!
- “Justify” allocation request.

<table>
<thead>
<tr>
<th>Page Limit</th>
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</tr>
</thead>
<tbody>
<tr>
<td>3</td>
<td>Progress report</td>
</tr>
<tr>
<td>10</td>
<td>New or Renewal</td>
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<td>15</td>
<td>Over 10 Million SUs</td>
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</tbody>
</table>

Pg. limit: DOES NOT INCLUDE FIGURES & TABLES.
Extended Collaborative Support (ECS) (https://portal.xsede.org/ecss-justification)

- Porting applications to new resources
- Providing help for portal and gateway development
- Improving scalability of codes to higher processor counts
- Optimizing codes to efficiently utilize specific resources
- Assisting with visualization, workflow, data analysis, and data transfer
Login at portal.xsede.org
Our reach will forever exceed our grasp, but, in stretching our horizon, we forever improve our world.
Backup Slides for Allocations Submissions
Example Form: New Project

XSEDE Resource Allocation System XRAS

Available Opportunities
Listed below are the currently open/available submission opportunities to which you may submit an allocation request.

XRAC - September 2014 Research
Start a New Submission

Campus Champions Campus Champions
Start a New Submission

Educational Educational
Start a New Submission

Software Testbeds Software Testbeds

Requests
No requests to display!
Select from the Available Opportunities on the left to start a new Request.
Example Form: Getting Info in order

XSEDE Resource Allocation System (XRAS)

Research Request

Research allocations may be requested for any compute, visualization, or storage resource and require a formal request document and CVs (for PI/Co-PIs). Research allocations are typically appropriate as follow-ons to Startups; but a PI need not request a Startup prior to submitting a Research request. A PI may submit a Research allocation request at any time during an active Startup allocation, if the PI has fulfilled his or her startup needs. A successful Research allocation will supersede any Startup allocation and start a new 12-month allocation period.

To complete this request you should have the following information ready:

- Title
- Abstract
- Keywords
- PI
- Field of science
- Documents (Main Document, Code Perf & Scaling)
- Resources

Start Submission  Advanced Submission  Cancel
New Request
Submission for XRAC - September 2014

Personnel / Roles

By default you are added to the request as an Allocation Manager. You can update your role to be PI or Co-PI, if applicable. Add other people this request by looking them up by their XSEDE Portal Username. Then you can select the person’s role for the request.

Note: Each person to be added to the request must already have a portal account and must provide you with their XSEDE Portal Username. For security reasons, we do not permit you to search to find portal usernames; you must provide a valid username. After providing a username, the person's full name, email address, institution, and phone number are shown for confirmation.

PI, Co-PIs, and Allocation Managers

Enter username to lookup

Person
Vivian Benton <benton@psc.edu>
Carnegie Mellon University
412-268-6355

Role
Allocation Manager
Example proposal submission: Personnel/Roles

New Request
Submission for XRAC - September 2014

Personnel / Roles

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PI, Co-PIs, and Allocation Managers

Enter username to lookup

Role

Allocation Manager

Person
Vivian Benton <benton@psc.edu>
Carnegie Mellon University
412-268-6355

Person
Ken Hackworth <hackworth@psc.edu>
Pittsburgh Supercomputing Center
412-268-7081
Example proposal submission: Title/Abstract/FOS

XSEDE Resource Allocation System

New Request
Submission for XRAC - September 2014

Title, Abstract, Field of Science

Here is where you specify the title and abstract for your allocation request. In the abstract please describe your research in a clear and concise manner. Someone outside of your field of research should be able to understand your proposal. This section also enables you to specify a primary field of science and, if applicable, any additional fields of science.

Title

Predictions for outcome of British Open

Abstract

We will analyze the play of the participants for the British Open to see who has the best chance of winning the British Open.
Example proposal submission: Resource request

New Request
Submission for XRAC - September 2014

Specify Resources

Here are the compute, visualization, and storage resources that are available for this submission opportunity. From the Available Resources list, you can select each resource you want to request and fill out the available related information. Certain resources have secondary requirements, please make sure to pay attention to those. For detailed resource information please visit the XSEDE Resource listing.

- Indiana University Gateway/Web Service Hosting (Quarry)
- Indiana University HP DL580 Large Memory Cluster (Mason)
- Open Science Grid (OSG)
- PSC Persistent disk storage (Data SuperCell)
- PSC SGI Altix UV (Blacklight)
- SDSC Appro Linux Cluster (Trestles)
- SDSC Appro with Intel Sandy Bridge Cluster (Coriern Compute Cluster)
Example proposal submission: Resources request

New Request
Submission for XRAC - September 2014

Specify Resources

Here are the compute, visualization, and storage resources that are available for this submission opportunity. From the Available Resources list, you can select each resource you want to request and fill out the available related information. Certain resources have secondary requirements, please make sure to pay attention to those. For detailed resource information please visit the XSEDE Resource listing.

Indiana University Gateway/Web Service Hosting (Quarry)
Indiana University HP DL580 Large Memory Cluster (Mason)
Open Science Grid (OSG)
PSC Persistent disk storage (Data SuperCell)
PSC SGI Altix UV (Blacklight)
SDSC Appro Linux Cluster (Trestles)
SDSC Appro with Intel Sandy Bridge Cluster (Gordon Compute Cluster)
SDSC Medium-term disk storage (Data Oasis)

PSC SGI Altix UV (Blacklight)

In order to request this resource, you must also request one of the following resources:

- PSC Persistent disk storage (Data SuperCell)

Amount requested

30,000 SUs

Comments


Example proposal submission: Saving and Final Submission

XSEDE Resource Allocation System  
XRAS

New Request
Submission for XRAC - September 2014

Request Ready to Submit
Congratulations! Your request is ready for submission. Click below to submit your request. If you are not quite ready to submit your request you can save and return to submit it at a later time.

✓ Submit Request  ○ Save for Later

← Previous
Example proposal submission: Successful submission

XSEDE Resource Allocation System  XRAS

Your request has been submitted!

Predictions for outcome of British Open
Submission for XRAC - September 2014

Number  DMS140036
Status  Submitted
Type  New
Abstract  —  We will analyze the play of the participants for the British Open to see who has the best chance of winning the British Open.

Keywords  —  British Open, GOLF
Pending Request

XSEDE Resource Allocation System  XRAS

Available Opportunities
Listed below are the currently open/available submission opportunities to which you may submit an allocation request.

XRAC - September 2014  Research

Start a New Submission

Requests
Submitted 1

Predictions for outcome of British Open
New, Submitted
XRAC - September 2014  Research
PI: Haikworth, Ken
Allocation Manager: Benton, Vivian

Start a New Submission
Predictions for outcome of British Open
Submission for XRAC - September 2014  View Opportunity

Number DMS140036
Status Under Review
Type New
Abstract — We will analyze the play of the participants for the British Open to see who has the best chance of winning the British Open.

Keywords — British Open, GOLF

Fields of Science
Statistics and Probability primary

Personnel
PI
Ken Hackworth <hackworth@psc.edu>
Pittsburgh Supercomputing Center
412-268-7083

Allocation Manager
Vivian Benton <benton@psc.edu>
Carnegie Mellon University
412-268-5355