

Xpert Network Panel Tool Directory for CDI Science December 17, 2020

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XSEDE

Extreme Science and Engineering
Discovery Environment



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Background - JP Navarro

- ❖ Work at Argonne National Lab. and the Univ. of Chicago
- ❖ Part of XSEDE's Cyberinfrastructure Integration "XCI" area
- ❖ Manage the Requirements Analysis and Capability Delivery "RACD" team
 - Deliver software and online services to users, HPC operators, and XSEDE operations
 - XSEDE cyberinfrastructure integrating software and online service
- ❖ Lead XSEDE Information Services efforts
 - Includes software tools publishing and discovery capabilities



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TeraGrid & XSEDE Tool Directories History

- ❖ *Coordinated TeraGrid Software & Services “CTSS” V1 in 2003*
 - Soup to nuts (kernel to user tools) software list (MS Word) coordinated by operators
 - First automated publishing of user tools available on HPC resources
- ❖ *Transition to XSEDE 1 ~2011*
 - Improve automated publishing of user tools available on HPC resources
 - Software catalog leverages more open source tools
- ❖ *Transition to XSEDE 2 ~2016*
 - Expanded beyond user tools available on XSEDE HPC resource
 - Expanded to tools outside the XSEDE environment



XSEDE

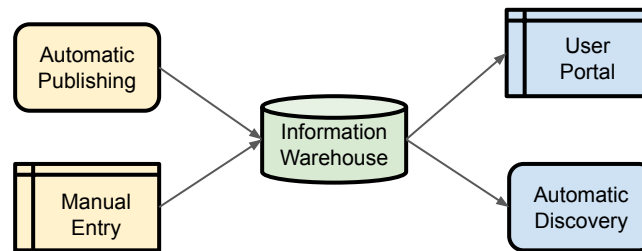
XSEDE's Tools Directory

Motivating Use Cases

- Enable the (XSEDE) community to publish, **discover**, and **use** software and online services
- Enable XSEDE itself to track elements of XSEDE's cyberinfrastructure

Tool categories

- Software on integrated HPC resources
- Edge services for accessing HPC resources
- Central services (Portals, Gateways, Globus)
- Software packages
- Cluster building toolkits
- Cloud images
- Container repositories



XSEDE Research Software Portal

Motivating Use Case

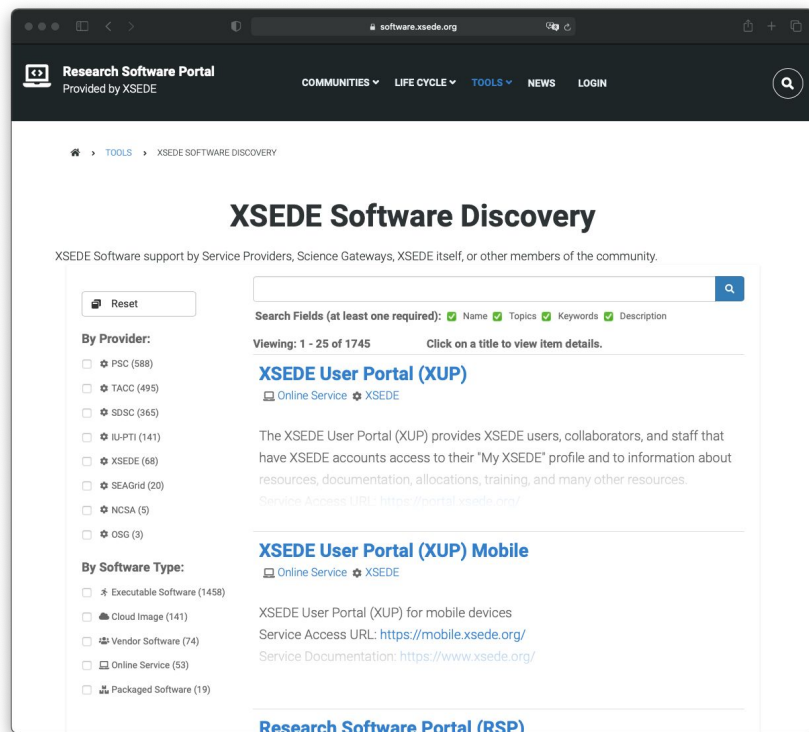
Enable the XSEDE community to share and discover all forms of software

Services:

<https://software.xsede.org/>

Interesting bits:

- Mostly aggregated automatically
- AWS hosted
- Elasticsearch capability



The screenshot shows the XSEDE Software Discovery portal. The header includes the XSEDE logo, the text "Research Software Portal Provided by XSEDE", and navigation links for "COMMUNITIES", "LIFE CYCLE", "TOOLS", "NEWS", and "LOGIN". The main content area is titled "XSEDE Software Discovery" and includes a search bar with a "Reset" button. Below the search bar, there are two sections: "By Provider:" and "By Software Type:". The "By Provider:" section lists various providers with their respective counts: PSC (588), TACC (495), SDSC (365), IU-PTI (141), XSEDE (68), SEAGrid (20), NCSA (5), and OSG (3). The "By Software Type:" section lists software types with their counts: Executable Software (1458), Cloud Image (141), Vendor Software (74), Online Service (53), and Packaged Software (19). On the right side, there is a search results area showing "XSEDE User Portal (XUP)" and "XSEDE User Portal (XUP) Mobile" with links to their respective online services and documentation.



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XSEDE and UIUC IT Services Join Forces

Motivating Use Case

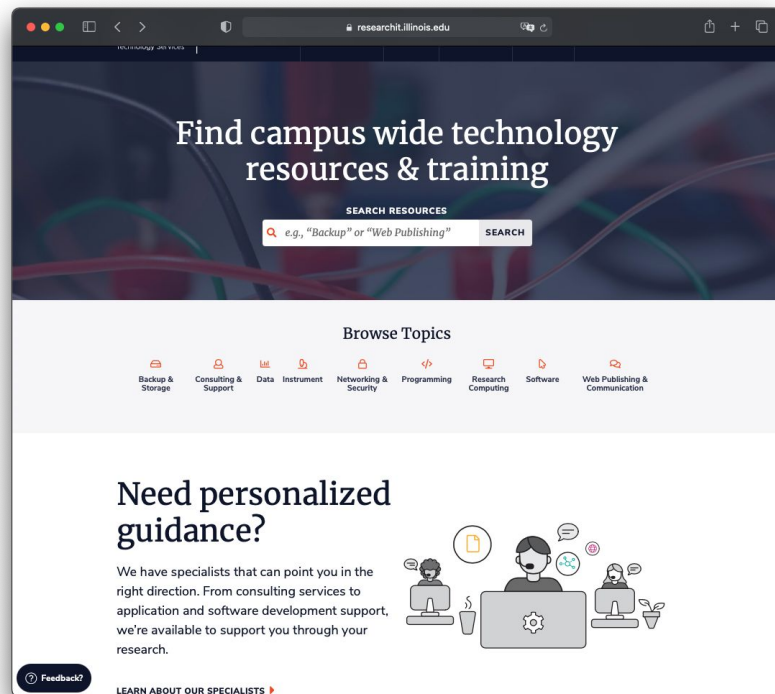
Enable research enhancing resource discovery
across organizational boundaries

Services:

<https://researchit.illinois.edu>

Resources like:

- Software tools
- Computing resources
- Training and events
- Consulting and support services
- Resource guides



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Proposed Questions - 1

Can a directory of tools facilitate the development of computational and data-intensive science?

- Would easily sharing and discovering research software tools across infrastructures, campuses, and agencies help?
- Or, are reading papers, word of mouth, and Google search good enough?

What attributes should a directory of tools (for RSEs) show?

- **What** does the tool do?
- **Where** is it?
- **Who** can access the tool, **who** provides it?
- **How** to access and use it?
- **Take me there** pointers
- **Identifiers** for publications and attribution



Proposed Questions - 2

Can/should such a directory be organized in a distributed way?

- Yes, projects, organizations, platforms need local directories
- **We also need quality, up-to-date, accessible aggregation directories**



Proposed Questions - 3

How narrow or broad should the list (directory) be?

→ Depends on which users we are targeting

How can related efforts best be cross-referenced?

1. Need a formal collaborative initiative or project
2. Where requirements can be shared
3. Where a shared solution can be designed

XSEDE collaborations that brought us to where we are:

- Federated HPC operators
- UIUC
- SGCI



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