# *XSEDE Overview*

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# What is XSEDE

XSEDE (Extreme Science and Engineering Discovery Environment) is a five-year, $121-million project supported by the National Science Foundation. The goal is to provide a single virtual system that scientists can use to interactively share computing resources, data, and expertise.

Although the XSEDE name explicitly says “Science and Engineering”, it serves a broader community that includes the social sciences, humanities and other fields

XSEDE

Extreme Science and Engineering Discovery Environment

# What Does XSEDE do?

- Centralizes many of the functions that are common to all of the participating supercomputer centers (more generally service providers)
  - Allocations, accounting & peer review of proposals
  - Help desk / ticketing system
  - Documentation
  - Web site, portal, security and authentication
- Advanced support through ECSS program
- Coordinate networking and shared XSEDE wide file system
- Education, outreach & training
- Annual meeting
- Gateways and middle ware
- Campus champions – representatives to campuses

# How SDSC fits into XSEDE

- SDSC is not a division of XSEDE nor does it work for XSEDE. Although XSEDE is an important funding source for SDSC, it is by no means the largest or dominant.

- SDSC and the other centers (TACC, PSC, NICS, etc.) are autonomous organizations that compete for supercomputing resources. Typically this is through the NSF Track 2 program, with the condition that most of cycles will be made available through the XSEDE allocations process.

- SDSC is an Organized Research Unit (ORU) at UCSD and is involved in many independent projects that are distinct and unrelated to XSEDE.

# *Who is XSEDE?*

Total of 17 organizations that provide compute, storage and other resources along with training, software and expertise





# XSEDE resources – what's available

High performance computing resources ranging from 100-6000 TFlop peak


Visualization

High throughput computing

Open Science Grid


Future Grid

Distributed test beds

4-11 PB parallel file systems, XSEDE Wide File System, 60-170 PB tape archives

# Getting an allocation

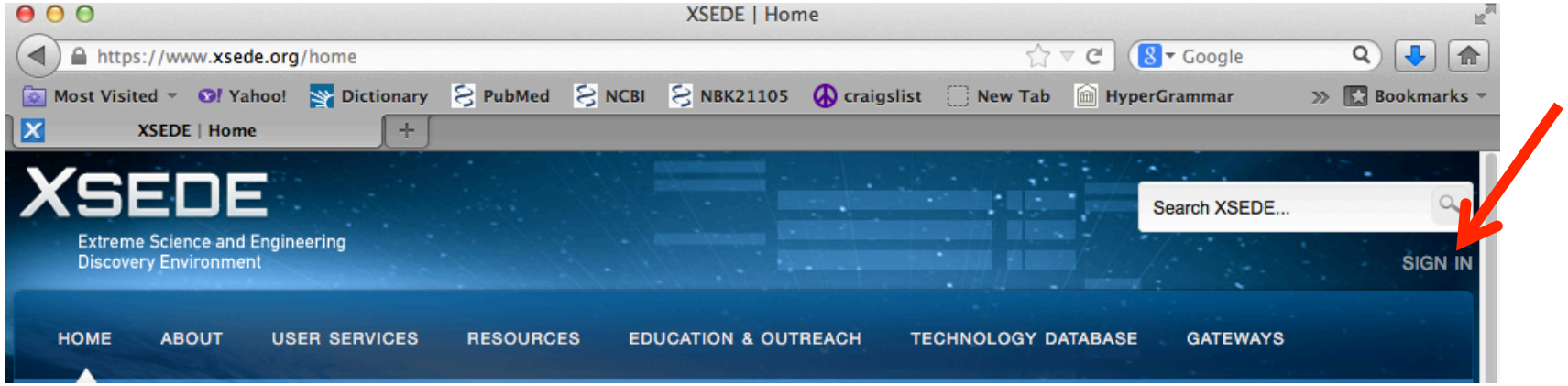
***The WRONG way***

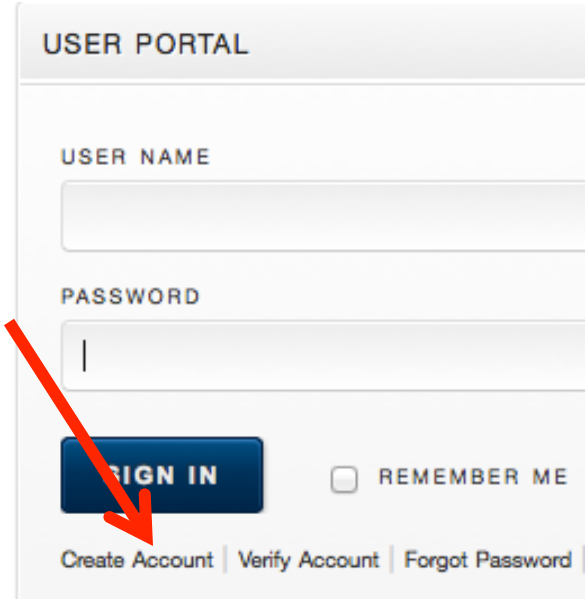
- Send email to someone you know at SDSC
- Who will then forward your email to me asking if I can help a new user who wants to get started with SDSC or XSEDE resources
- I'll then send you an email explaining what XSEDE is and why you need to go through the standard allocations channels

***The RIGHT way***

- Register at the XSEDE portal and submit your proposal through POPS

# Allocations step 1 – create a portal account

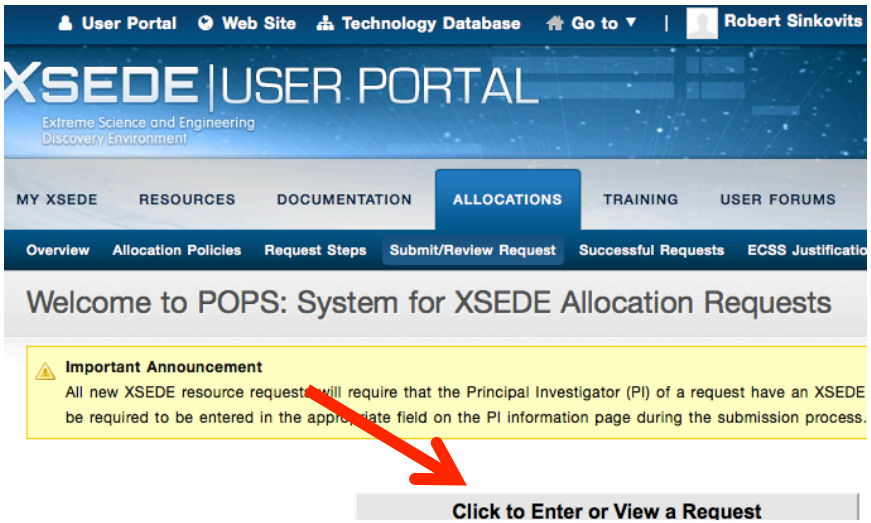


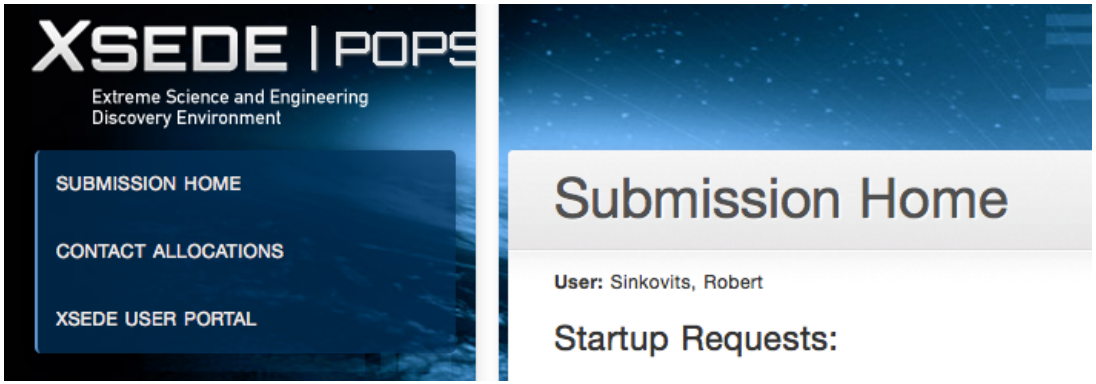




All users must create a portal account in order to use any of the XSEDE resources

# *Allocations step 2 – Navigate to POPS*

https://www.xsede.org/group/xup/submit-request



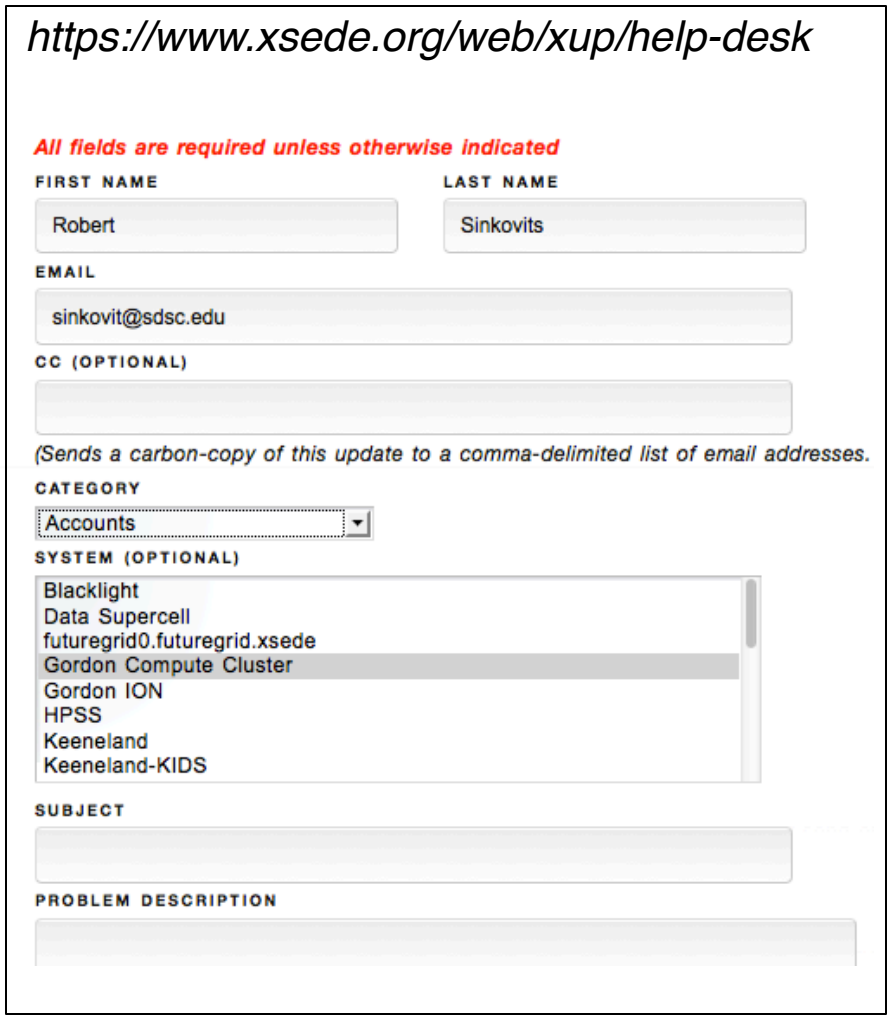

Only the PI needs to apply for an allocation. The PI can then add an arbitrary number of users to the project.

Students cannot serve as PIs, except for NSF Graduate Research Fellows and Honorable Mention awardees.

# Getting help through XSEDE

## The RIGHT way

*https://www.xsede.org/web/xup/help-desk*




## The WRONG way

Send email to someone you know at SDSC, who will

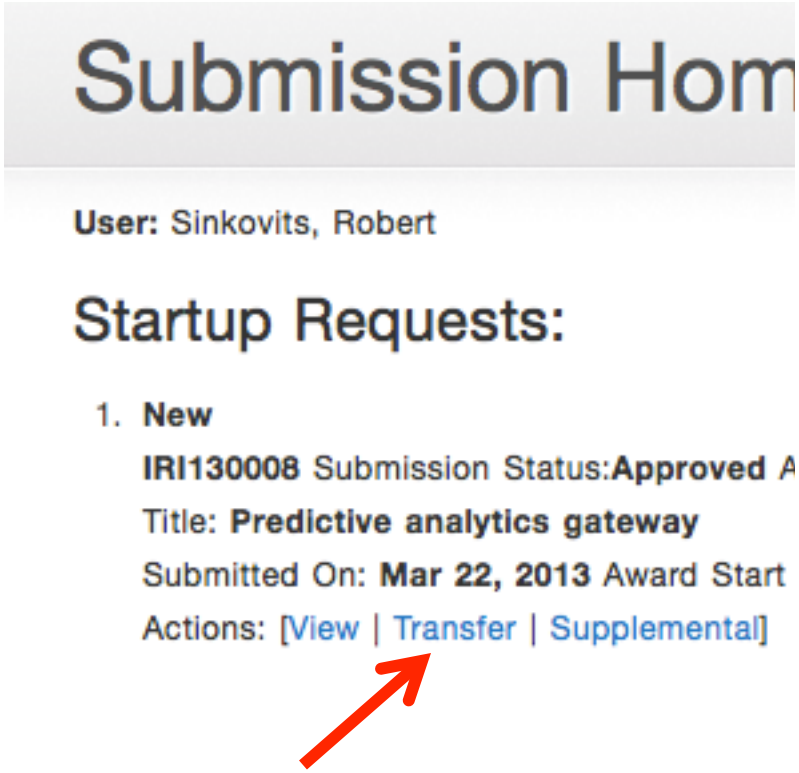
Forward to someone who they think can help, who will eventually tell you to submit a ticket through the XSEDE … or write your problem on a sticky note, which gets forgotten or falls behind desk

Requests submitted to the XSEDE ticketing system will be logged, tracked and assigned to the person best suited to handle your problem

# Moving time between XSEDE systems

***The RIGHT way***

*https://pops-submit.xsede.org/auth/TGUP_POPS/main/cgi/index.cgi*




***The WRONG way***

Send email to someone you know at SDSC, who will …

# *Extended Collaborative Support Services (ECSS)*

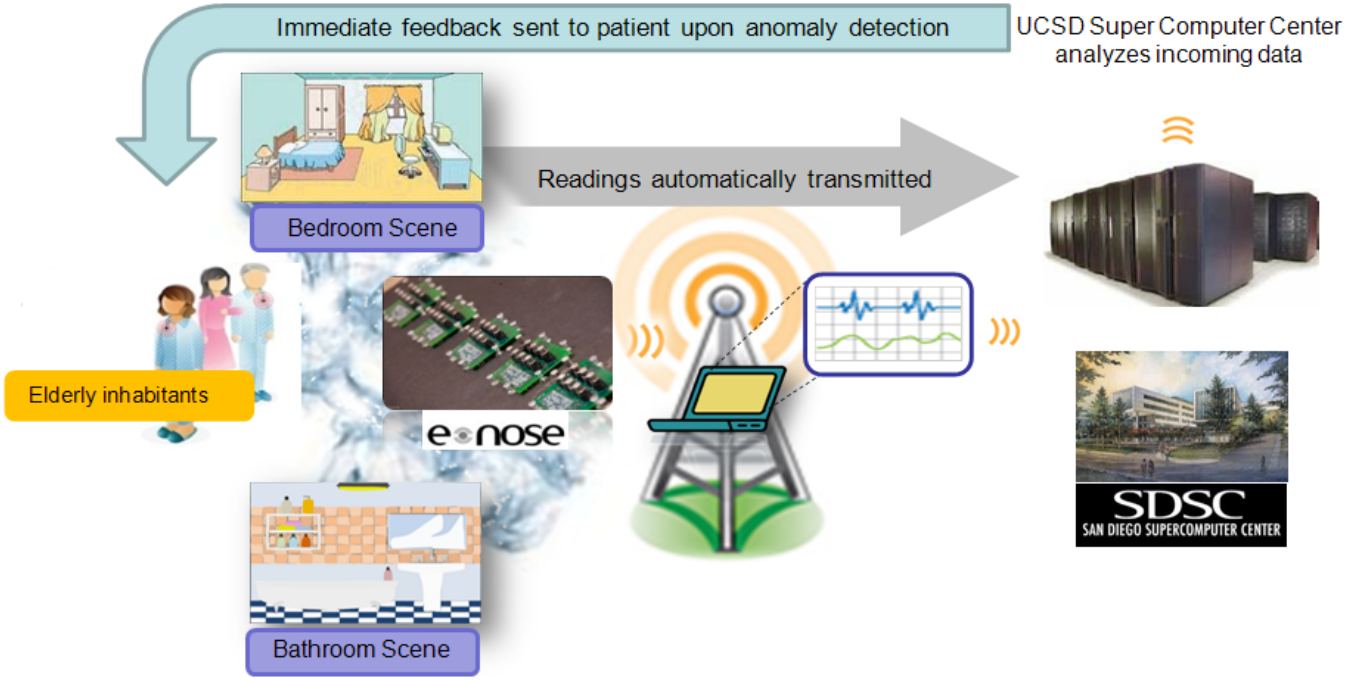
XSEDE provides much more than storage and compute cycles. Through the ECSS program, you can get help from expert staff to

- Make the transition from workstation to supercomputer
- Develop parallel versions of serial codes
- Optimize performance to make best use of XSEDE hardware
- Develop science gateways that allow entire communities of users to transparently access supercomputing resources
- Create workflows or other solutions that maximize throughput

Users normally ask for ECSS when they submit their allocations proposals, but it can be requested at any time

# ECSS example - classification of time series data

Chemical sensors (e-noses) will be placed in the homes of elderly participants in an effort to continuously and non-intrusively monitor their living environments. Time series classification algorithms will then be applied to the sensor data to detect anomalous behavior that may suggest a change in health status.




In preparation for pilot study, time series classification software developed by the Huerta lab has been ported to Gordon.

After optimizing code, linking Intel's MKL and parallelizing key loops, calculations that had taken 15-1/2 hours on a local workstation can now be completed in 4 minutes on a single Gordon compute node.

***Source:*** *Herb Hauser (U. Scranton) and Ramon Huerta (UCSD) Used by permission. 2012*

# ECSS example - classification of time series data

Original version of code was serial, compiled using GNU C++ compiler and linked to default LAPACK libraries. By changing the compiler and compiler options, linking MKL, enabling threaded execution, eliminating redundant calculations and parallelizing loops, obtained 167x speedup

| Notes | cores | Run time | Speedup |
|---|---|---|---|
| Original code, GNU compiler | 1 | 11:22:00 | - |
| Switch to Intel compiler and enable AVX | 1 | 05:41:49 | 2.0 |
| Link threaded MKL library, run in parallel | 16 | 00:14:46 | 46.2 |
| OpenMP directives in loops in kAR and kARtest | 16 | 00:13:10 | 52.5 |
| Remove duplicate call to kARtest | 16 | 00:07:58 | 85.6 |
| Optimization of DYSRK operations | 16 | 00:04:04 | 167.7 |

Reported speedups are relative to single core on Gordon. Porting from Huerta lab workstation (Intel Nehalem) to Gordon resulted in 1.3x reduction in runtime

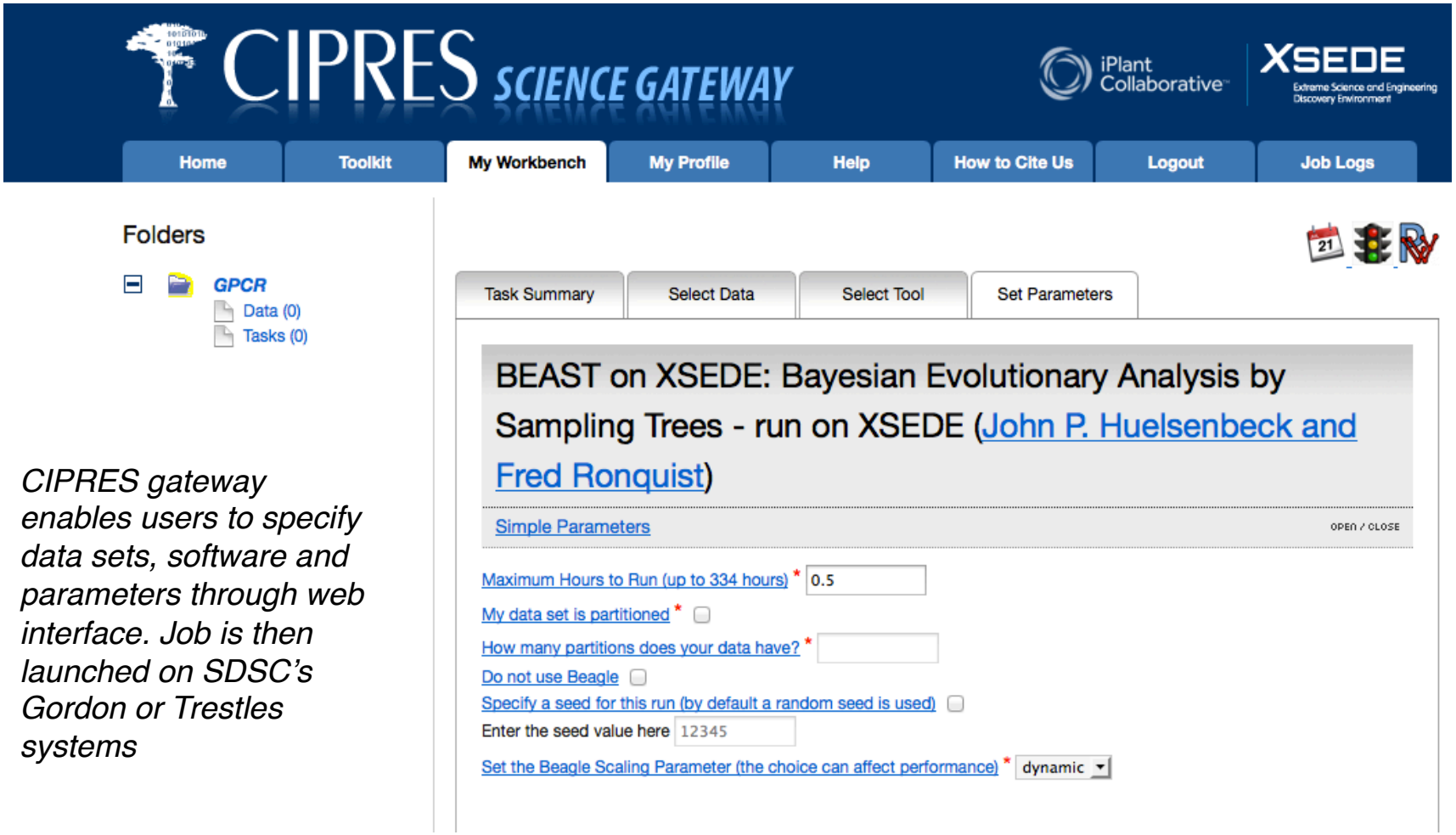
# Gateways

Gateways allow users to submit jobs that will subsequently be run on XSEDE resources through a web interface. In most cases a single allocation to the PI serves an entire community of users.

*https://www.xsede.org/web/guest/gateways-listing*

| TITLE | FIELD OF SCIENCE ▲ | PORTAL HOMEPAGE |
|---|---|---|
| Massive Pulsar Surveys using the Arecibo L-band Feed Array (ALFA) | Astronomical Sciences | Visit Portal |
| Center for Multiscale Modeling of Atmospheric Processes | Atmospheric Sciences | Visit Portal |
| Community Climate System Model (CCSM) TeraGrid Gateway | Atmospheric Sciences | Visit Portal |
| Biodrugscore: A portal for customized scoring and ranking of molecules docked to the human proteome | Biochemistry and Molecular Structure and Function | Visit Portal |
| Chemical Informatics and Cyberinfrastructure Collaboratory | Biochemistry and Molecular Structure and Function | Visit Portal |

# Gateway example - CIPRES




*CIPRES gateway enables users to specify data sets, software and parameters through web interface. Job is then launched on SDSC's Gordon or Trestles systems*

# XSEDE Wrap up

- XSEDE centralizes many of the essential service. Users do not need to figure out a different set of policies, web sites, etc. in order to work across multiple sites.

- Get used to going through the proper XSEDE channels for allocations, transfers, adding users to accounts and submitting help tickets

- XSEDE is much more than hardware. Our staff have expertise in a wide range of higher performance computing topics.