

# **SDSC HPC/CI User Training 2022**

## **HPC/CI Basic Concepts: Accessing Expanse**

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**EXPANSE**  
COMPUTING WITHOUT BOUNDARIES

**SAN DIEGO SUPERCOMPUTER CENTER**



NSF Award 1928224



# Outline

- Expanse overview
- Overview of Basic Skills Needed to Use HPC/CI Systems
- Expanse overview
- Logging on to Expanse
- Modules
- Account Management

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# Expanse





# EXPANSE

COMPUTING WITHOUT BOUNDARIES  
5 PETAFLOP/S HPC and DATA RESOURCE

## HPC RESOURCE

13 Scalable Compute Units  
728 Standard Compute Nodes  
52 GPU Nodes: 208 GPUs  
4 Large Memory Nodes

## LONG-TAIL SCIENCE

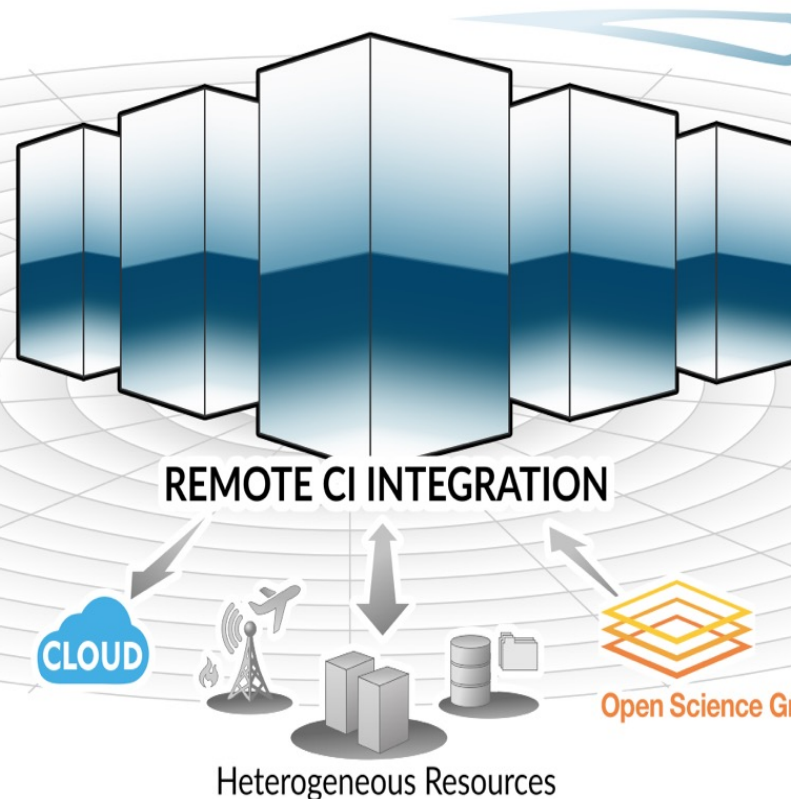
Multi-Messenger Astronomy  
Genomics  
Earth Science  
Social Science

## DATA CENTRIC ARCHITECTURE

12PB Perf. Storage: 140GB/s, 200k IOPS  
Fast I/O Node-Local NVMe Storage  
7PB Ceph Object Storage  
High-Performance R&E Networking

## INNOVATIVE OPERATIONS

Composable Systems  
High-Throughput Computing  
Science Gateways  
Interactive Computing  
Containerized Computing  
Cloud Bursting

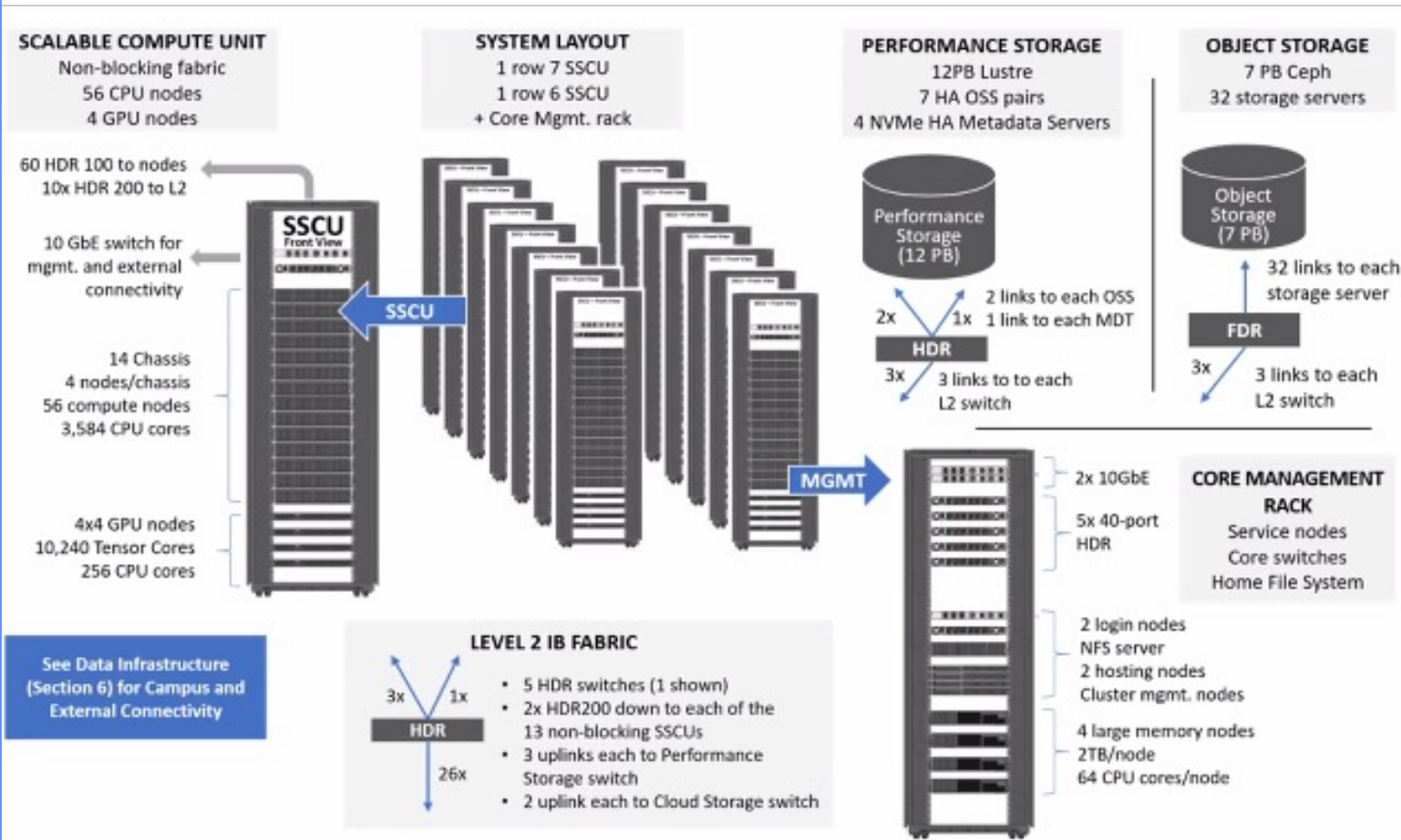


For more details see the Expanse user guide @ [https://www.sdsc.edu/support/user\\_guides/expanse.html](https://www.sdsc.edu/support/user_guides/expanse.html)  
and the "Introduction to Expanse" webinar @ [https://www.sdsc.edu/event\\_items/202006\\_Introduction\\_to\\_Expanse.html](https://www.sdsc.edu/event_items/202006_Introduction_to_Expanse.html)

# Expanse Heterogeneous Architecture

## System Summary

- 13 SDSC Scalable Compute Units (SSCU)
- 728 x 2s Standard Compute Nodes
- 93,184 Compute Cores
- 200 TB DDR4 Memory
- 52x 4-way GPU Nodes w/NVLINK
- 208 V100s
- 4x 2TB Large Memory Nodes
- HDR 100 non-blocking Fabric
- 12 PB Lustre High Performance
- Storage
- 7 PB Ceph Object Storage
- 1.2 PB on-node NVMe
- Dell EMC PowerEdge
- Direct Liquid Cooled



# Expanse User Portal

<https://portal.expanse.sdsc.edu>

- Provides Web based access to interactive applications including Jupyter Notebooks & Jupyter Lab, Matlab, Rstudio.
- Access using XSEDE portal account

The image is a composite of four screenshots illustrating the workflow for using the Expanse User Portal:

- (1) Log onto the Portal:** A screenshot of the Expanse Portal homepage. The URL in the browser is `portal.expanse.sdsc.edu/sun/sdsc/portal`. The page features the SDSC logo and a navigation menu with options like 'Files', 'Jobs', 'Clusters', and 'Interactive Apps'.
- (2) Fill out form inputs:** A screenshot of the 'Jupyter Session' configuration page. It shows a form where users can specify their account (e.g., 'sdsc154'), partition, and other session parameters. The 'Open OnDemand / Jupyter Session' button is visible.
- (3) Copy the URL and paste into Web browser:** A screenshot showing the URL generated after session creation: `https://dipping-either-pureblood.expanse-user-content.sdsc.edu/?token=e5cb992765d875d33875ad`. The page title is 'Jupyter Session'.
- (4) Monitor status window: may take a long time:** A screenshot of the 'SDSC Expanse' job status monitor. It shows a progress bar with four stages: 'In Queue', 'Running', 'Mapped', and 'Proxied'. The 'In Queue' stage is highlighted, with a note: 'Job has not yet started.' Below this, a 'Running' status is indicated.
- (5) Access your Jupyter Service:** A screenshot of a Jupyter Notebook interface. The notebook is titled 'numpy\_intro.ipynb' and displays a plot of a normal distribution curve. The code cell shows the generation of random data and a linear algebra example using NumPy.

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# Basic Skills Needed to Use HPC/CI Systems

[https://github.com/sdsc-hpc-training-org/basic\\_skills](https://github.com/sdsc-hpc-training-org/basic_skills)

- Overview of the HPC system you want to work on: e.g. The Expanse cluster:
  - [https://drive.google.com/file/d/1i1zwOFOz438y0SWcjkDp2zd6FJXjVyY\\_/view?usp=sharing](https://drive.google.com/file/d/1i1zwOFOz438y0SWcjkDp2zd6FJXjVyY_/view?usp=sharing)
- Security and Authentication
- Using Github
- Unix/Linux
- Understand HPC system environment (accounts, modules, etc)

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# Logging onto Expanse

- Expanse supports Single Sign-On through the XSEDE User Portal
- From the command line using an XSEDE-wide password,
- From the Expanse User Portal (<https://portal.expanse.sdsc.edu>).
- Note that CPU and GPU resources are **allocated separately**, but the login nodes are the same.
- To log in to Expanse from the command line
  - hostname: login.expanse.sdsc.edu
  - Secure shell (SSH) command examples:

```
ssh <user_name>@login.expanse.sdsc.edu  
ssh -l < user_name > login.expanse.sdsc.edu
```

- When you log onto *login.expanse.sdsc.edu*, you will be assigned one of the two login nodes login0[1-2]-expanse.sdsc.edu. Both systems are identical.

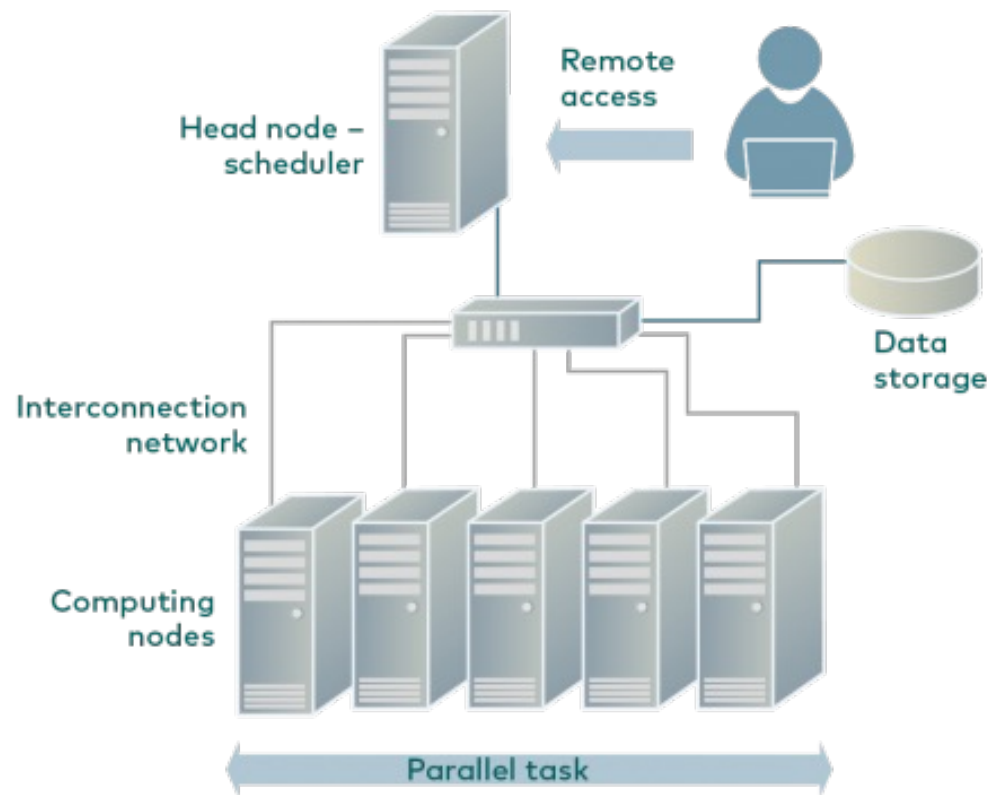
# Using SSH Keys

- You can append your public key (e.g. from your laptop) to your `~/.ssh/authorized_keys` file to enable access from authorized hosts without having to enter your password.
- RSA, ECDSA and ed25519 keys are accepted.
- Make sure you have a **strong passphrase** on the private key on your local machine.
- You can use *ssh-agent* forwarding to avoid repeatedly typing the private key password:
  - [https://github.com/sdsc-hpc-training-org/hpc-security/blob/master/ssh\\_methods/connect-using-ssh-agent.md](https://github.com/sdsc-hpc-training-org/hpc-security/blob/master/ssh_methods/connect-using-ssh-agent.md)
- Hosts which try to connect to SSH more frequently than ten times per minute may get blocked for a short period of time
- See the SDSC webinar: Indispensable Security: Tips to Use SDSC's HPC Resources Securely:
  - **2021 Webinar:** [https://www.sdsc.edu/event\\_items/202007\\_CometWebinar.html](https://www.sdsc.edu/event_items/202007_CometWebinar.html)
  - 2022 Webinar scheduled for April, 2022. Watch the training pages:
    - [https://www.sdsc.edu/education\\_and\\_training/training\\_hpc.html](https://www.sdsc.edu/education_and_training/training_hpc.html)



# System Access: Clients

- Linux/Mac –
  - use terminal + installed ssh app
- Windows:
  - Win10 terminal app + installed ssh app
  - Older Windows OS's: ssh clients apps Putty, Cygwin
- Login hostname for SDSC Expanse:
  - [login.expense.sdsc.edu](https://login.expense.sdsc.edu)
  - 198.202.113.252



Source: <https://hpc.rtu.lv/hpc/introduction-to-hpc/?lang=en>

For more on SDSC security, see: <https://github.com/sdsc-hpc-training-org/hpc-security>

# Example of a terminal connection:

```
Warning: No xauth data; using fake authentication data for X11 forwarding.  
Welcome to Bright release      9.0
```

```
Based on CentOS Linux 8  
ID: #000002
```

```
-----  
WELCOME TO
```

```
  / _ _ / // _ _ V | / / / _ _ // _ _ /  
 / _ / | // / / / / / // ^ _ V _ /  
 // _ / // _ _ / _ _ // / / _ _ // _ _  
 / _ _ // / / / / / / / / / / / / /
```

```
-----  
Use the following commands to adjust your environment:
```

```
'module avail'      - show available modules  
'module add <module>' - adds a module to your environment for this session  
'module initadd <module>' - configure module to be loaded at every login
```

```
-----  
Last login: Fri Jan 28 12:00:38 2022 from 12.345.678.90  
[username@login02 ~]$
```

The logon message you see is called the MOTD (message of the day, located in /etc/motd).



# Using Login Nodes Properly

- The login nodes are meant for file editing, simple data analysis, & tasks that use minimal compute resources.
- All computationally demanding jobs should be submitted and run through the batch queuing system.
- **Do not use the login nodes for:**
  - computationally intensive processes,
  - as hosts for running workflow management tools
  - as primary data transfer nodes for large or numerous data transfers
  - as servers providing other services accessible to the Internet.
  - running Jupyter notebooks
- **Login nodes are not the same as the batch nodes.**
  - Users should request an interactive sessions to compile ;arge programs.

# Expanse User Portal

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- Access using XSEDE portal account

(1) Log onto the Portal

(2) Fill out form inputs

(3) Copy the URL and paste into Web browser

(4) Monitor status window: may take a long time

(5) Access your Jupyter Service

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- **Modules**
- Account Management



# Expanse Environment Modules

- Expanse uses *Lmod*, a *Lua* based module system.
  - [https://lmod.readthedocs.io/en/latest/010\\_user.html](https://lmod.readthedocs.io/en/latest/010_user.html)
- Users setup custom environments by loading available modules into the shell environment, *including needed compilers and libraries* and the batch scheduler.
- What modules let you do:
  - Dynamic modification of your shell environment
  - User can set, change, or delete environment variables
  - User chooses between different versions of the same software or different combinations of related codes.

# Modules on Expanse

- Users will need to load the scheduler (e.g. slurm)
- Users will *not* see all available modules when they run command "module available" *without loading a compiler*.
- Use the command "**module spider**" option to see if a particular package exists and can be loaded, run command
  - `module spider <package>`
  - `module keywords <term>`
- For additional details, and to identify module dependencies modules, use the command: `module spider <application_name>`
- The **module paths are different** for the CPU and GPU nodes. Users can enable the paths by loading the following modules:
  - `module load cpu` (for cpu nodes)
  - `module load gpu` (for gpu nodes)
  - avoid loading both modules

# Modules: Popular commands

Command	Description
module list	List the modules that are currently loaded
module avail	List the modules that are available in environment
module spider	List of the modules and extensions currently available
module display <module_name>	Show the environment variables used by <module name> and how they are affected
module unload <module name>	Remove <module name> from the environment
module load <module name>	Load <module name> into the environment
module swap <module one> <module two>	Replace <module one> with <module two> in the environment
module help	get a list of all the commands that module knows about do:
Shorthand notation:    ml foo ml -bar	“ml” == module load foo “ml -bar” == module unload bar

*SDSC Guidance: add module calls to your environment and batch scripts*



# Module Command Examples

```
[username@login02 ~]$ module reset
Resetting modules to system default. Resetting $MODULEPATH back to system default. All extra directories will be removed from $MODULEPATH.
```

```
[username@login02 ~]$ module list
```

```
Currently Loaded Modules:
```

```
1) cpu/0.15.4 2) slurm/expense/20.02.3 3) intel/19.1.1.217
```

List Current environment

```
username@login02 ~]$ module avail
```

```
----- /cm/shared/apps/spack/cpu/lmod/linux-centos8-x86_64/intel/19.1.1.217 -----
bamtools/2.5.1      grace/5.1.25      libpng/1.6.37      openmpi/4.0.4 (D)
bedtools2/2.27.1    gsl/2.5           libtirpc/1.2.6     papi/6.0.0.1
[SNIP]
eigen/3.3.7         jasper/2.0.16     openmpi/3.1.6

----- /cm/shared/apps/spack/cpu/lmod/linux-centos8-x86_64/Core -----
abaqus/2018          emboss/6.6.0      gmp/6.1.2           parallel/20200822
anaconda3/2020.11    freesurfer/7.1.1  go/1.15.1           pciutils/3.7.0
[SNIP]
cmake/3.18.2         gcc/9.2.0         mpfr/4.0.2          zstd/1.4.5
curl/7.72.0          gcc/10.2.0        nbo/7.0-openblas    (D)
doxygen/1.8.17       gh/1.13.1         openjdk/11.0.2

----- /cm/local/modulefiles -----
boost/1.71.0  cmjob  lua/5.3.5  shared  singularitypro/3.5  slurm/expense/20.02.3 (L)
----- /cm/shared/apps/xsede/modulefiles -----
cue-login-env  xdinfo/1.5-1  xdusage/2.1-1
----- /usr/share/modulefiles -----
DefaultModules  cpu/0.15.4 (L)  gct/6.2  globus/6.0  gpu/0.15.4  nostack/0.15.4
----- /cm/shared/modulefiles -----
AMDuProf/3.4.475  default-environment  sdsc/1.0
```

Show available modules

```
Where:
```

```
L: Module is loaded
```

```
D: Default Module
```

# Module Command Examples

Use “module show” to find out what a particular module will change in the environment

```
[username@login02 ~]$ module show cmake
```

```
-----  
/cm/shared/apps/spack/cpu/lmod/linux-centos8-x86_64/Core/cmake/3.18.2.lua:  
-----
```

```
whatis("Name : cmake")  
whatis("Version : 3.18.2")  
whatis("Target : zen")  
whatis("Short description : A cross-platform, open-source build system. CMake is a family of tools designed to  
build, test and package software. ")  
help([[A cross-platform, open-source build system. CMake is a family of tools  
designed to build, test and package software.]])  
prepend_path("PATH", "/cm/shared/apps/spack/cpu/opt/spack/linux-centos8-zen/gcc-8.3.1/cmake-3.18.2-  
rfzatdti4qlsrf2zezwad75fnccy4f7d/bin")  
prepend_path("ACLOCAL_PATH", "/cm/shared/apps/spack/cpu/opt/spack/linux-centos8-zen/gcc-8.3.1/cmake-3.18.2-  
rfzatdti4qlsrf2zezwad75fnccy4f7d/share/aclocal")  
prepend_path("CMAKE_PREFIX_PATH", "/cm/shared/apps/spack/cpu/opt/spack/linux-centos8-zen/gcc-8.3.1/cmake-3.18.2-  
rfzatdti4qlsrf2zezwad75fnccy4f7d/")  
setenv("CMAKEHOME", "/cm/shared/apps/spack/cpu/opt/spack/linux-centos8-zen/gcc-8.3.1/cmake-3.18.2-  
rfzatdti4qlsrf2zezwad75fnccy4f7d")
```

```
[username@login02 ~]$
```

# Module: check Environment

Once you have loaded the modules, you can check the system variables that are available for you to use.

```
[username@login01 ~]$ module load gcc/9.2.0
[username@login01 ~]$ module show gcc/9.2.0
-----
/cm/local/modulefiles/gcc/9.2.0:
-----
whatis("adds GNU Cross Compilers to your environment variables ")
prepend_path("PATH", "/cm/local/apps/gcc/9.2.0/bin")
prepend_path("LD_LIBRARY_PATH", "/cm/local/apps/gcc/9.2.0/lib:/cm/local/apps/gcc/9.2.0/lib64")
help([[ Adds GNU Cross Compilers to your environment variables,
]])

[username@login01 ~]$ which gcc
/cm/local/apps/gcc/9.2.0/bin/gcc
[username@login01 ~]$
```



# Module: command not found

- Sometimes happens when switching from one shell to another or attempting to run the module command from within a shell script or batch job.
- Module command may not be inherited to the shell
- To keep this from happening, execute the following:
  - From the command line (interactive shells)
    - [source /etc/profile.d/modules.sh](#)
  - OR add to your shell script (including Slurm batch scripts)

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# Multiple Allocations

- Many users will have access to multiple accounts and hence *projects*:
  - an allocation for a research project and a separate allocation for classroom or educational use
- Users should verify that the correct *project* is designated for all batch jobs.
- Awards are granted for a specific purposes and should not be used for other *projects*.
- To charge your job to one of your *projects*, replace << project >> with one from your list and put this PBS directive in your job script:
  - #SBATCH -A << project >>
  - *srun* -account=<< project >>



# Allocation Information

```
module load sdsc
expanse-client user
expanse-client user -r expanse_gpu
```

```
[username@login02 ~]$ module load sdsc
[username@login02 ~]$ expanse-client user
```

Resource expanse

	NAME	PROJECT	TG PROJECT	USED	AVAILABLE	USED BY PROJECT
1	username	ddp363		65	50000	2223
2	username	sds173	TG-CCR190013	6	1000	4750
3	username	sds184	TG-TRA210003	121	100000	56336
4	username	abc123		1596	5050000	3267835

```
[username@login02 ~]$ expanse-client user -r expanse_gpu
```

Resource expanse\_gpu

	NAME	PROJECT	TG PROJECT	USED	AVAILABLE	USED BY PROJECT
1	username	ddp363		0	2500	58
2	username	sds173	TG-CCR190013	0	100	47
3	username	sds184	TG-TRA210003	0	5000	1172
4	username	abc123		42	269000	62058

# Charging

- Charge unit for all SDSC machines, including Expanse, is the Service Unit (SU).
  - 1 CPU core using  $\leq 2\text{G}$  of data for 1 hour
  - 1 GPU using  $< 96\text{G}$  of data for 1 hour
  - 'shared' partitions: based on either # of cores or fraction of memory requested, whichever is larger
- Charges based on resources used by job regardless of use.
- Charges are based on either # of cores or fraction of the memory requested, whichever is larger.
- **Minimum charge for any job is 1 SU:**
  - *Can quickly use up SUs if you run a lot of very short jobs.*
- More details in Expanse user guide:  
[https://www.sdsc.edu/support/user\\_guides/expanse.html#charging](https://www.sdsc.edu/support/user_guides/expanse.html#charging)

# Useful Links

- Expanse User Guide:
  - [https://www.sdsc.edu/support/user\\_guides/expanse.html](https://www.sdsc.edu/support/user_guides/expanse.html)
- Expanse Overview:
  - [https://education.sdsc.edu/training/interactive/202201\\_parallel\\_computing\\_concepts/index.html](https://education.sdsc.edu/training/interactive/202201_parallel_computing_concepts/index.html)
- You need to have an Expanse account in order to access the system. There are a few ways to do this:
  - Submit a proposal through the [XSEDE Allocation Request System](#)
  - A PI on an active allocation can add you to their allocation (if you are collaborators working on the same project).
  - Request a trial account: instructions @ <https://portal.xsede.org/allocations/startup>.
- Online repo and information:
  - <https://github.com/sdsc-hpc-training-org/expanse-101>
  - <https://hpc-training.sdsc.edu/expanse-101/>

# Resources

- Expanse User Guide & Tutorial
  - [https://www.sdsc.edu/support/user\\_guides/expanse.html](https://www.sdsc.edu/support/user_guides/expanse.html)
  - <https://hpc-training.sdsc.edu/expanse-101/>
- Clone code examples for this tutorial:
  - <https://github.com/sdsc-hpc-training-org/expanse-101>
- SDSC Training Resources
  - [https://www.sdsc.edu/education\\_and\\_training/training\\_hpc.html](https://www.sdsc.edu/education_and_training/training_hpc.html)
- XSEDE Training Resources
  - <https://www.xsede.org/for-users/training>
  - <https://cvw.cac.cornell.edu/expanse/>

# Thank You