

Cyberinfrastructure-Enabled Machine Learning Summer Institute

June 18, June 25-27 2024

CIML SI24 Day 1: Prep Day

Accounts, Login, Environments, Running Jobs,
Logging into Expanse User Portal

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Outline

- Expanse Overview & Innovative Features
- Getting Started/Logging on
- Environments & Modules
- Account Management
- Compiling and Running Jobs
- Expanse User Portal
- Hands-on Examples
- Conclusions

Basic Information

- Expanse User Guide:
 - https://www.sdsc.edu/support/user_guides/expanse.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](#)
 - 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>.
 - Training accounts expire, save your data.
- Online repo and information:
 - <https://github.com/sdsc-hpc-training-org/expanse-101>
 - <https://hpc-training.sdsc.edu/expanse-101/>

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Expanse



SDSC
SAN DIEGO SUPERCOMPUTER CENTER

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

DATA CENTRIC ARCHITECTURE

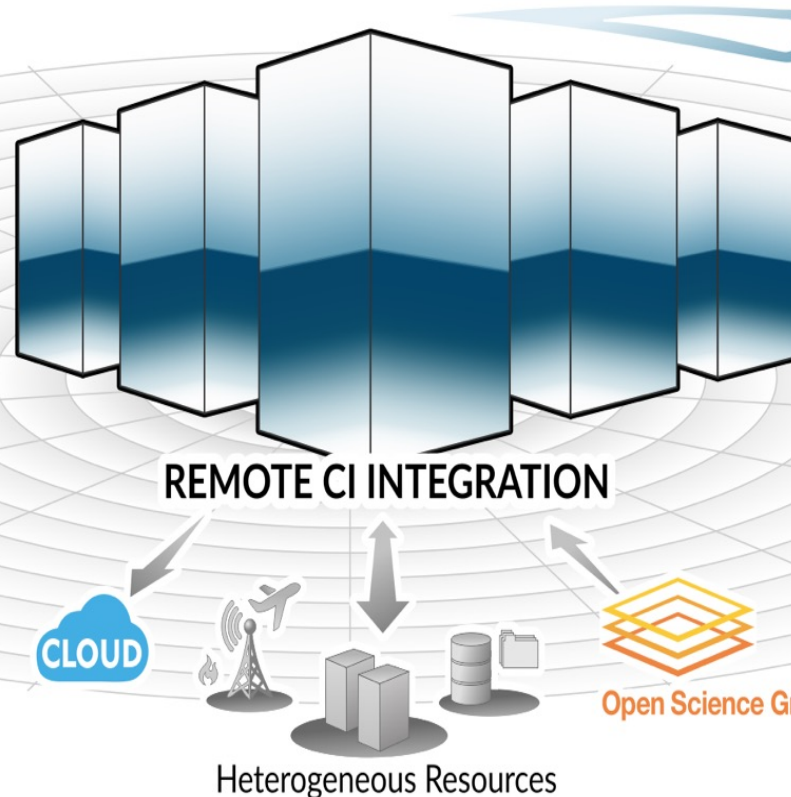
12PB Perf. Storage: 140GB/s, 200k IOPS
Fast I/O Node-Local NVMe Storage
7PB Ceph Object Storage
High-Performance R&E Networking

LONG-TAIL SCIENCE

Multi-Messenger Astronomy
Genomics
Earth Science
Social Science

INNOVATIVE OPERATIONS

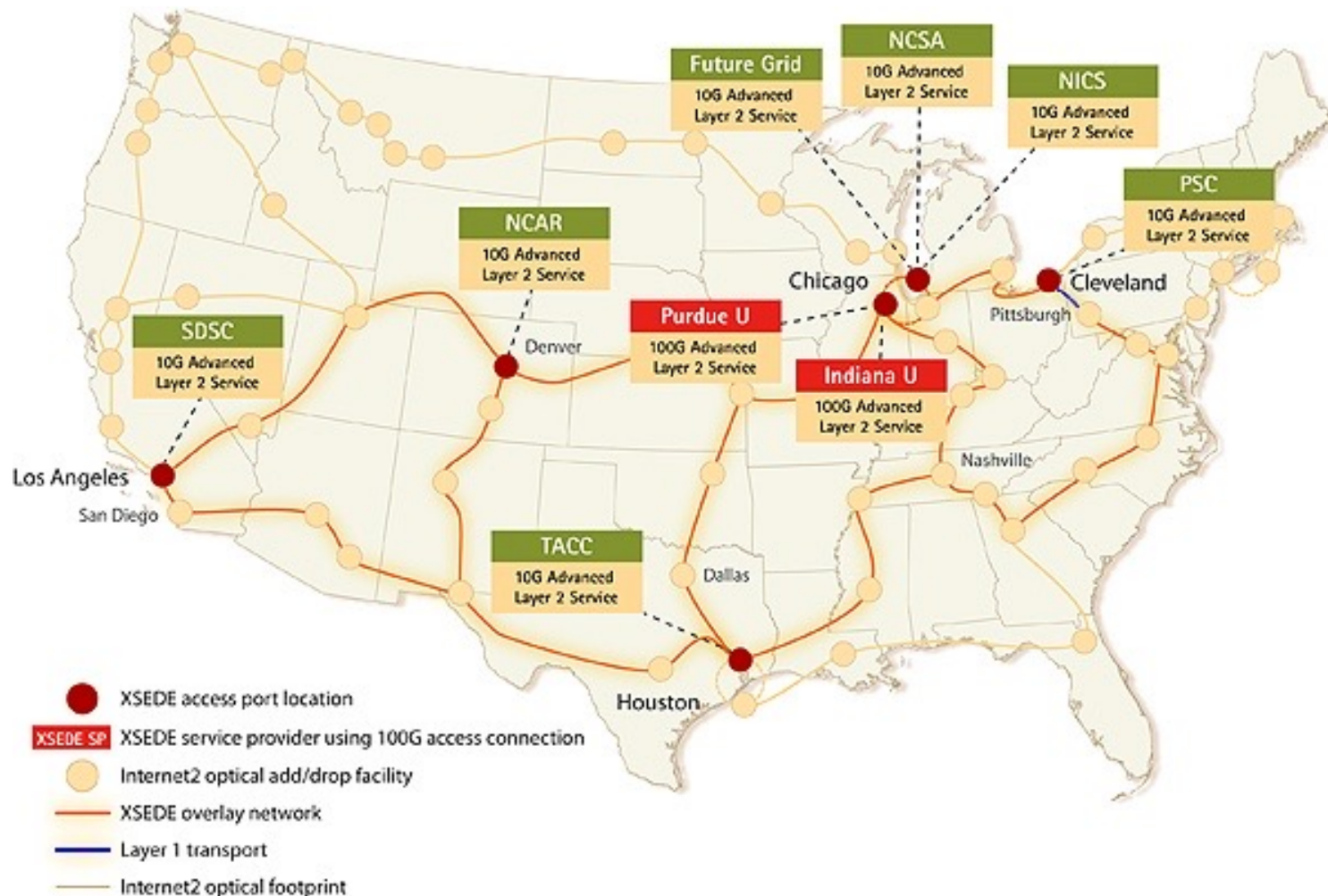
Composable Systems
High-Throughput Computing
Science Gateways
Interactive Computing
Containerized Computing
Cloud Bursting



For more details see the Expanse user guide @ https://www.sdsc.edu/support/user_guides/expanse.html
and the "Introduction to Expanse" webinar @ https://www.sdsc.edu/event_items/202006_Introduction_to_Expanse.html

Expanse: part of NSF Funded ACCESS

Extreme Science and Engineering Discovery Environment (XSEDE)



Map of XSEDE Access Ports: advanced computing resource made available to researchers

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Logging into Expanse

- Expanse supports Single Sign-On through the ACCESS User Portal
- From the command line using an ACCESS password,
 - Coming soon the Expanse User Portal.
- CPU and GPU resources are allocated separately, the login nodes are the same.
- To log in to Expanse from the command line, use the hostname:
 - login.expanse.sdsc.edu
- Secure shell (SSH) command examples:

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

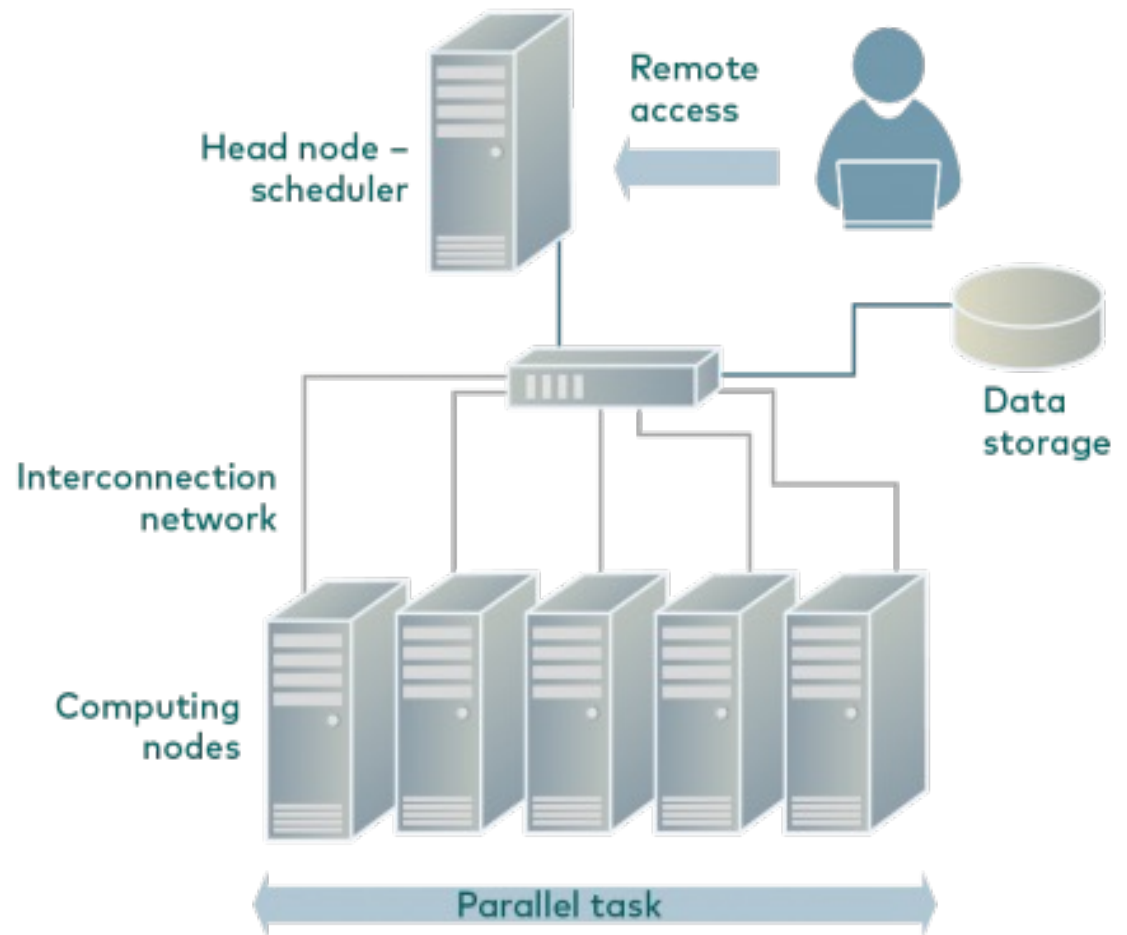
- When you log in to *login.expanse.sdsc.edu*, you will be assigned one of the two login nodes login0[1-2]-expanse.sdsc.edu. Both systems are identical.

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` or `keychain` to avoid repeatedly typing the private key password.
- Hosts which connect to SSH more frequently than ten times per minute may get blocked for a short period of time
- See the SDSC Security *repo*:
 - <https://github.com/sdsc-hpc-training-org/hpc-security>

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
- Expanse login hostname:
 - login.expanse.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:

```
Welcome to Bright release          9.0

                                     Based on Rocky Linux 8
                                     ID: #000002

-----

                        WELCOME TO

      /_____/ |// // _ \ / | / | / / ____// ____/
     /___/ | // // _ / / | / | / \_ \ \___/
    /___/ | // ____/ ____ |// | /___/ // ___/
   /____// // |// // _ / |// | /____/ ____/

-----

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: Mon Jun 17 15:34:22 2024 from 75.80.45.222
connect /private/tmp/com.apple.launchd.HbagVgBfXZ/org.xquartz:0: Connection refused
[train111@login01 ~]$ whoami
train111
[train111@login01 ~]$ date
Mon Jun 17 19:16:27 PDT 2024
[train111@login01 ~]$ hostname
login01
[train111@login01 ~]$
```

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,
 - hosts for running workflow management tools
 - primary data transfer nodes for large or numerous data transfers
 - 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 large programs.

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Expanse Environment Modules

- Expanse uses *Lmod*, a *Lua* based module system.
 - 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 *not* see all available modules when they run command "module available" – need to load *dependent/related modules*.
- 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

Module Command Examples

```
[train111@login01 ~]$ module reset
Resetting modules to system default. Resetting $MODULEPATH back to system default. All extra
directories will be removed from $MODULEPATH.
[train111@login01 ~]$ module list
Currently Loaded Modules:
  1) shared      2) cpu/0.17.3b (c)   3) slurm/expense/23.02.7  4) sdsc/1.0    5) DefaultModules
Where:
  c:  built natively for AMD Rome
[train111@login01 ~]$ module avail
----- /cm/shared/apps/spack/0.17.3/cpu/b/share/spack/lmod/linux-rocky8-x86_64/Core --
anaconda3/2021.05/q4munrg          git-lfs/2.11.0/kmruniy          pigz/2.6/bgymyl
aocc/3.2.0/io3s466                 git/2.31.1/ldetm5y             rclone/1.56.2/mldjorr
aria2/1.35.0/q32jtg2               intel/19.1.3.304/6pv46so        sratoolkit/2.10.9/rn4hu
mf
entrezdirect/10.7.20190114/6pkkpx2  matlab/2022b/lefe4oq           subversion/1.14.0/qpzq6
zs
Where:
L:  Module is loaded
c:  built natively for AMD Rome
e:  not architecture specific
g:  built natively for Intel Skylake
D:  Default Module

Module defaults are chosen based on Find First Rules due to Name/Version/Version modules
found in the module tree.
See https://lmod.readthedocs.io/en/latest/060\_locating.html for details.
```


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

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Allocations

- Some users will have more than one login account.
- Many users will have access to multiple allocations (*projects*), for example:
 - an allocation for a research project, classroom or educational use
- Users should verify that the correct *project* is designated for all Expanse (batch) jobs.
- Awards are granted for a specific purpose and should not be used for other *projects*.
- In general, for Expanse commands, to charge your job to one of your *projects*, replace << project123 >> with one from your list and put this PBS directive in your job script:
 - #SBATCH -A << project123 >>

Allocation Information

```
module load sdsc
expance-client user
expance-client user -r expance_gpu
```

```
[train111@login02 ~]$ module load sdsc
[train111@login02 ~]$ expance-client user
```

Resource expance

	NAME	STATE	PROJECT	TG PROJECT	USED	AVAILABLE	USED BY PROJECT
1	train111	allow	gue998	TG-CIE960001S	7	200000	78392

```
[train111@login02 ~]$ expance-client user -r expance_gpu
```

Resource expance_gpu

	NAME	STATE	PROJECT	TG PROJECT	USED	AVAILABLE	USED BY PROJECT
1	train111	allow	gue998	TG-CIE960001S	13	6000	649

```
[train111@login02 ~]$
```

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Supported Compilers on Expanse

- CPU nodes
 - GNU, Intel, AOCC (AMD) compilers
 - multiple MPI implementations (OpenMPI, MVAPICH2, and IntelMPI).
 - A majority of applications have been built using *gcc/10.2.0* which *features AMD Rome* specific optimization flags (-march=znver2).
 - Intel, and AOCC compilers all have flags to support Advanced Vector Extensions 2 (AVX2).
- GPU Compiling:
 - Expanse GPU nodes have GNU, Intel, and PGI compilers.
 - Note: Expanse login nodes are not the same as the GPU nodes → all GPU codes must be compiled by requesting an interactive session on the GPU nodes.

For updated information, see: https://www.sdsc.edu/support/user_guides/expanse.html#compiling

AMD AOCC Compilers: CPU Only

Language	Serial	MPI	OpenMP	MPI + OpenMP
Fortran	flang	mpif90	ifort -openmp	mpif90 -openmp
C	clang	mpiclang	icc -openmp	mpicc -openmp
C++	clang++	mpiclang	icpc -openmp	mpicxx -openm

The AMD Optimizing C/C++ Compiler (AOCC) is only available on CPU nodes. AMD compilers can be loaded using the module load command:

\$ module load aocc

For more information on the AMD compilers:

\$ [flang | clang] -help

Intel Compilers: GPU and GPU

- Default/Suggested Compilers to used based on programming model and languages:

	Serial	MPI	OpenMP	MPI + OpenMP
Fortran	ifort	mpif90	ifort -openmp	mpif90 -openmp
C	icc	mpicc	icc -openmp	mpicc -openmp
C++	icpc	mpicxx	icpc -openmp	mpicxx -openmp

- In this tutorial, we include Optional: Hands-on Examples that cover many of the cases in the table:
 - (1) MPI
 - (2) OpenMP
 - (3) HYBRID

GNU Compilers: CPU and GPU

- The GNU compilers can be loaded by executing the following commands at the Linux prompt or placing in your startup files (`~/.cshrc` or `~/.bashrc`)

```
[train111@login01 MPI]$ module purge
[train111@login01 MPI]$ module load slurm
[train111@login01 MPI]$ module load cpu
[train111@login01 MPI]$ module load gcc/10.2.0
[train111@login01 MPI]$ module load openmpi/4.0.4
[train111@login01 MPI]$ module list
Currently Loaded Modules:

  1) slurm/expense/20.02.3  2) cpu/1.0  3) gcc/10.2.0  4) openmpi/4.0.4
```

- For AVX support, compile with `-mavx`.
- Note that AVX support is only available in version 4.7 or later, so it is necessary to explicitly load the `gnu/4.9.2` module until such time that it becomes the default.
- For more information on the GNU compilers: `man [gfortran | gcc | g++]`

Using the GNU Compilers

Table of recommended GNU compilers:

	Serial	MPI	OpenMP	MPI+OpenMP
Fortran	gfortran	mpif90	gfortran -fopenmp	mpif90 -fopenmp
C	gcc	mpicc	gcc -fopenmp	mpicc -fopenmp
C++	g++	mpicxx	g++ -fopenmp	mpicxx -fopenmp

Running Jobs on Expanse

- When you run in the batch mode, you submit jobs to be run on the compute nodes using the sbatch command as described below.
- *Remember that computationally intensive jobs should be run only on the compute nodes and not the login nodes.*
- Expanse places limits on the number of jobs queued and running on a per group (allocation) and partition basis.
- Please note that submitting a large number of jobs (especially very short ones) can impact the overall scheduler response for all users.

Methods for Running Jobs on Expanse

- Expanse uses the **Simple Linux Utility for Resource Management (SLURM)** batch environment.
 - **Batch Jobs:** Submit batch scripts to Slurm from the login nodes:
 - Partition (queue)
 - Time limit for the run (maximum of 48 hours)
 - Number of nodes, tasks per node; Memory requirements (if any)
 - Job name, output file location; Email info, configuration
- **Interactive Jobs:** Use the *srun* command to obtain nodes for 'live,' command line interactive access:
 - **CPU:**

```
srun --partition=debug --account=XYZ123 --pty --nodes=1 --ntasks-per-node=128 --mem=248 -t 00:30:00 --wait=0 --export=ALL /bin/bash
```
 - **GPU:**

```
srun --pty --account=XYZ123 --nodes=1 --ntasks-per-node=1 --cpus-per-task=10 -p gpu-debug --gpus=1 -t 00:10:00 /bin/bash
```

Slurm Partitions on Expanse

Partition limits subject to change based on Early User Period evaluation

Partition Name	QOS	Max Walltime	Max Nodes/Job	Max RunningJobs	Max Running + Queued Jobs	Charge Factor	Comments
compute	normal	48 hrs	32	64	128	1	Used for exclusive access to regular compute nodes
shared	shared-normal	48 hrs	1	4096	4096	1	Single-node jobs using fewer than 128 cores
gpu	gpu-normal	48 hrs	4	16	24	1	Used for exclusive access to the GPU nodes
gpu-shared	gpu-shared-normal	48 hrs	1	16	24	1	Single-node job using fewer than 4 GPUs
large-shared	large-shared-normal	48 hrs	1	1	4	1	Single-node jobs using large memory up to 2 TB (minimum memory required 256G)
debug	debug-normal	15 min	2	1	2	1	Priority access to compute nodes set aside for testing of jobs with short walltime and limited resources
gpu-debug	gpu-debug-normal	15 min	2	1	2	1	** Priority access to gpu nodes set aside for testing of jobs with short walltime and limited resources
preempt	preempt-normal	7 days	32		128	.8	Discounted jobs to run on free nodes that can be pre-empted by jobs submitted to any other queue (NO REFUNDS)
preempt-gpu	preempt-gpu-normal	7 days	1			.8	Discounted jobs to run on unallocated nodes that can be pre-empted by jobs submitted to higher priority queues (NO REFUNDS)

Common Slurm Commands

- Submit jobs using the sbatch command:

```
$ sbatch mycode-slurm.sb
```

Submitted batch job 8718049

- Check job status using the squeue command:

```
$ squeue -u $USER
```

JOBID	PARTITION	NAME	USER	ST	TIME	NODES	NODELIST(REASON)
8718049	compute	mycode	user	PD	0:00	1	(Priority)

- Once the job is running:

```
$ squeue -u $USER
```

JOBID	PARTITION	NAME	USER	ST	TIME	NODES	NODELIST(REASON)
8718049	debug	mycode	user	R	0:02	1	expans-14-01

- Cancel a running job:

```
$ scancel 8718049
```

General Steps: Compiling/Running Jobs

- Change to a working directory (for example the `expanse101` directory):

```
cd /home/$USER/expanse101/MPI
```

- **Verify** that the correct modules are loaded:

```
module list
```

Currently Loaded Modulefiles:

```
1) slurm/expanse/20.02.3 2) cpu/1.0 3) gcc/10.2.0 4) openmpi/4.0.4
```

- **Compile** the MPI hello world code:

```
mpif90 -o hello_mpi hello_mpi.f90
```

- **Verify** executable has been created (check that date):

```
ls -lt hello_mpi
```

```
-rwxr-xr-x 1 user sdsc 721912 Mar 25 14:53 hello_mpi
```

- **Submit job**

```
sbatch hello_mpi_slurm.sb
```

MPI Hello World

- Change to the MPI examples directory:

```
[train111@login01 MPI]$ cat hello_mpi.f90
! Fortran example
program hello
include 'mpif.h'
integer rank, size, ierror, tag, status(MPI_STATUS_SIZE)

call MPI_INIT(ierror)
call MPI_COMM_SIZE(MPI_COMM_WORLD, size, ierror)
call MPI_COMM_RANK(MPI_COMM_WORLD, rank, ierror)
print*, 'node', rank, ': Hello world!'
call MPI_FINALIZE(ierror)
end
[train111@login01 MPI]$
```

MPI Hello World: Compile

Set the environment and
then compile the code

```
[train111@login01 MPI]$ cat README.txt  
[1] Compile:
```

```
# Load module environment  
module purge  
module load slurm  
module load cpu  
module load gcc/10.2.0  
module load openmpi/4.0.4
```

```
mpif90 -o hello_mpi hello_mpi.f90
```

[2a] Run using Slurm:

```
sbatch hellompi-slurm.sb
```

[2b] Run using Interactive CPU Node

```
srun --partition=debug --pty --account=use300 --nodes=1 --ntasks-per-node=128 --mem=248G -t  
00:30:00 --wait=0 --export=ALL /bin/bash
```

```
[train111@login01 MPI]$ module list
```

Currently Loaded Modules:

1) cpu/1.0 2) slurm/expansive/20.02.3

```
[train111@login01 MPI]$ module purge
```

```
[train111@login01 MPI]$ module load slurm
```

```
[train111@login01 MPI]$ module load cpu
```

```
[train111@login01 MPI]$ module load gcc/10.2.0
```

```
[train111@login01 MPI]$ module load openmpi/4.0.4
```

```
[train111@login01 MPI]$ module list
```

Currently Loaded Modules:

1) slurm/expansive/20.02.3 2) cpu/1.0 3) gcc/10.2.0 4) openmpi/4.0.4

```
[train111@login01 MPI]$ mpif90 -o hello_mpi hello_mpi.f90
```

```
[train111@login01 MPI]$
```

MPI Hello World: Batch Script

- To run the job, use the **batch script submission** command.
- Monitor the job until it is finished using the **squeue** command.

```
[train111@login01 MPI]$ cat hellompi-slurm-gnu.sb
#!/bin/bash
#SBATCH --job-name="hellompi-gnu"
#SBATCH --output="hellompi-gnu.%j.%N.out"
#SBATCH --partition=compute
#SBATCH --nodes=2
#SBATCH --ntasks-per-node=128
#SBATCH --export=ALL
#SBATCH -t 00:10:00

#This job runs with 2 nodes,
128 cores per node for a total of 256 cores.

## Environment
module purge
module load slurm
module load cpu
module load gcc/10.2.0
module load openmpi/4.0.4

## Use srun to run the job

srun --mpi=pmi2 -n 256 --cpu-bind=rank ./hello_mpi_gnu

[train111@login01 MPI]$
```

```
[train111@login01 MPI]$ sbatch hellompi-slurm-gnu.sb; squeue -u train111
Submitted batch job 108910
      JOBID PARTITION  NAME  USER ST   TIME  NODES NODELIST(REASON)
    108910  compute hellompi train111 PD   0:00    2 (None)
[train111@login01 MPI]$ cat hellompi-gnu.108910.exp-12-54.out
node      4 : Hello world!
node      5 : Hello world!
node      7 : Hello world!
node      0 : Hello world!
node      2 : Hello world!
node      3 : Hello world!
node      9 : Hello world!
node     10 : Hello world!

[SNIP]

node     247 : Hello world!
node     248 : Hello world!
node     249 : Hello world!
node     186 : Hello world!
node     220 : Hello world!
node     203 : Hello world!
node     135 : Hello world!
```


Using An Interactive mode

```
[train111@login01 MPI]$ module purge
[train111@login01 MPI]$ module load slurm
[train111@login01 MPI]$ module load cpu
[train111@login01 MPI]$ module load gcc/10.2.0
[train111@login01 MPI]$ module load openmpi/4.0.4
[train111@login01 MPI]$ srun --pty --nodes=1 --ntasks-per-node=24 -p debug -t 00:30:00 --wait 0 /bin/bash
[train111@exp-9-55 MPI]$ module list
```

Request
interactive
node for 30
minutes

```
[train111@exp-9-55 MPI]$ mpirun -np 16 ./hello_mpi
```

```
node    1 : Hello world!
node   15 : Hello world!
node    7 : Hello world!
node   14 : Hello world!
node   11 : Hello world!
node    6 : Hello world!
node    4 : Hello world!
node    5 : Hello world!
node   12 : Hello world!
node   13 : Hello world!
node    0 : Hello world!
node    8 : Hello world!
node    9 : Hello world!
node   10 : Hello world!
node    2 : Hello world!
node    3 : Hello world!
```

- Exit interactive session when your work is done or you will be charged CPU time.
- Beware of oversubscribing your job: asking for more cores than you have. Intel compiler allows this, but your performance will be degraded.

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Expanse User Portal

File Browsing, editing, creation, upload, download, etc.

Interactive Services

Job Script Editing and Submission

Active Job monitoring and Management

OOD 2.0 Features

SDSC
The Expanse portal provides an integrated, and easy to use interface to access Expanse HPC resource.

With the portal, researchers can manage files (create, edit, move, upload and download), view job templates for various applications, submit and monitor jobs, run interactive applications, and connect via SSH. The portal has no end-user installation requirements other than access to a modern up-to-date web browser.

Pinned Apps A featured subset of all available apps

- Active Jobs
- Home Directory
- Job Composer
- Expanse Shell Access
- MATLAB
- RSTUDIO
- Allocation and Usage Information
- Jupyter

Active Jobs

ID	Name	User	Access	Time	Status	Cluster
6880300	testjob	testuser	test@sdsc	2020-03-07 10:00:00	Completed	exp@sdsc
6880301	testjob	testuser	test@sdsc	2020-03-07 10:00:00	Completed	exp@sdsc
6880302	testjob	testuser	test@sdsc	2020-03-07 10:00:00	Completed	exp@sdsc
6880303	testjob	testuser	test@sdsc	2020-03-07 10:00:00	Completed	exp@sdsc
6880304	testjob	testuser	test@sdsc	2020-03-07 10:00:00	Completed	exp@sdsc
6880305	testjob	testuser	test@sdsc	2020-03-07 10:00:00	Completed	exp@sdsc
6880306	testjob	testuser	test@sdsc	2020-03-07 10:00:00	Completed	exp@sdsc
6880307	testjob	testuser	test@sdsc	2020-03-07 10:00:00	Completed	exp@sdsc
6880308	testjob	testuser	test@sdsc	2020-03-07 10:00:00	Completed	exp@sdsc
6880309	testjob	testuser	test@sdsc	2020-03-07 10:00:00	Completed	exp@sdsc
6880310	testjob	testuser	test@sdsc	2020-03-07 10:00:00	Completed	exp@sdsc

Jobs

Job Details

Job Name: (default) Simple Sequential Job

Submitted to: exp@sdsc

Cluster: exp@sdsc

Status: Pending

Script location: /home/testuser/.ssh/config

Script name: main_job.sh

Folder contents: main_job.sh

<https://portal.expanse.edu>

Expanse Portal – Training Account Log-in

CIML SI24 Link: <https://portal.expanse.edu/training>

The left screenshot shows the login page for the Expanse Portal. The URL in the browser is https://training-auth.sdsc.edu/authorize.php?response_type=code&scope=openid&clie.... The page has a red header with the text "SDSC TRAINING ACCOUNT LOG-IN". Below the header, there is a form with two input fields: "Training Account Name" (containing "trainXX or etrainYY") and "Password" (containing "account.password"). A blue button labeled "Log In With Training Account" is positioned below the password field. A yellow oval highlights the "Log In With Training Account" button.

The right screenshot shows the main portal interface. The navigation bar includes "Expanse Portal", "Apps", "Files", "Jobs", "Clusters", "Interactive Apps", and "My Interactive Sessions". The SDSC logo is prominently displayed. Below the logo, a message states: "The Expanse portal provides an integrated, and easy to use interface to access Expanse HPC resource. With the portal, researchers can manage files (create, edit, move, upload, and download), view job templates for various applications, submit and monitor jobs, run interactive applications, and connect via SSH. The portal has no end-user installation requirements other than access to a modern up-to-date web browser". A section titled "Pinned Apps A featured subset of all available apps" displays a grid of app icons. The apps shown are: Active Jobs, Desktop, Home Directory, Job Composer, expanse Shell Access, MATLAB, RSTUDIO, Allocation and Usage Information, and Jupyter.

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- **Hands-on Examples**
- Conclusions

Hands-on Examples

- Collection of working codes can be found in several places:
- HPC Training Github repo:
 - <https://github.com/sdsc-hpc-training-org/hpctr-examples>
- On Expanse:

```
[train111@login02 ~]$ ll /cm/shared/examples/sdsc
total 0
drwxrwxr-x 2 mahidhar use300 4 May 29 09:40 abaqus
drwxrwxr-x 2 mahidhar use300 6 May 10 2023 abinit
drwxrwxr-x 2 mahidhar use300 5 Sep 12 2023 alphafold
drwxrwxr-x 7 mahidhar use300 5 Oct 5 2023 amber
drwxrwxr-x 2 mahidhar use300 1 Apr 29 2021 bintest
drwxr-xr-x 6 mkandes use300 4 Jun 12 14:32 ciml
drwxrwxr-x 4 mahidhar use300 2 Apr 14 2022 classes
[snip]
drwxrwxr-x 2 mahidhar use300 3 Feb 24 2022 hadoop
drwxrwxr-x 5 mahidhar use300 23 Aug 11 2022 hpcg
drwxrwxr-x 3 mahidhar use300 7 Sep 10 2021 hpl
[snip]
drwxrwxr-x 6 mahidhar use300 4 Dec 7 2023 matlab
drwxrwxr-x 2 mahidhar use300 6 Nov 22 2021 mpi
drwxrwxr-x 2 mahidhar use300 5 Oct 28 2020 mpi-openmp-hybrid
[snip]
drwxrwxr-x 2 mahidhar use300 2 Feb 24 2022 nwchem
drwxrwxr-x 2 mahidhar use300 6 Oct 13 2020 openacc
drwxrwxr-x 2 mahidhar use300 6 Oct 13 2020 openmp
drwxrwxr-x 4 mahidhar use300 2 Jul 1 2023 orca
drwxrwxr-x 3 mahidhar use300 3 Mar 12 13:35 paraview
drwxrwxr-x 3 mahidhar use300 1 Jun 20 2023 pyscf
[snip]
drwxr-xr-x 2 mkandes use300 1 Oct 27 2021 visit
drwxrwxr-x 4 mahidhar use300 2 Nov 23 2021 wannier90
drwxrwxr-x 5 mahidhar use300 3 Dec 20 2020 xpmem
```


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When Things Go Wrong, Check Your User Environment

- Do you have the right modules loaded?
- What software versions do you need?
- Is your code compiled and updated
 - Did you compile it last year? Have the libraries changed?
- Are you running your job from the right location?
 - \$HOME versus \$WORK?

Run jobs from the right location

- Lustre scratch filesystem:
 - /oasis/scratch/expanse/\$USER/temp_project
 - Preferred: Scalable large block I/O)
- Compute/GPU node local SSD storage:
 - /scratch/\$USER/\$SLURM_JOBID
 - Meta-data intensive jobs, high IOPs)
- Lustre projects filesystem:
 - /oasis/projects/nsf
- /home/\$USER:
 - Only for source files, libraries, binaries.
 - *Do not* use for I/O intensive jobs.

Thank You

Basic Information

- Expanse User Guide:
 - https://www.sdsc.edu/support/user_guides/expanse.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](#)
 - 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>.
 - Training accounts expire, save your data.
- Online repo and information:
 - <https://github.com/sdsc-hpc-training-org/expanse-101>
 - <https://hpc-training.sdsc.edu/expanse-101/>

Resources

- Expanse User Guide
 - https://www.sdsc.edu/support/user_guides/expanse.html
- Expanse-101 Tutorial:
 - <https://hpc-training.sdsc.edu/expanse-101/>
- GitHub Repo: clone example code:
 - <https://github.com/sdsc-hpc-training-org/hpctr-examples>
- SDSC Training Resources
 - https://www.sdsc.edu/education_and_training/training
- ACCESS Training Resources
 - <https://www.xsede.org/for-users/training>