CIML SI25 Day 1: Prep Day

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

By Mary Thomas

Outline

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

Basic Information

- Check out the 0_Prep doc – contains important information:
  - https://github.com/ciml-org/ciml-summer-institute-2025/tree/main/0_preparation
- 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:
  - You have been assigned a training accounts: they expire, save your data.
  - Request a trial account, instructions @ https://portal.xsede.org/allocations/startup.
  - Reach out to a PI with an active allocation can add you to their allocation.
  - Submit a proposal through the XSEDE Allocation Request System.
- Online repo and information:
  - https://github.com/sdsc-hpc-training-org/expanse-101
  - https://hpc-training.sdsc.edu/expanse-101/

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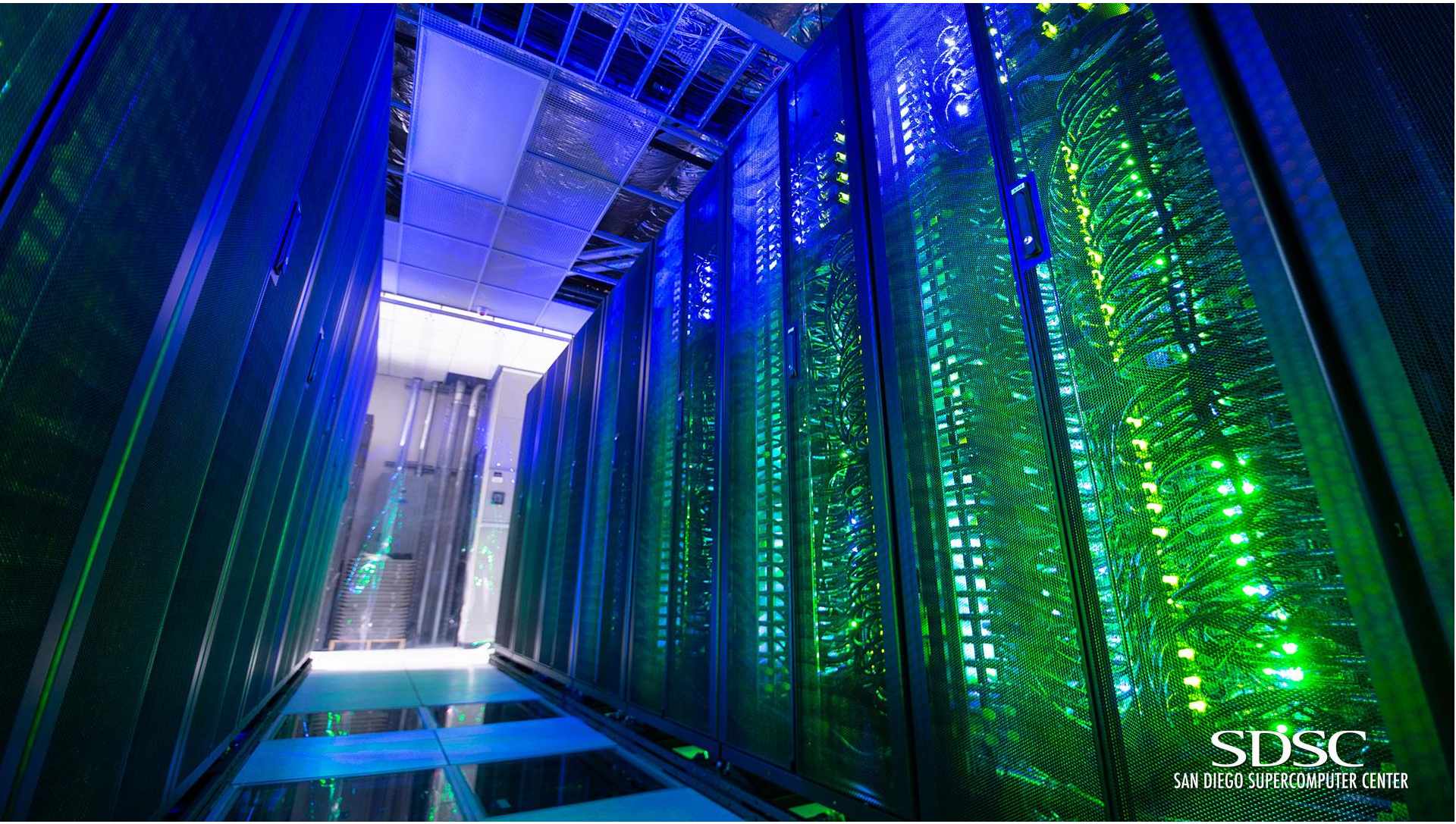
Expanse

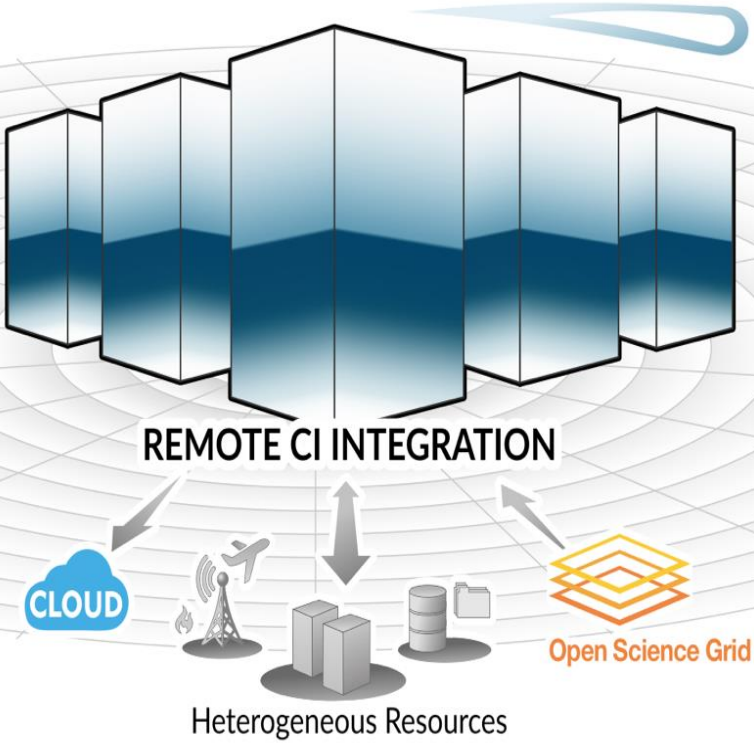


EXPANSE

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



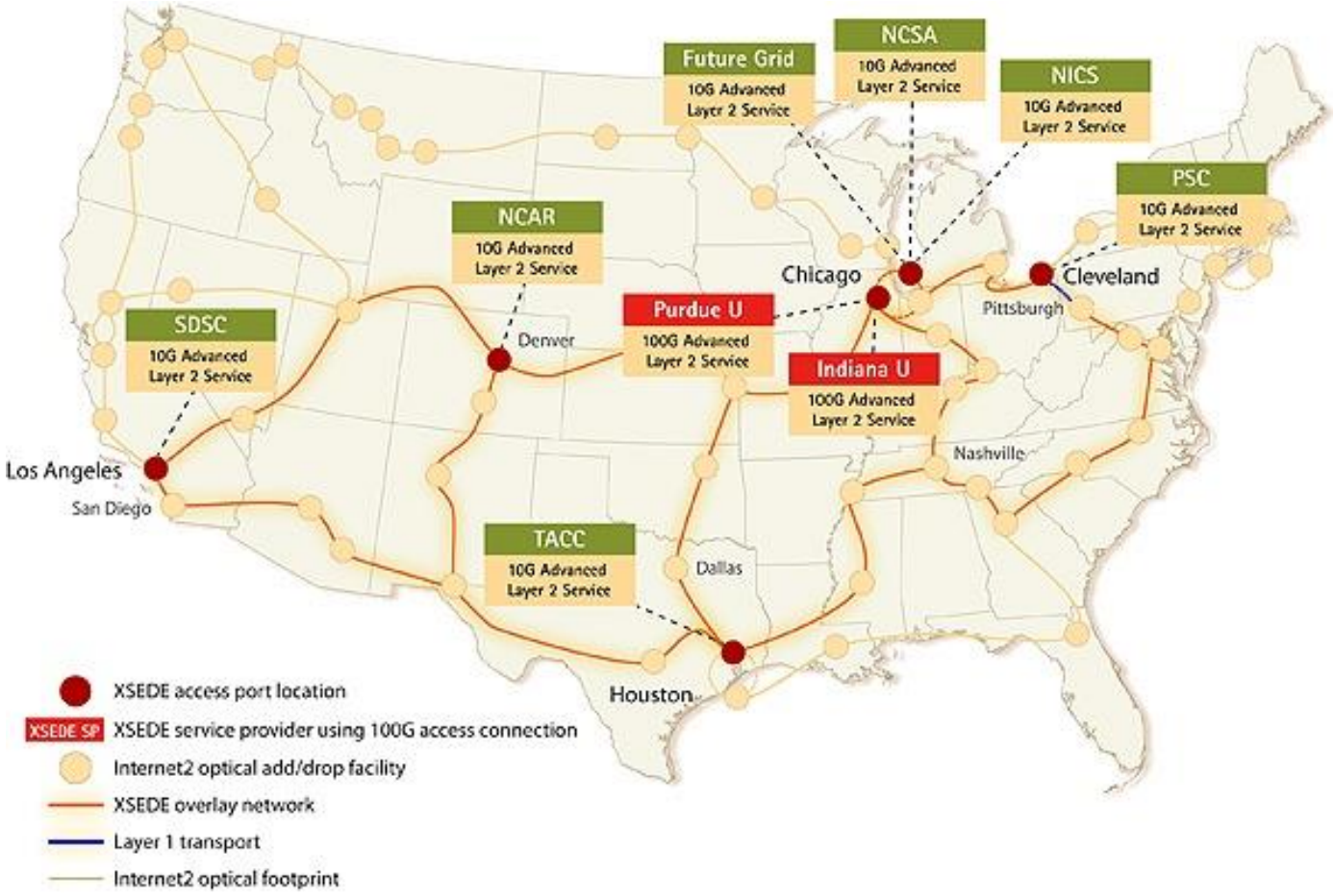
LONG-TAIL SCIENCE
Multi-Messenger Astronomy
Genomics
Earth Science
Social Science

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 ACESS

Extreme Science and Engineering Discovery Environment (XSEDE)



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

COMPLECS: Introductory Webinar Series

COMPLECS (COMPrehensive Learning for end-users to Effectively utilize CyberinfraStructure): SDSC program where training will cover non-programming skills needed to effectively use supercomputers.

- Parallel computing concepts
- Intermediate Linux and shell scripting
- Linux tools for file processing
- HPC Security and getting help
- Code migration
- Getting Started with Batch Job Scheduling: Slurm Edition
- HPC hardware overview
- Interactive computing
- Data management: Part 1 & 2
- High-Throughput and Many Task Computing Worksflows: Slurm Edition

https://www.sdsc.edu/education/training-programs/COMPLECS.html

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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.

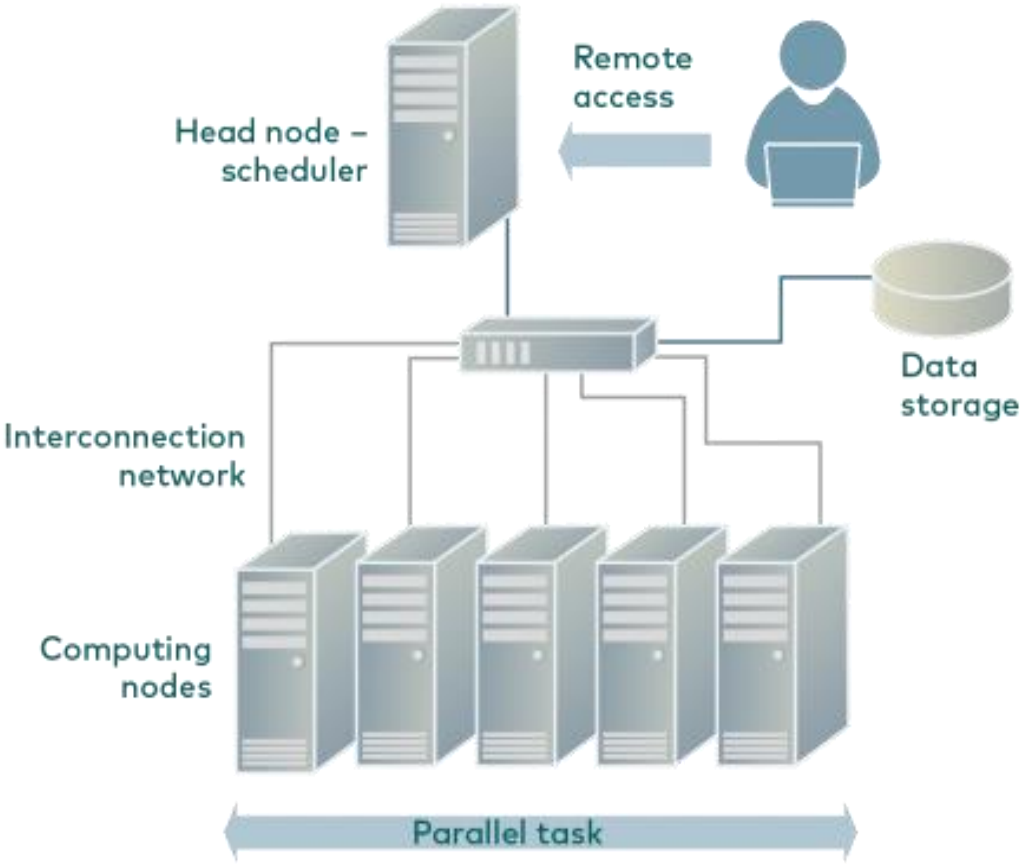
Using SSH Keys

- 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. Reseting $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/expanse/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/bgymyil
   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 that 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 purposes 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
expanse-client user
expanse-client user -r expanse_gpu

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

 Resource  expanse
```

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

```
[train111@login02 ~]$ expanse-client user -r expanse_gpu

 Resource  expanse_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/expanse/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.
- Expanse code examples:
  - https://github.com/sdsc-hpc-training-org/hpctr-examples

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:
  - ***Make sure you have the right module environment***

CPU	srun --partition=debug --pty --account=<<project>> --nodes=1 --ntasks-per-node=4 --mem=8G -t 00:30:00 --wait=0 --export=ALL /bin/bash
GPU	login01$ srun --partition=gpu-debug --pty --account=<<project>> --ntasks-per-node=10 --nodes=1 --mem=96G --gpus=1 -t 00:30:00 --wait=0 --export=ALL /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 then 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 then 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 submited 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**)

cified using -p option in batch script.

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        expanse-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]$
```

Code Examples: https://github.com/sdsc-hpc-training-org/hpctr-examples

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/expanse/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/expanse/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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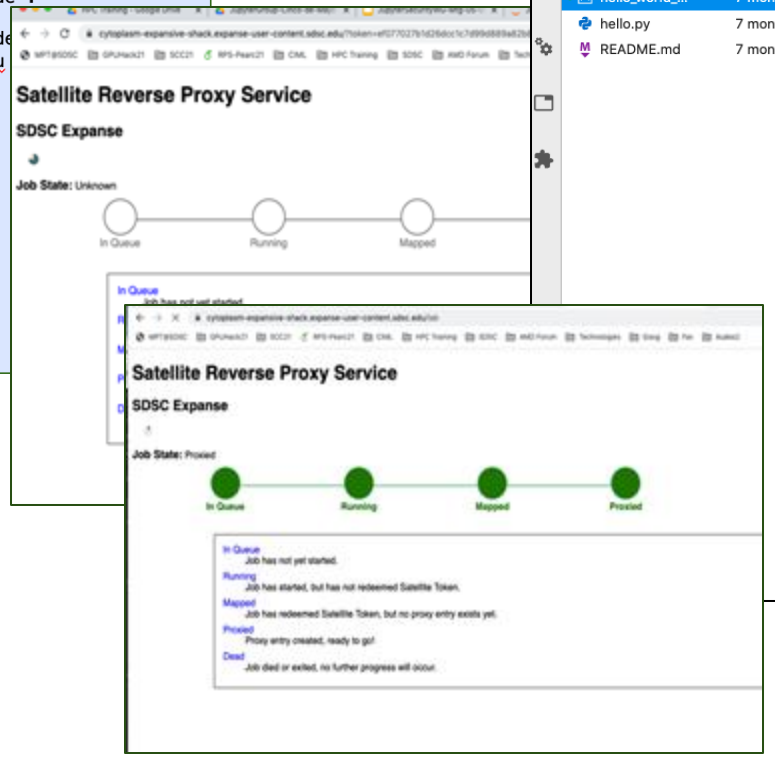
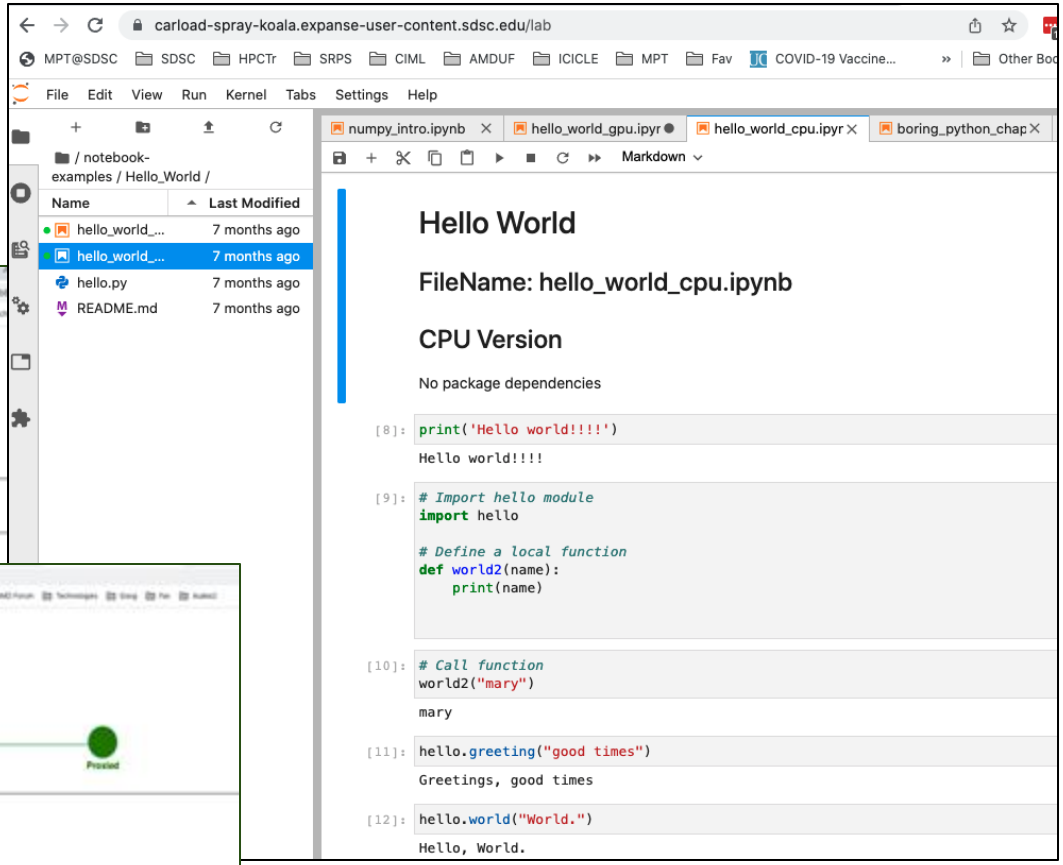
Launch Secure Notebooks Using galyleo

https://github.com/sdsc/galyleo

```
[username@login01 ~]export
PATH="/cm/shared/apps/sdsc/galyleo:${PATH}"

[username@login01 ~]$ galyleo.sh --help
USAGE: galyleo.sh launch [command-line
option] {value}
command-line option      : value
    -A | --account         :
    -R | --reservation     :
    -p | --partition       :
    -q | --qos             :
    -N | --nodes           :
    -n | --ntasks-per-node :
    -c | --cpus-per-task
    -M | --memory-per-node
    -m | --memory-per-cpu
    -G | --gpus
       | --gres
    -t | --time-limit
    -j | --jupyter
    -d | --notebook-dir
    -r | --reverse-proxy
    -D | --dns-domain
    -s | --sif
    -B | --bind
       | --nv
    -e | --env-modules
       | --conda-env
    -Q | --quiet
```

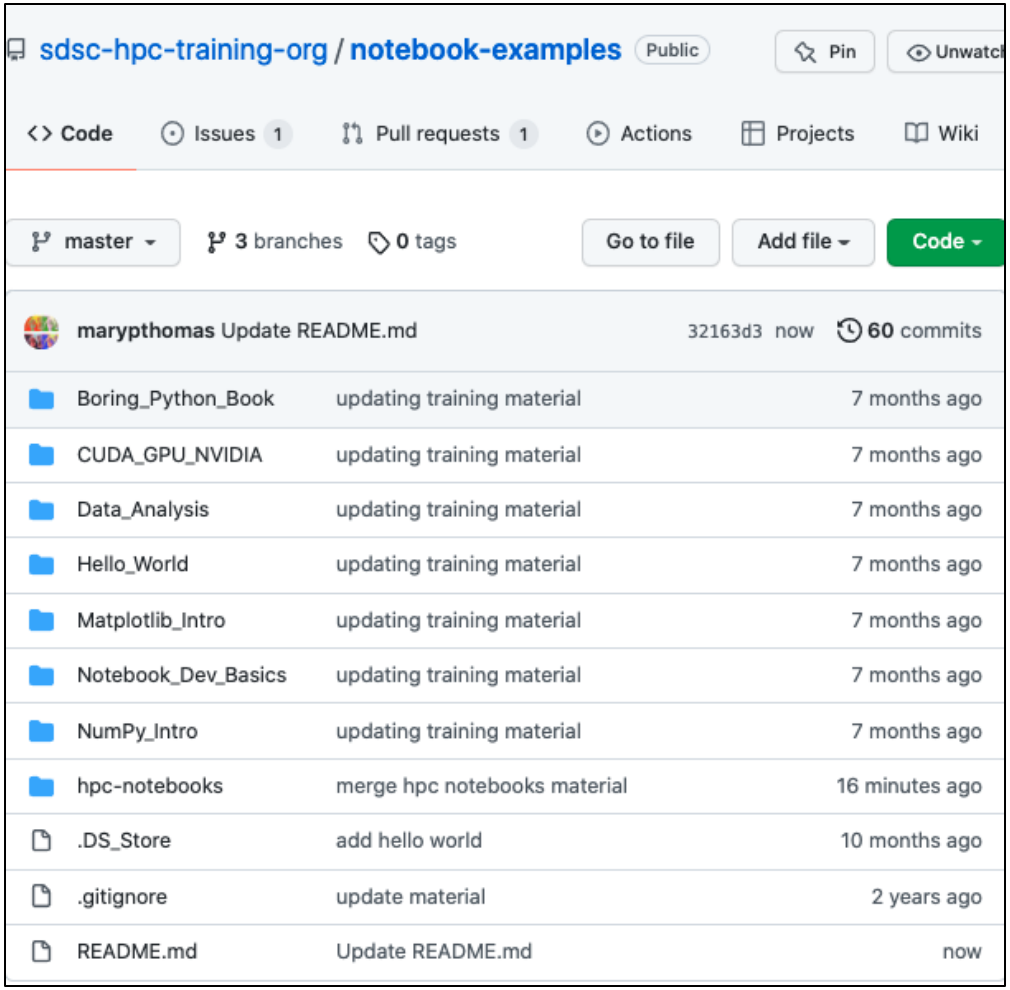




Notebook Examples

https://github.com/sdsc-hpc-training-org/notebook-examples

- Collection of tested, working notebooks tested on Expanse and other SDSC HPC systems
- Includes range of materials from “hello world” to Spark ML notebooks.
- Note: collection changes often, based on testing and contributions



Outline

- Expanse Overview & Innovative Features
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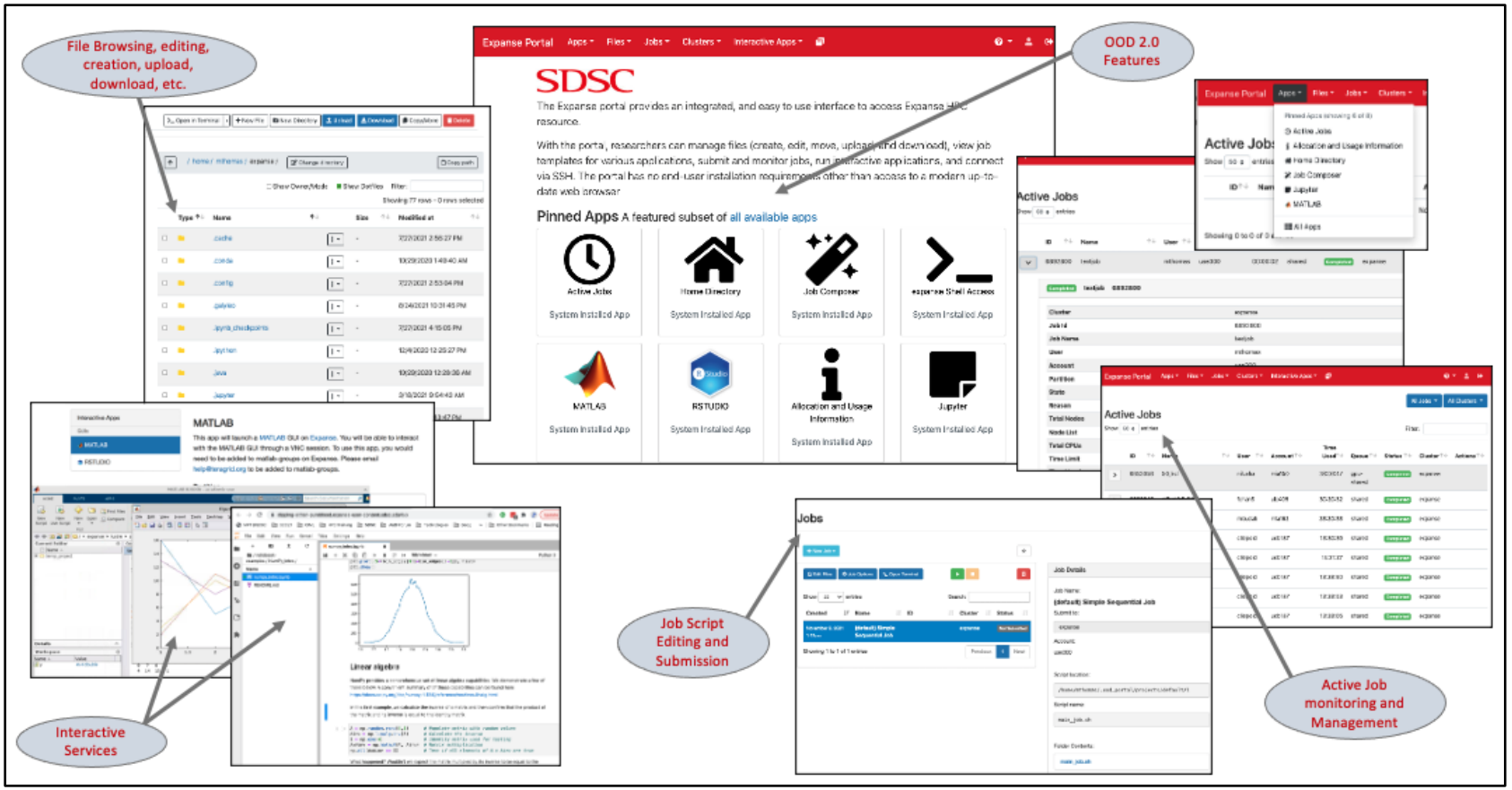
- Environments & Modules
- Account Management
- Compiling and Running Jobs
- Jupyter Notebooks
- **Expanse User Portal**
- Hands-on Examples
- Conclusions

Expanse User Portal

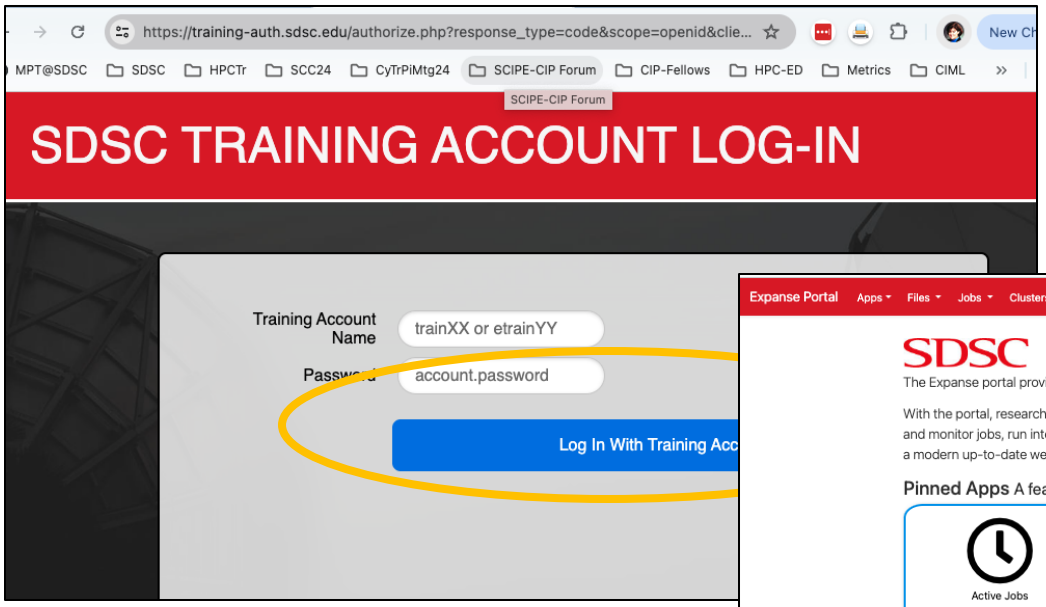


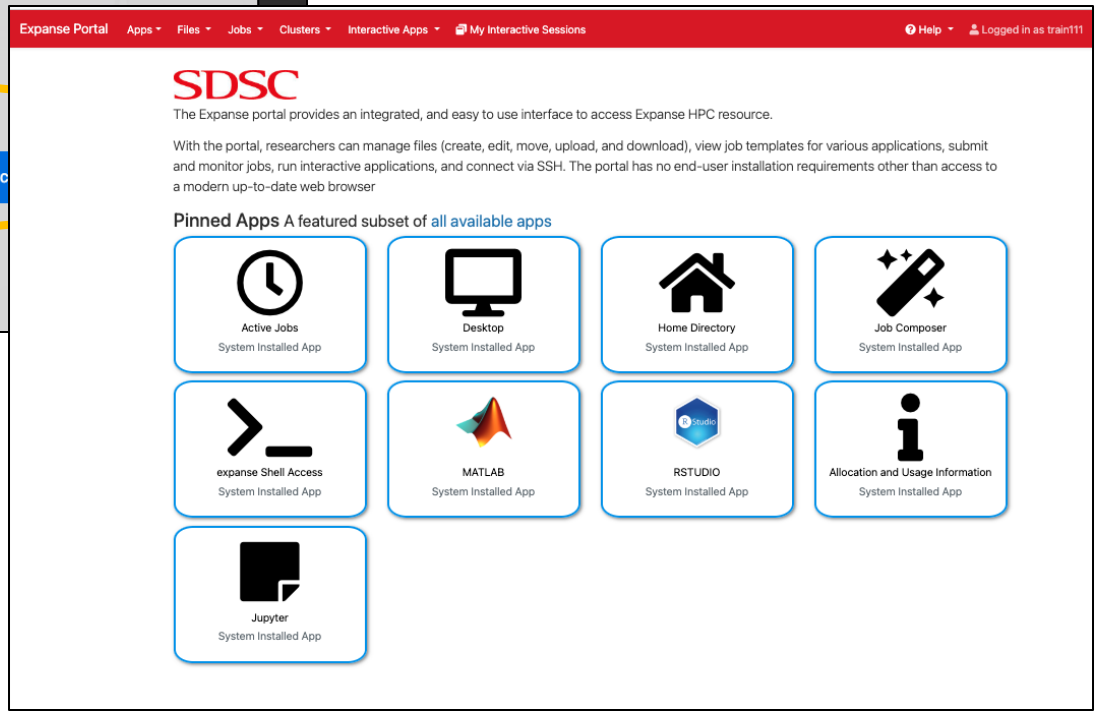
https://portal.expanse.sdsc.edu

For the CIML SI25 use: https://portal.expanse.sdsc.edu/training

Expanse Portal – Training Account Log-in

CIML Summer Institute: https://portal.expanse.sdsc.edu/training





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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-hybri
[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?
- Reach out to consult@sdsc.edu

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.

Resources

- GitHub Repo for this webinar: clone code examples for this tutorial – clone example code:
  - https://github.com/ciml-org/ciml-summer-institute-2025
- SDSC Training Resources
  - https://www.sdsc.edu/support/user_guides/expanse.html
  - https://education.sdsc.edu/training/interactive/
  - https://www.sdsc.edu/events/index.html
  - https://github.com/sdsc-hpc-training-org/hpctr-examples
  - https://github.com/sdsc-hpc-training-org/notebook-examples
- ACCESS Training Resources
  - https://support.access-ci.org/events

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/

Thank You