Running jobs on Expanse
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EXPANSE
COMPUTING WITHOUT BOUNDARIES

SAN DIEGO SUPERCOMPUTER CENTER

NSF Award 1928224

Outline

- System overview and login
- Slurm scheduler – partition information
- Running jobs
    - MPI
    - OpenMP
    - MPI/OpenMP hybrid
    - GPU jobs
- Filesystems
    - Example local scratch usage
- Summary

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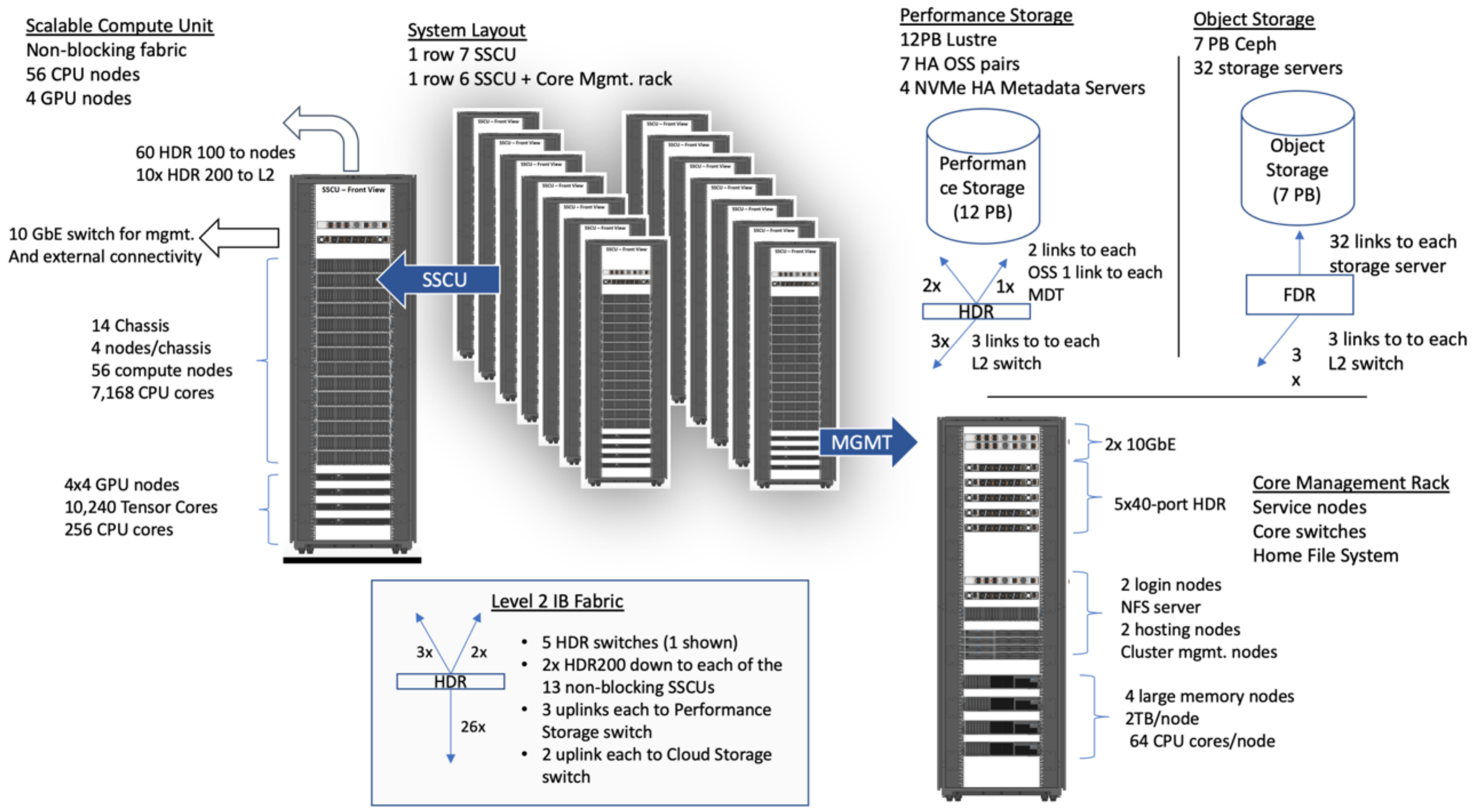
Expanse is a heterogeneous architecture designed for high performance, reliability, flexibility, and productivity

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*



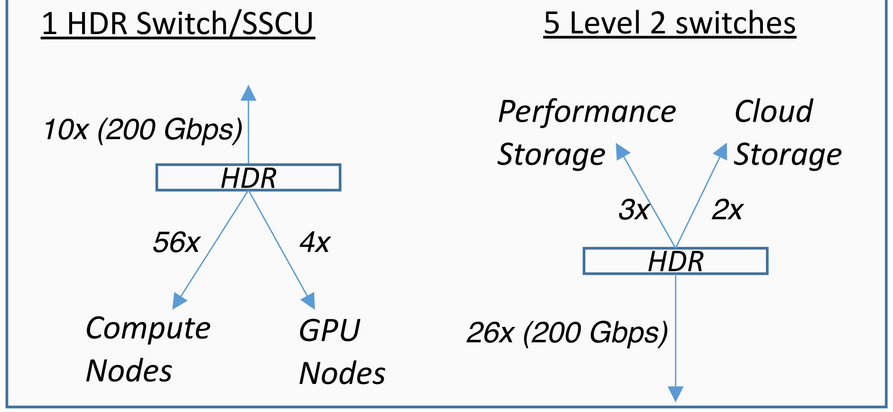
The SSCU is Designed for the Long Tail Job Mix, Maximum Performance, Efficient Systems Support, and Efficient Power and Cooling

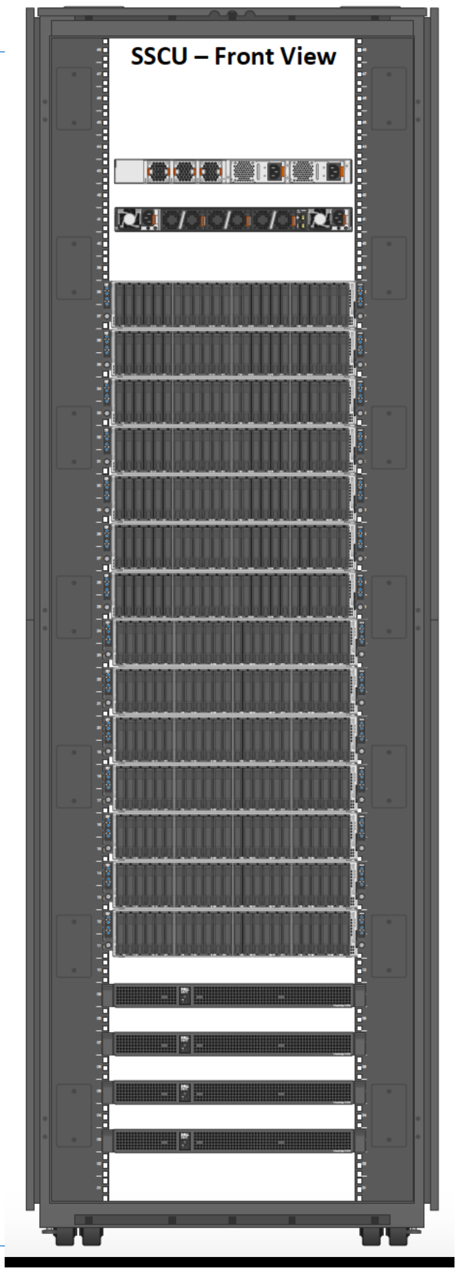
Standard Compute Nodes
- *2x AMD EPYC 7742 @2.25 GHz*
- *128 Zen2 CPU cores*
- *PCIe Gen4*
- *256 GB DDR4*
- *1 TB NVME*

GPU Nodes
- *4x NVIDIA V100/follow-on*
- *10,240 Tensor Cores*
- *32 GB GDDR*
- *1.6 TB NVMe*
- *Intel CPUs*

SSCU Components
- *56x CPU nodes*
- *7,168 Compute Cores*
- *4x GPU nodes*
- *1x HDR Switch*
- *1x 10GbE Switch*
- *HDR 100 non-blocking fabric*
- *Wide rack for serviceability*
- *Direct Liquid Cooling to CPU nodes*

Non-blocking Interconnect





Logging into Expanse

- 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

- Users can login directly using the Secure shell (SSH) command or a ssh client (such as putty). Example:

```
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 nodes are identical.
- Users can also login via the XSEDE single sign on host (login.xsede.org):

```
ssh your_xsede_portal_username@login.xsede.org
gsissh login.expanse.sdsc.edu
```

- ***Access via Expanse User Portal (See Subha's talk later today).***

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 SDSC Security Webinar:
  - https://www.sdsc.edu/event_items/202007_CometWebinar.html

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

Appropriate use of Login Nodes

- The login nodes are meant for file editing, simple data management, and other 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 intensive 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
- For GPU codes, users should request interactive sessions on batch nodes for compilations (the host CPU is different from the login node).

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Expanse Scheduler Information

- Expanse uses the **Simple Linux Utility for Resource Management (SLURM)** batch environment.
- 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
```

Expanse Scheduler Information

- Expanse has both node exclusive and shared partitions (just like Comet). Partitions that are familiar from Comet:
    - compute – CPU nodes, exclusive access. Careful since this is now 128 cores => will be using up SUs very quickly. Make sure to use the full node resources efficiently.
    - shared – CPU nodes, shared access for jobs needing < 128 cores
    - gpu – GPU nodes, exclusive access
    - gpu-shared – GPU nodes, shared access for jobs needing < 4 GPUs
    - large-shared - Large memory nodes
    - debug – for shorts tests, quick access
- New partitions on Expanse:
    - gpu-debug – for short tests, compilation tasks
    - preempt - discounted jobs to run on free nodes that can be pre-empted by jobs in other partitions (compute, shared)
    - gpu-preempt - discounted jobs to run on free nodes that can be pre-empted by jobs in other partitions (gpu, gpu-shared)

Expanse Partitions

Partition Name	*Max Walltime*	*Max Nodes/Job*	*Max Running Jobs*	*Max Running + Queued Jobs*	*Charge Factor*	*Comments*
compute	48 hrs	32	64	128	1	* Used for exclusive access to regular compute nodes
shared	48 hrs	1	4096	4096	1	Single-node jobs using fewer than 128 cores
gpu	48 hrs	4	16	24	1	Used for exclusive access to the GPU nodes
gpu-shared	48 hrs	1	16	24	1	Single-node job using fewer than 4 GPUs
large-shared	48 hrs	1	1	4	1	Single-node jobs using large memory up to 2 TB (minimum memory required 256G)
debug	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	15 min	2	1	2	1	** Priority access to gpu nodes set aside for testing of jobs with short walltime and limited resources
preempt	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**)
gpu-preempt	7 days	1			.8	

Expanse Scheduler – required parameters

--partition (-p)

--nodes (-N)

--ntasks-per-node OR --ntasks (-n): If both are specified SLURM picks ntasks

--wallclock (-t)

--account (-A): Unlike Comet we do *not* pick a default

--gpus : Total number of GPUs needed by job (unlike Comet where were setting –gres).

Note**: --mem, --mem-per-cpu, --mem-per-gpu are not required. However, it is recommended to explicitly request (using one of these options) what is needed –* ***even on the "compute" and "gpu" partitions which are exclusive.

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Interactive Jobs

- You can request an interactive session using the srun command. The following example will request one regular compute node, 128 cores, in the debug partition for 30 minutes:

```
srun --partition=debug --pty --nodes=1 --ntasks-per-node=128 --mem=248G -t
00:30:00 -A xyz123 --wait=0 --export=ALL /bin/bash
```

- The following example will request a GPU node, 10 cores, 1 GPU and 90G (all the memory) in the debug partition for 30 minutes:

```
srun --partition=gpu-debug --pty --nodes=1 --ntasks-per-node=10 --mem=90G --
gpus=1 -A xyz123 -t 00:30:00 --wait=0 --export=ALL /bin/bash
```

Example batch script: MPI Job
(/cm/shared/examples/sdsc/mpi)

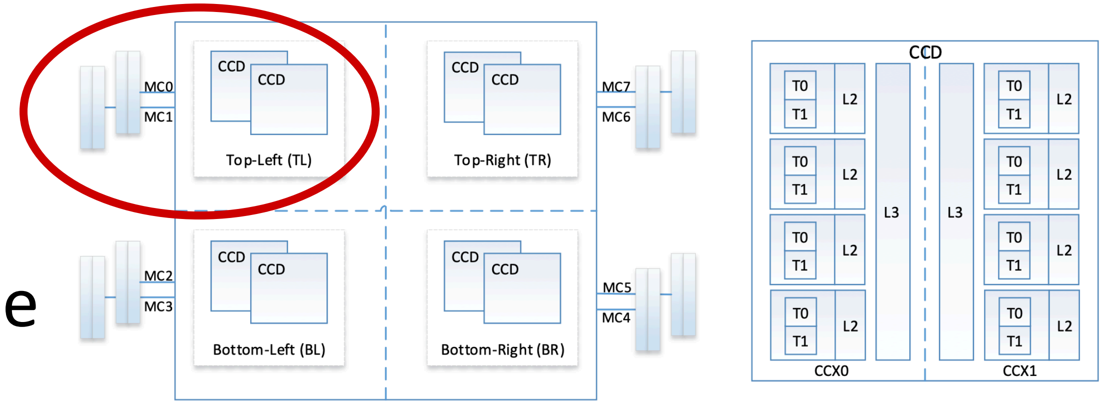
```
#!/bin/bash
#SBATCH --job-name="hellompi"
#SBATCH --output="hellompi.%j.%N.out"
#SBATCH --partition=compute
#SBATCH --nodes=2
#SBATCH --ntasks-per-node=128
#SBATCH --mem-per-cpu=1800M
#SBATCH --account=XYZ123
#SBATCH --export=ALL
#SBATCH -t 00:10:00

#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
```

Example batch script: OpenMP Job
(/cm/shared/examples/sdsc/openmp)

```
#!/bin/bash
#SBATCH --job-name="hell_openmp_shared"
#SBATCH --output="hello_openmp_shared.%j.%N.out"
#SBATCH --partition=shared
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=1
#SBATCH --cpus-per-task=16
#SBATCH --mem=32G
#SBATCH --export=ALL
#SBATCH -t 01:30:00

# AOCC environment

module purge
module load slurm
module load cpu
module load aocc

#SET the number of openmp threads
export OMP_NUM_THREADS=16

#Run the openmp job
./hello_openmp
```

For Hybrid MPI/OpenMP jobs: recall NPS4 Configuration

- The processor is partitioned into four NUMA domains.
- Each logical quadrant is a NUMA domain.
- Memory is interleaved across the two memory channels
- PCIe devices will be local to one of four NUMA domains (the IO die that has the PCIe root for the device)
- ***Important to keep NUMA architecture in mind. Specifically for hybrid MPI/OpenMP jobs.***



https://developer.amd.com/wp-content/resources/56338_1.00_pub.pdf

Example batch script: Hybrid MPI/OpenMP Job

/cm/shared/examples/sdsc/mpi-openmp-hybrid

```
#!/bin/bash
#SBATCH --job-name="hellohybrid"
#SBATCH --output="hellohybrid.%j.%N.out"
#SBATCH --partition=shared
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=2
#SBATCH --cpus-per-task=16
#SBATCH --account=XYZ123
#SBATCH --export=ALL
#SBATCH -t 01:30:00

#Environment
module purge
module load slurm
module load cpu
module load intel
module load intel-mpi

#Run
export OMP_NUM_THREADS=16
mpirun -genv I_MPI_PIN_DOMAIN=omp:compact ./hello_hybrid
```

Example batch script: Hybrid MPI/OpenMP Job

```
#! /bin/bash
#SBATCH --job-name="hpl-2node"
#SBATCH -o hpl.%j.out
#SBATCH -e hpl.%j.err
#SBATCH --partition=compute
#SBATCH --nodes=2
#SBATCH --ntasks-per-node=32
#SBATCH --cpus-per-task=4
#SBATCH --mem-per-cpu=1800M
#SBATCH -A use300
#SBATCH --export=ALL
#SBATCH -t 10:00:00
module purge
module load cpu
module load slurm
module load aocc
module load openmpi
XHPL=xhpl
mpirun -x OMP_NUM_THREADS  --mca pml ucx --mca osc ucx  --map-by l3cache ./xhpl
```

Example batch script: OpenACC job on GPU nodes

```
#!/bin/bash
#SBATCH --job-name="OpenACC"
#SBATCH --output="OpenACC.%j.%N.out"
#SBATCH --partition=gpu-shared
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=1
#SBATCH --account=XYZ123
#SBATCH --gpus=1
#SBATCH -t 01:00:00


#Environment
module purge
module load slurm
module load gpu
module load pgi


#Run the job
./laplace2d.openacc.exe
```

Example batch script: Multi-node GPU job

```
#!/bin/bash
#SBATCH --job-name="test"
#SBATCH -o test.%j.out
#SBATCH --qos=gpu-unlim
#SBATCH -e test.%j.err
#SBATCH --partition=gpu
#SBATCH --nodes=4
#SBATCH --ntasks-per-node=4
#SBATCH --cpus-per-task=10
#SBATCH --mem=370G
#SBATCH --gpus=16
#SBATCH --export=None
#SBATCH -t 04:00:00

## Modules
module purge
module load gpu
module load slurm
module load intel
module load openmpi
module load cuda10.2/toolkit

srun --mpi=pmi2 -n 180 --cpus-per-task=10 $HPL_DIR/bin/CUDA/xhpl
```

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Home File System

- After logging in, users are placed in their home directory, /home, also referenced by the environment variable $HOME.
- The home directory is limited in space and should be used only for source code, binaries, and small input files.
- Users will have a quota of 100GB in /home.
- Do **not** run jobs doing intensive IO to/from the home file system, as it is not set up for high performance throughput. Job scripts should use Lustre or local scratch for IO.

Parallel Lustre Filesystems

- Global parallel filesystem:
  - 12 PB Lustre parallel file system
  - 140 GB/second performance

- Two Lustre filesystems locations on Expanse (both are part of the *same* filesystem):
  - Lustre scratch location: /expanse/lustre/scratch/$USER (purged for files older than 90 days based on create date)
  - Lustre projects location: /expanse/lustre/projects/groupid/$USER (usage tracked to comply with group allocation).

- SDSC limits the number of files that can be stored in /lustre/scratch filesystem to 2 million files per user.

- Users should contact user support for assistance at help@xsede.org, if their workflow requires extensive small I/O, to avoid causing system issues associated with load on the metadata server.

Node local NVMe based scratch filesystem

- All Expanse nodes feature NVMe based local scratch storage. The disk sizes vary based on then nodes:
  - Regular compute nodes: 1TB (~900 GB usable)
  - Large memory nodes: 3.2TB (~2.9TB usable)
  - GPU nodes: 1.6TB (~1.4TB usable)
- NVMe based storge is excellent for IOPs intensive workloads. Also can be useful for scratch files (small and large) generated on a per task basis.
- Users can access the SSDs only during job execution under the following directories local to each compute node:

  /scratch/$USER/job_$SLURM_JOBID
- The location is *purged* at the end of a job so any important data must be copied out.

Example batch script: local scratch usage (Gaussian application)

```
#!/bin/bash
#SBATCH --job-name="gaussian"
#SBATCH --output="gaussian.%j.%N.out"
#SBATCH --partition=shared
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=1
#SBATCH --cpus-per-task=32
#SBATCH --account=XYZ123
#SBATCH --export=ALL
#SBATCH -t 00:10:00

module purge
module load cpu
module load gaussian/16.C.01
exe=`which g16`
export GAUSS_SCRDIR=/scratch/$USER/job_$SLURM_JOBID

filename=water_opt_32c.dat
bash ./getcpusets $$
cat $$.out $filename >file.tmp.$$
/usr/bin/time $exe < file.tmp.$$ > $filename.out
rm -f $$.out file.tmp.$$
```

Summary

- Expanse uses SLURM for scheduling jobs.
- All jobs on Expanse must be run via the scheduler. *Do not run on the login nodes.*
- Expanse supports both node exclusive (“compute”, “gpu”, “preempt”) and shared partitions (“shared”, “large-shared”, “gpu-shared”,”debug”,”gpu-debug”).
- Account information is required in job scripts (no default unlike Comet).
- Filesystem options – Lustre parallel filesystem, NVMe based node local scratch filesystem.
- **Early access period ongoing**. *Production November, 2020*.
- Follow all things Expanse at https://expanse.sdsc.edu !