SDSC HPC/CI User Training 2022

HPC/CI Basic Concepts: Job Submission on Expanse

EXPANSE

COMPUTING WITHOUT BOUNDARIES

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SAN DIEGO SUPERCOMPUTER CENTER

NSF Award 1928224

SDSC SAN DIEGO SUPERCOMPUTER CENTER

UC San Diego

Outline

- **Introduction**
- Compiling and Linking Code
- Running Jobs
- Additional Examples
  - CPU Jobs
  - GPU/CUDA Jobs
- Final Comments

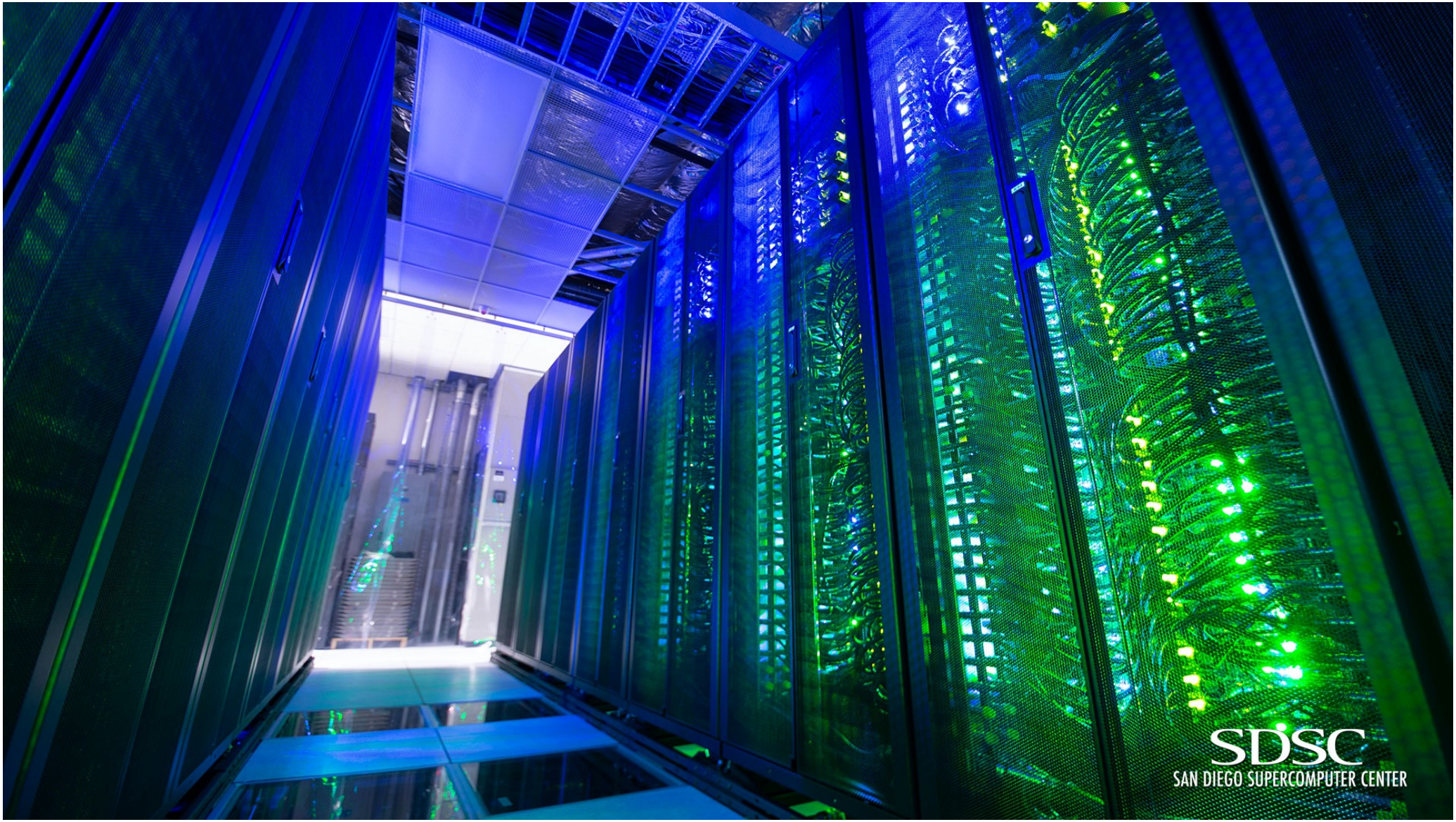
Basic Information

- 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
  - 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/

Expanse

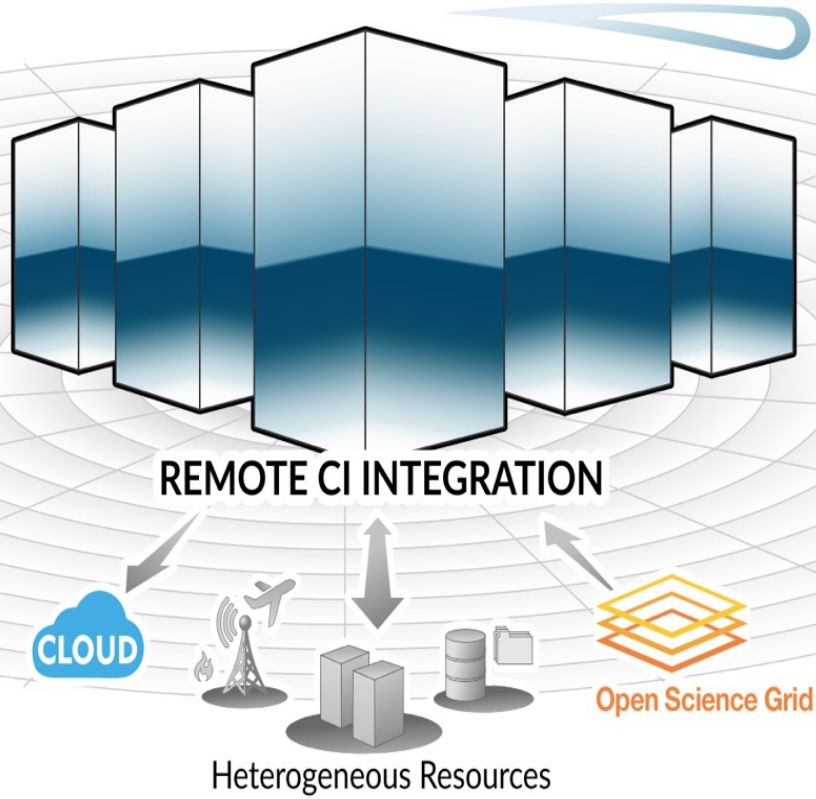


EXPANSE

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

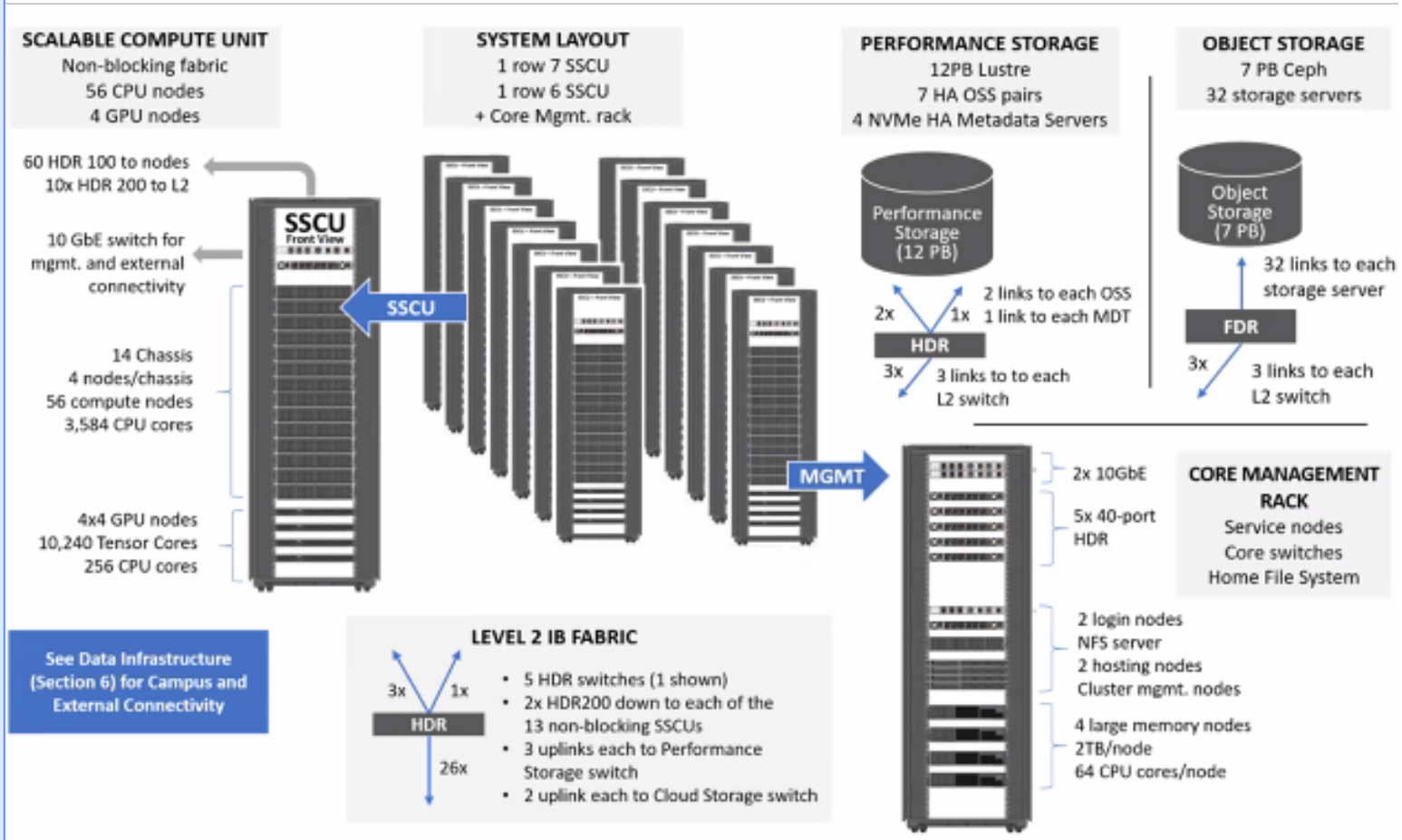
INNOVATIVE OPERATIONS
Composable Systems
High-Throughput Computing
Science Gateways
Interactive Computing
Containerized Computing
Cloud Bursting

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 Heterogeneous Architecture

System Summary

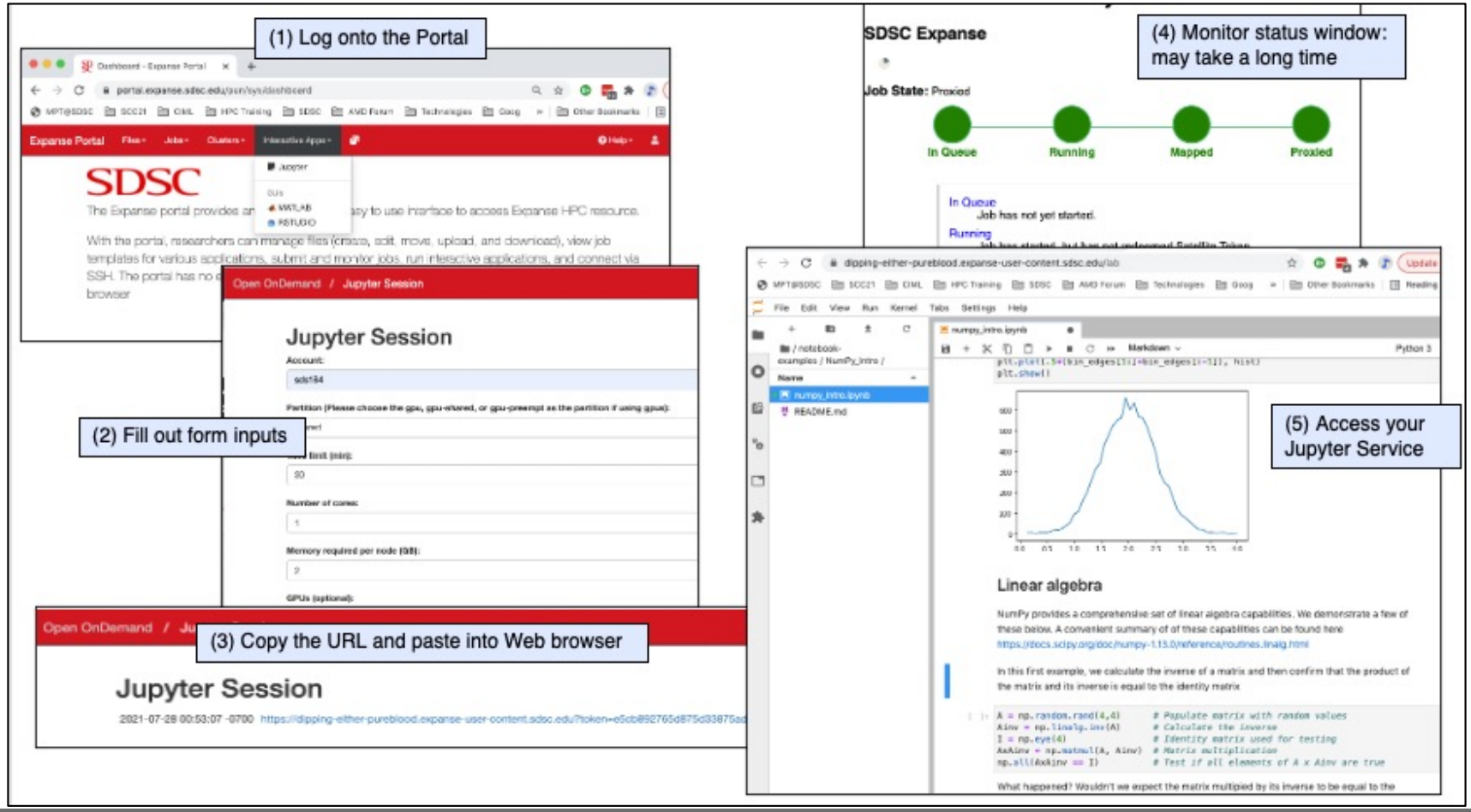
- *13 SDSC Scalable Compute Units (SSCU)*
- *728 x 2s Standard Compute Nodes*
- *93,184 Compute Cores*
- *200 TB DDR4 Memory*
- *52x 4-way GPU Nodes w/NVLINK*
- *208 V100s*
- *4x 2TB Large Memory Nodes*
- *HDR 100 non-blocking Fabric*
- *12 PB Lustre High Performance*
- *Storage*
- *7 PB Ceph Object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



Outline

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- Running Jobs
- Additional Examples
  - CPU Jobs
  - GPU/CUDA Jobs
- Final Comments

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.

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

Using the AOCC Compilers

- If you have modified your environment, you can change your environment by swapping modules or executing the module purge & load commands at the Linux prompt
- Place the load commands in your startup file (~/.cshrc or ~/.bashrc) or batch script

```
[username@login02 ~]$ module list
Currently Loaded Modules:
  1) shared   2) cpu/1.0   3) DefaultModules   4) hdf5/1.10.1   5) intel/ 19.1.1.217
## need to change multiple modules
[username@login02 ~]$ module purge
[username@login02 ~]$ module list
No modules loaded
[username@login02 ~]$ module load slurm
[username@login02 ~]$ module load cpu
[username@login02 ~]$ module load aocc
[username@login02 ~]$ module load openmpi/4.0.4
[username@login02 ~]$ module list
Currently Loaded Modules:
  1) slurm/expanse/20.02.3   2) cpu/1.0   3) aocc/2.2.0   4) openmpi/4.0.4
[username@login02 MPI]$ module swap intel aocc
Due to MODULEPATH changes, the following have been reloaded:
  1) openmpi/4.0.4
[username@login02 ~]$ module list
Currently Loaded Modules:
  1) slurm/expanse/20.02.3   2) cpu/1.0   3) aocc/2.2.0   4) openmpi/4.0.4
[username@login02 ~]$
```

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

The Intel compilers and the MVAPICH2 MPI compiler wrappers can be loaded by executing the following commands at the Linux prompt:

$module load intel mvapich2

For more information on the Intel compilers:

$[ifort | icc | icpc] -help

Using the Intel Compilers

- If you have modified your environment, you can change your environment by swapping modules or executing the module purge & load commands at the Linux prompt
- Place the load commands in your startup file (~/.cshrc or ~/.bashrc) or batch script

```
[username@login02 ~]$ module list
[username@login02 MPI]$ module list
Currently Loaded Modules:
  1) slurm/expanse/20.02.3   2) cpu/1.0   3) aocc/2.2.0   4) openmpi/4.0.4
[username@login02 ~]$ module purge
[username@login02 ~]$ module list
No modules loaded
[username@login02 ~]$ module load slurm
[username@login02 ~]$ module load cpu
[username@login02 ~]$ module load intel
[username@login02 ~]$ module load openmpi/4.0.4
[username@login02 ~]$ module list
Currently Loaded Modules:
  1) slurm/expanse/20.02.3   2) cpu/1.0   3) aocc/2.2.0   4) openmpi/4.0.4
[username@login02 ~]$
```

```
[username@login02 MPI]$ module list
Currently Loaded Modules:
  1) slurm/expanse/20.02.3   2) cpu/1.0   3) aocc/2.2.0   4) openmpi/4.0.4
[username@login02 ~]$ module swap aocc intel
Due to MODULEPATH changes, the following have been reloaded:
  1) openmpi/4.0.4
[username@login02 ~]$ module list
Currently Loaded Modules:
  1) slurm/expanse/20.02.3   2) cpu/0.15.4   3) intel/19.1.1.217   4) openmpi/4.0.4
[username@login02 ~]$ [username@login02 ~]$ which mpirun
/cm/shared/apps/spack/cpu/opt/spack/linux-centos8-zen2/intel-19.1.1.217/openmpi-
4.0.4-f5mc6sg2jtrw7qqdksf6tru4vo4tawrv/bin/mpirun
```

Accessing Intel Compiler Features

- Advanced Vector Extensions (AVX2): to enable AVX2 support
  - compile with the `-march=core-avx2` option.
  - https://en.wikipedia.org/wiki/Advanced_Vector_Extensions (128/256bit SIMD, Vector ops (MPI broadcast, gather, …)
  - Note that -march=core-avx2 alone does not enable aggressive optimization, so compilation with -O3 is also suggested.

- Intel Math Kernal Lib (MKL) libraries are available as part of the "intel" modules on Expanse.
  - Once this module is loaded, the environment variable INTEL_MKLHOME points to the location of the mkl libraries and
  - Use MKL Link Advisor to see what libraries are recommended for your compiler and system configuration:
  - https://software.intel.com/content/www/us/en/develop/articles/intel-mkl-link-line-advisor.html

PGI Compilers

- PGI (formerly The Portland Group, Inc.), was a company that produced a set of commercially available Fortran, C and C++ compilers for high-performance computing systems.
- It is now owned by NVIDIA.
- To compile code, you need to obtain an interactive node.
- For AVX support, compile with -fast

	Serial	MPI	OpenMP	MPI+OpenMP
Fortran	pgf90	mpif90	pgf90 -mp	mpif90 -mp
C	pgcc	mpicc	pgcc -mp	mpicc -mp
C++	pgCC	mpicxx	pgCC -mp	mpicxx -mp

- For more information on the PGI compilers run:

$ man [pgf90 | pgcc | pgCC]

PGI Compilers: GPU Only

```
[username@login02 ~]$ module reset
[username@login02 ~]$ module load gpu
[username@login02 ~]$ module load pgi
[username@login02 ~]$
[username@login02 ~]$ which pgcc
/cm/shared/apps/spack/gpu/opt/spack/linux-centos8-skylake_avx512/gcc-8.3.1/pgi-20.4-
2tsjnv2icisxmgdy4mijl4t5mkbr32ea/linux86-64/20.4/bin/pgcc
[username@login02 ~]$ which mpicc
/cm/shared/apps/spack/gpu/opt/spack/linux-centos8-skylake_avx512/gcc-8.3.1/pgi-20.4-
2tsjnv2icisxmgdy4mijl4t5mkbr32ea/linux86-64/20.4/mpi/openmpi-3.1.3/bin/mpicc
```

PGI supports the following high-level languages:

- Fortran 77, 90/95/2003, 2008 (partial)
- High Performance Fortran (HPF)
- ANSI C99 with K&R extensions
- ANSI/ISO C++
- CUDA Fortran
- OpenCL
- OpenACC
- OpenMP

GNU Compilers: CPU & GPU

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

- For AVX support, compile with -mavx.
- AVX support only available in version 4.7 or later --> explicitly load the gnu/4.9.2 module
- For more information on the GNU compilers:

    $*man [gfortran | gcc | g++]*

GNU Compilers

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

```
[username@login02]$ module purge
[username@login02]$ module load slurm
[username@login02]$ module load cpu
[username@login02]$ module load gcc/10.2.0
[username@login02]$ module load openmpi/4.0.4
[username@login02]$ 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
```

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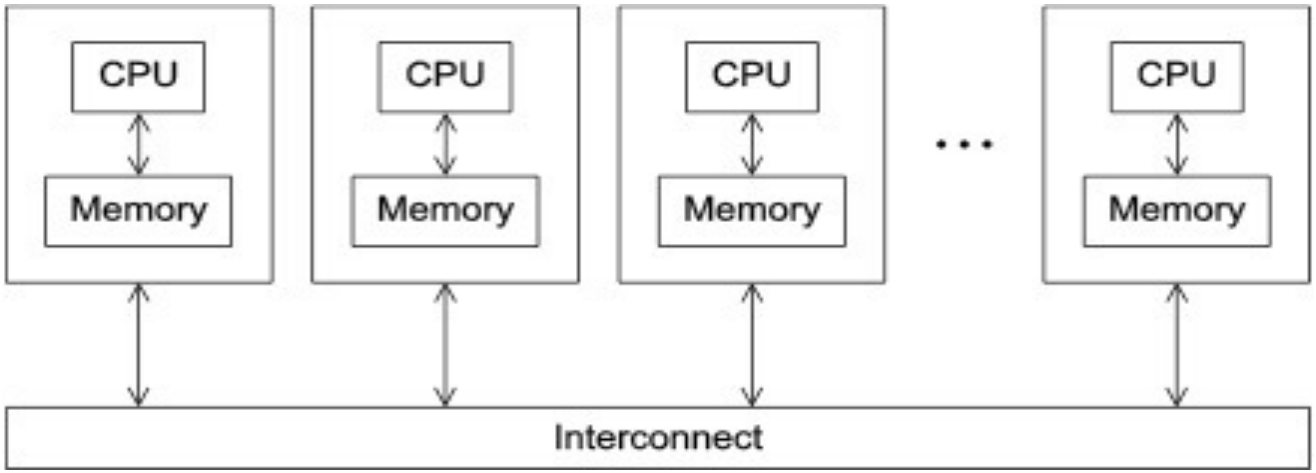
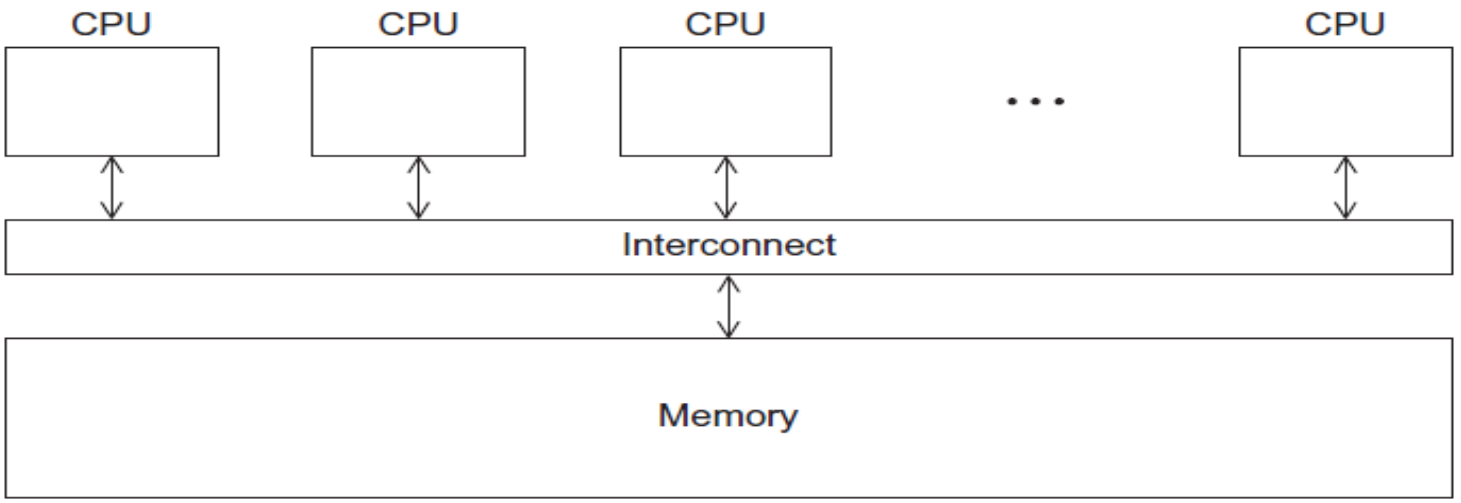
Parallel Models: Distributed Memory



- Programs that run asynchronously, pass messages for communication and coordination between resources.
- Examples include: SOA-based systems, massively multiplayer online games, peer-to-peer apps.
- Different types of implementations for the message passing mechanism: HTTP, RPC-like connectors, message queues
- HPC historically uses the Message Passing Interface (MPI)

Parallel Models: Shared Memory



- CPUs all share same localized memory (SHMEM);
  - Coordination and communication between tasks via interprocessor communication (IPC) or virtual memory mappings.
- May use: uniform or non-uniform memory access (UMA or NUMA); cache-only memory architecture (COMA).
- Most common HPC API's for using SHMEM:
  - Portable Operating System Interface (POSIX); Open Multi-Processing (OpenMP) designed for parallel computing – best for multi-core computing.

Running Jobs on Expanse

A few observations:

- 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 Runing Jobs on Expanse

- **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

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

- **Interactive Jobs:** Use the *srun* command to request 'live' nodes from Slurm for 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
    ```

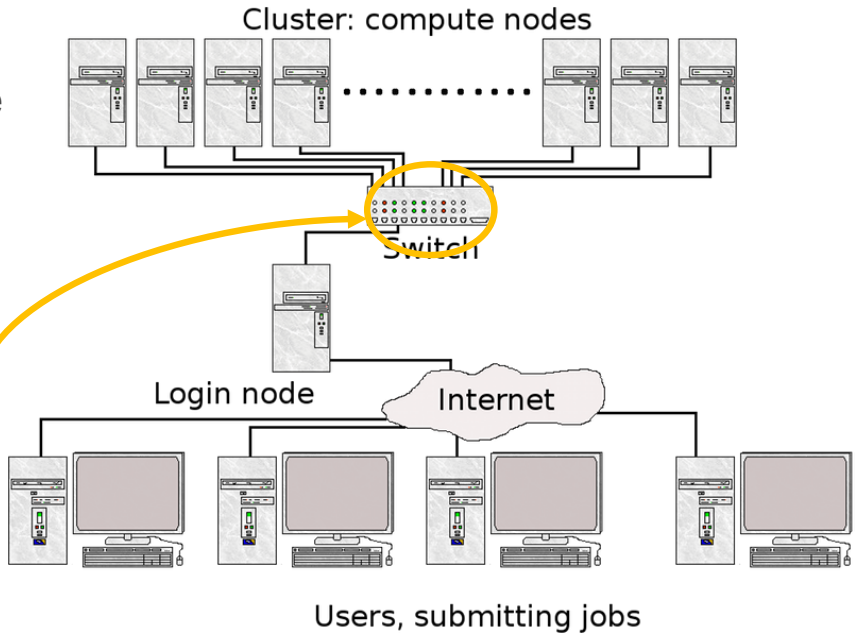
  - GPU:

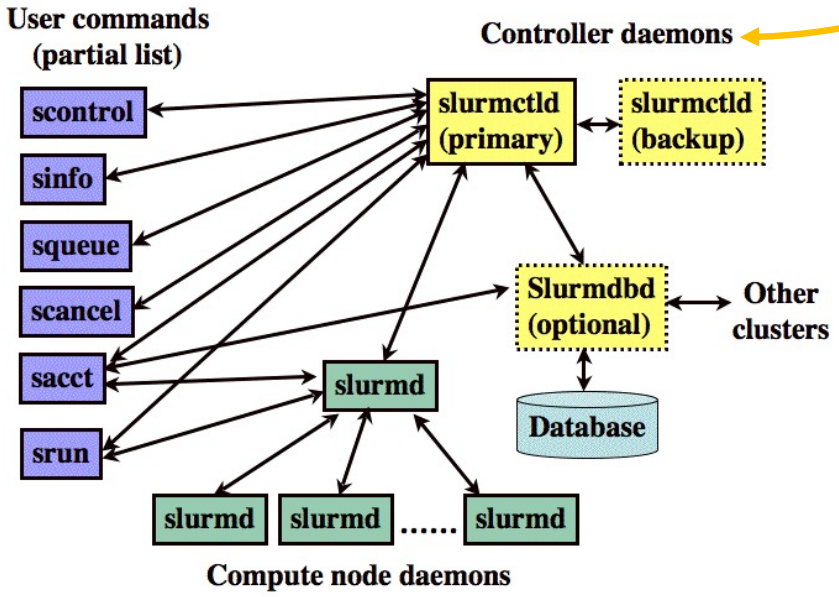
    ```
    srun  --pty --account=XYZ123 --nodes=1  --ntasks-per-node=1  --cpus-per-task=10  -p gpu-debug  --gpus=1  -t 00:10:00 /bin/bash
    ```

Slurm Resource Manager

Simple Linux Utility for Resource Management

- "Glue" for parallel computer to schedule and execute jobs
- Role: Allocate resources within a cluster
  - Nodes (unique IP address)
  - Interconnect/switches
  - Generic resources (e.g. GPUs)
  - Launch and otherwise manage jobs





- Functionality:
  - Prioritize queue(s) of jobs;
  - decide when and where to start jobs;
  - terminate job when done;
  - Appropriate resources;
  - manage accounts for jobs

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, monitor it's state:

  $ 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

https://slurm.schedmd.com/sbatch.html

Slurm Partitions on Expanse

https://www.sdsc.edu/support/user_guides/expanse.html#running

Partition Name	Max Walltime	Max Nodes/Job	Max Running Jobs	Max Running + Queued Jobs	Charge Factor	Notes
compute	48 hrs	32	32	64	1	Used for exclusive access to regular compute nodes; *limit applies per group*
shared	48 hrs	1	4096	4096	1	Single-node jobs using fewer than 128 cores
gpu	48 hrs	4	4	8 (32 Tres GPU)	1	Used for exclusive access to the GPU nodes
gpu-shared	48 hrs	1	24	24 (24 Tres GPU)	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	30 min	2	1	2	1	Priority access to shared nodes set aside for testing of jobs with short walltime and limited resources
gpu-debug	30 min	2	1	2	1	Priority access to gpu-shared nodes set aside for testing of jobs with short walltime and limited resources; *max two gpus per job*
preempt	7 days	32		128	.8	Non-refundable discounted jobs to run on free nodes that can be pre-empted by jobs submitted to any other queue
gpu-preempt	7 days	1		24 (24 Tres GPU)	.8	Non-refundable discounted jobs to run on unallocated nodes that can be pre-empted by higher priority queues

Last updated 9/14/21

https://slurm.schedmd.com/sbatch.html

Example Batch Script

```
[uswername@login02 calc-prime]$ cat mpi-prime-slurm.sb
#!/bin/bash
#SBATCH --job-name="mpi_prime"
#SBATCH --output="mpi_prime.%j.%N.out"
####SBATCH --partition=compute
#SBATCH --partition=debug
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=24
#SBATCH --export=ALL
#SBATCH -t 00:10:00
#SBATCH -A use300

#This job runs with 1 node, 24 cores per node for a total of 24 cores.
## Environment
module purge
module load slurm
module load cpu
module load gcc/10.2.0
module load openmpi/4.0.4

## echo job name and id:
echo "SLURM_JOB_NAME:  $SLURM_JOB_NAME"
echo "SLURM_JOB_ID:    $SLURM_JOB_ID"
d=`date`
echo "DATE:  $d"

## Use srun to run the job, pass variable to code
srun --mpi=pmi2 -n 24 --cpu-bind=rank ./mpi_prime
```

Simple batch script showing environment, date, etc.

```
[mthomas@login02 calc-prime]$ sbatch --export=NLO=1000 mpi-prime-slurm.sb
Submitted batch job 9113467
[mthomas@login02 calc-prime]$ !sq
squeue -u mthomas
             JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON
           9113467     debug mpi_prim  mthomas  R       0:04      1 exp-9-55
```

Output: mpi-prime

```
28 January 2022 12:21:30 PM
PRIME_MPI
 n_hi= 262144
  C/MPI version
  An MPI example program to count the number of primes.
  The number of processes is 24

         N        Pi          Time
         1         0      0.025196
         2         1      0.001954
         4         2      0.024015
         8         4      0.025980
        16         6      0.025996
        32        11      0.026022
        64        18      0.025977
       128        31      0.025999
       256        54      0.025999
       512        97      0.026009
      1024       172      0.013043
      2048       309      0.012683
      4096       564      0.028262
      8192      1028      0.025999
     16384      1900      0.025998
     32768      3512      0.041243
     65536      6542      0.213824
    131072     12251      0.676576
    262144     23000      1.570949


PRIME_MPI - Master process:    Normal end of execution.
```

SLURM Environment Variables

https://slurm.schedmd.com/sbatch.html#lbAJ

Internal ENV vars that exist when job submitted:

INPUT ENVIRONMENT VARS

https://slurm.schedmd.com/sbatch.html#lbAJ

- Upon startup, sbatch will read and handle the options set in the following environment variables.
- SBATCH_JOB_NAME
  - Same as -J, --job-name
- SBATCH_ACCOUNT
  - Same as -A, --account
- SBATCH_TIMELIMIT
  - Same as -t, --time

OUTPUT ENVIRONMENT VARS

https://slurm.schedmd.com/sbatch.html#lbAK

- The Slurm controller will set the following variables in the environment of the batch script.
- SLURM_EXPORT_ENV
  - Same as --export.
- SLURM_JOB_ID
  - The ID of the job allocation.
- SLURM_JOB_NAME
  - Name of the job.

Passing values into the batch script

- Passing variables into a SLURM job when you submit the job
- Use the --export flag.
- Examples
  - pass the value of two variables x and B into the job script named jobscript.sbatch:
    - sbatch --export=x=7,B='mystring' jobscript.sb
  - OR: sbatch --export=ALL,x=7,B= mystring ' jobscript.sbatch
- The first example will replace the user's environment with a new environment containing only values for x and B and the SLURM_* environment variables. The second will add the values for A and b to the existing environment.
-

Example: Passing Vars to Batch Script

```
[uswername@login02 calc-prime]$ cat mpi-prime-slurm.sb
#!/bin/bash
#SBATCH --job-name="mpi_prime"
#SBATCH --output="mpi_prime.%j.%N.out"
####SBATCH --partition=compute
#SBATCH --partition=debug
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=24
#SBATCH --export=ALL
#SBATCH -t 00:10:00
#SBATCH -A use300

#This job runs with 1 node, 24 cores per node for a total of 24 cores.
## Environment
module purge
module load slurm
module load cpu
module load gcc/10.2.0
module load openmpi/4.0.4

## echo job name and id:
echo "SLURM_JOB_NAME:  $SLURM_JOB_NAME"
echo "SLURM_JOB_ID:    $SLURM_JOB_ID"
d=`date`
echo "DATE:  $d"
echo "Var NLO:  $NLO"

## Use srun to run the job, pass variable to code
srun --mpi=pmi2 -n 24 --cpu-bind=rank ./mpi_prime Y
```

Batch script showing environment, date, and passing variable

```
[mthomas@login02 calc-prime]$ sbatch --export=NLO=1000 mpi-prime-slu
Submitted batch job 9113467
[mthomas@login02 calc-prime]$ !sq
squeue -u mthomas
             JOBID PARTITION     NAME     USER ST       TIME  NODES NOD
           9113467     debug mpi_prim  mthomas  R       0:04      1 exp-9-55
```

What is Interactive HPC-Computing

- In **computer** science, **interactive computing** refers to software which accepts input from the user as it runs.
  - commonly used programs, such as word processors or spreadsheet applications.
- **Interactive HPC computing** involves *real-time* user inputs to perform tasks on a set of compute node(s) including:
  - Code development, real-time data exploration, and visualizations.
  - Used when applications have large data sets or are too large to download to local device, software is difficult install, etc.
  - User inputs come via command line interface or application GUI (Jupyter Notebooks, Matlab, R-studio).
  - Actions performed on remote compute nodes as a result of user input or program out.
- Expanse supports running applications via command line and Web-based services (Jupyter Notebooks, Matlab, R-studio)

Running Interactive Jobs - CPU

Obtaining an interactive CPU node with 1 node, 128 cores, and 249GB:

```
[username@login01 ~]$ srun --partition=debug --account=abc123 --pty --nodes=1 --ntasks-per-node=128
--mem=248 -t 00:30:00 --wait=0 --export=ALL /bin/bash
srun: job 5825986 queued and waiting for resources
srun: job 5825986 has been allocated resources
[username@exp-9-55 ~]$ hostname
exp-9-55
[username @exp-9-55 ~]$

[username@exp-9-55 ~]$ module list
Currently Loaded Modules:
  1) slurm/expanse/20.02.3   2) cpu/0.15.4   3) intel/19.1.1.217   4) openmpi/4.0.4
[username@exp-9-55 ~]$ module purge
modul[username@exp-9-55 ~]$ module restore
Restoring modules from user's default
[username @exp-9-55 ~]$ module list
Currently Loaded Modules:
  1) cpu/0.15.4   2) slurm/expanse/20.02.3   3) intel/19.1.1.217
[username @exp-9-55 ~]$ exit
[username@login01 ~]$
```

Running Interactive Jobs - GPU

The following example will request a GPU node, 10 cores, 1 GPU and 96G in the debug partition for 30 minutes. To ensure the GPU environment is properly loaded, please be sure run both the module purge and module restore commands.

```
[username@login02 ~]$ srun --partition=gpu-debug --pty --account=abc123 --ntasks-per-node=10
--nodes=1 --mem=96G --gpus=1 -t 00:30:00 --wait=0 --export=ALL /bin/bash
srun: job 5826039 queued and waiting for resources
srun: job 5826039 has been allocated resources
[username@exp-7-59 ~]$
[username@exp-7-59 ~]$ hostname
exp-7-59
[username@exp-7-59 ~]$ module purge
[username@exp-7-59 ~]$ module restore
Restoring modules from user's default
[username@exp-7-59 ~]$
```

```
[username@exp-7-59 ~]$ nvidia-smi
Thu Sep 16 00:09:41 2021
+-----------------------------------------------------------------------------+
| NVIDIA-SMI 460.32.03    Driver Version: 460.32.03    CUDA Version: 11.2     |
|-------------------------------+----------------------+----------------------+
| GPU  Name        Persistence-M| Bus-Id        Disp.A | Volatile Uncorr. ECC |
| Fan  Temp  Perf  Pwr:Usage/Cap|         Memory-Usage | GPU-Util  Compute M. |
|                               |                      |               MIG M. |
|===============================+======================+======================|
|   0  Tesla V100-SXM2...  On   | 00000000:18:00.0 Off |                    0 |
| N/A   32C    P0    41W / 300W |      0MiB / 32510MiB |      0%      Default |
|                               |                      |                  N/A |
+-------------------------------+----------------------+----------------------+

+-----------------------------------------------------------------------------+
| Processes:                                                                  |
|  GPU   GI   CI        PID   Type   Process name                  GPU Memory |
|        ID   ID                                                   Usage      |
|=============================================================================|
```

Outline

- **Introduction**
- Compiling and Linking Code
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  - GPU/CUDA Jobs
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Additional Examples

- Clone examples:
  - https://github.com/sdsc-hpc-training-org/expanse-101
- CPU Jobs
- GPU Jobs

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 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

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MPI Hello World

- Change to the MPI examples directory:

```
[username@login02 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
[username@login02 MPI]$
```

MPI Hello World: Compile

Set the environment and then compile the code

```
[username@login02 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 --account=sds184 --pty --nodes=1 --ntasks-per-
node=128 --mem=248 -t 00:30:00 --wait=0 --export=ALL /bin/bash
```

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

Currently Loaded Modules:
  1) cpu/1.0   2) slurm/expanse/20.02.3

[username@login02 MPI]$ module purge
[username@login02 MPI]$ module load slurm
[username@login02 MPI]$ module load cpu
[username@login02 MPI]$ module load gcc/10.2.0
[username@login02 MPI]$ module load openmpi/4.0.4
[username@login02 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

[username@login02 MPI]$ mpif90 -o hello_mpi hello_mpi.f90
[username@login02 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.

```
[username@login02 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 –A abc123
#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

[username@login02 MPI]$
```

```
[username@login02 MPI]$ sbatch hellompi-slurm-gnu.sb; squeue -u username
Submitted batch job 108910
             JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
            108910   compute hellompi  username PD       0:00      2 (None)
[username@login02 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

```
[username@login02 MPI]$ srun --partition=debug --account=s                    des=1 --ntasks-per-node=128 --
mem=248 -t 00:30:00 --wait=0 --export=ALL /bin/bash
[username@exp-9-55 MPI]$
[username@ exp-9-55 MPI]$ module purge
[username@ exp-9-55 MPI]$ module load slurm
[username@ exp-9-55 MPI]$ module load cpu
[username@ exp-9-55 MPI]$ module load gcc/10.2.0
[username@ exp-9-55 MPI]$ module load openmpi/4.0.4
```

Request interactive node for 30 minutes

```
[username@exp-9-55 MPI]$ mpif90 -o hello_mpi_f_gnu hello_mpi.f90
[username@exp-9-55 MPI]$ mpirun -np 8 ./hello_mpi_f_gnu
 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 GPU Hardware

GPU Nodes	
GPU Type	NVIDIA V100 SMX2
Nodes	52
GPUs/node	4
CPU Type	Xeon Gold 6248
Cores/socket	20
Sockets	2
Clock speed	2.5 GHz
Flop speed	34.4 TFlop/s
Memory capacity	*384 GB DDR4 DRAM
Local Storage	1.6TB Samsung PM1745b NVMe PCIe SSD
Max CPU Memory bandwidth	281.6 GB/s

Using GPU Nodes

- GPU nodes are allocated as a separate resource.
- Login nodes are not the same as the GPU nodes:

  → GPU codes must be compiled by requesting an interactive session on a GPU node.
- Batch: GPU nodes can be accessed via either the "gpu" or the "gpu-shared" partitions.
  - #SBATCH -p gpu
  - or #SBATCH -p gpu-shared
- Interactive GPU node:
  - srun --partition=gpu-debug --pty --account=abc123 --nodes=1 --ntasks-per-node=1 --cpus-per-task=10 --gpus=1 -t 00:10:00 /bin/bash

GPU/CUDA: Interactive Node

- Change to the OpenACC directory

```
[username@exp-7-59 OpenACC]$ ll
total 71
-rw-r--r-- 1 username abc123  2136 Oct  7 11:28 laplace2d.c
-rwxr-xr-x 1 username abc123 52056 Oct  7 11:28 laplace2d.openacc.exe
-rw-r--r-- 1 username abc123   234 Oct  7 11:28 OpenACC.108739.exp-7-57.out
-rw-r--r-- 1 username abc123   307 Oct  8 00:21 openacc-gpu-shared.sb
-rw-r--r-- 1 username abc123  1634 Oct  7 11:28 README.txt
-rw-r--r-- 1 username abc123  1572 Oct  7 11:28 timer.h
```

- Obtain an interactive node:

```
[username@login02 OpenACC]$ srun   --pty   --nodes=1   --ntasks-per-node=1   --
cpus-per-task=10   -p gpu-debug  --gpus=1  -t 00:10:00 /bin/bash
```

GPU/CUDA: Node Information

Check node configuration:

```
[username@exp-7-59 OpenACC]$ nvidia-smi
Thu Oct  8 03:58:44 2020
+-----------------------------------------------------------------------------+
| NVIDIA-SMI 450.51.05    Driver Version: 450.51.05    CUDA Version: 11.0     |
|-------------------------------+----------------------+----------------------+
| GPU  Name        Persistence-M| Bus-Id        Disp.A | Volatile Uncorr. ECC |
| Fan  Temp  Perf  Pwr:Usage/Cap|         Memory-Usage | GPU-Util  Compute M. |
|                               |                      |               MIG M. |
|===============================+======================+======================|
|   0  Tesla V100-SXM2...  On   | 00000000:18:00.0 Off |                    0 |
| N/A   32C    P0    41W / 300W |      0MiB / 32510MiB |      0%      Default |
|                               |                      |                  N/A |
+-------------------------------+----------------------+----------------------+

+-----------------------------------------------------------------------------+
| Processes:                                                                  |
|  GPU   GI   CI        PID   Type   Process name                  GPU Memory |
|        ID   ID                                                   Usage      |
|=============================================================================|
|  No running processes found                                                 |
+-----------------------------------------------------------------------------+
[username@exp-7-59 OpenACC]$
```

GPU: Compile on Interactive node

```
[username@login02 OpenACC]$
cat README.txt
[1] Compile Code:
(a) Get an interactive GPU debug node:
module load slurm
srun --partition=gpu-debug  --pty --account=abc123 --nodes=1   --ntasks-per-node=1   --cpus-per-task=10   --gpus=1  -t
00:10:00 /bin/bash
(b) On the GPU node:
module purge
module load slurm
module load gpu
module load pgi
pgcc -o laplace2d.openacc.exe -fast -Minfo -acc -ta=tesla:cc70 laplace2d.c

Compiler output:
GetTimer:
     20, include "timer.h"
          61, FMA (fused multiply-add) instruction(s) generated
laplace:
     47, Loop not fused: function call before adjacent loop
         Loop unrolled 8 times
         FMA (fused multiply-add) instruction(s) generated
     55, StartTimer inlined, size=2 (inline) file laplace2d.c (37)
[SNIP]
          75, #pragma acc loop gang, vector(4) /* blockIdx.y threadIdx.y */
         77, #pragma acc loop gang, vector(32) /* blockIdx.x threadIdx.x */
     88, GetTimer inlined, size=9 (inline) file laplace2d.c (54)
(Exit out of debug node after this)

[2] Run job:
sbatch openacc-gpu-shared.sb
```

GPU: Submit Batch Script on CPU node

```
[username@login02 OpenACC]$ cat openacc-gpu-shared.sb
#!/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 --gpus=1
#SBATCH –A abc123
#SBATCH -t 01:00:00

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

#Run the job
./laplace2d.openacc.exe

[username@login02 OpenACC]$ sbatch openacc-gpu-shared.sb
[username@login02 OpenACC]$ sbatch openacc-gpu-shared.sb ; squeue -u username
Submitted batch job 108915
             JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
            108915 gpu-share  OpenACC  username PD       0:00      1 (None)
```

```
[username@login02 OpenACC]$ cat OpenACC.108915.exp-7-57.out
main()
Jacobi relaxation Calculation: 4096 x 4096 mesh
    0, 0.250000
  100, 0.002397
  200, 0.001204
  300, 0.000804
  400, 0.000603
  500, 0.000483
  600, 0.000403
  700, 0.000345
  800, 0.000302
  900, 0.000269
 total: 1.084470 s
[username@login02 OpenACC]$
```

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Thank You

Resources

- Expanse User Guide & Tutorial
  - 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
- XSEDE Training Resources
  - https://www.xsede.org/for-users/training
  - https://cvw.cac.cornell.edu/expanse/