Quickly start using HPC resource at UCSB
- SLURM Array and Job Dependency
- Running Jupyter Notebook/Lab and VS Code on the Cluster
- NSF ACCESS allocation
- National & Commercial Cloud Computing Resources
Introduction to High-Performance Computing (HPC)

Paul Weakliem, Fuzzy Rogers, and Jay Chi

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Our Team

Paul Weakliem, PhD
Co-Director
Center for Scientific Computing & California Nanosystems Institute
Eling 3231
weakliem@cnsi.ucsb.edu

Fuzzy Rogers
Research Computing Administrator
Center for Scientific Computing & Materials Research Laboratory
MRL 2066B
fuz@mrl.ucsb.edu

Yu-Chieh “Jay” Chi, PhD
Research Computing Consultant
Center for Scientific Computing & Enterprise Technology Services
Elings 3229
jaychi@ucsb.edu
Our Research IT Partners

Mike Edwards
Director of Engineering Computing Infrastructure
3152A Harold Frank Hall
mcs@engineering.ucsb.edu

Michael Colee
Director of Earth Research Institute Computing (ERI)
6703 Ellison Hall
mtc@eri.ucsb.edu

Ted Cabeen
Director of Life Science Computing Group (LSCG)
2306 Life Science
ted.cabeeen@lscg.ucsb.edu

Andreas Boschke
Director of Infor. Infrastructure at Letter & Science IT (LSIT)
2306 Life Science
andreas@lsit.ucsb.edu
Agenda

● HPC Workflow
● SLURM Array
● SLURM Job Dependency
● Running Jupyter Notebook/Lab and VS Code on the cluster
  ○ Running Jupyter Notebook/lab on the POD/Braid2
  ○ Running VS Code on the POD/Braid2
  ○ Google Colab
  ○ Running Jupyter Lab on the SDSC Expanse
● Introduction to National HPC/Supercomputer resources
  ○ ACCESS allocation
  ○ Cloud Computing: JetStream2 from Indiana University
General HPC Workflow

1. `ssh`
2. `sbatch`
3. Job Runs on the Cluster
4. Job Running
5. Get Results
6. Grab Results

- Your local PC
- Login Node
- Slurm script
- SLURM Job Schedule
Job Arrays

- According to the Slurm Workload Manager, “Job arrays offer a mechanism for submitting and managing collections of similar jobs quickly and easily, … . All jobs must have the same initial options (e.g., size, time limit, etc.)”
- In general, job arrays are useful for applying the same processing routine to a collection of multiple input data files. Job arrays offer a very simple way to submit a large number of independent processing jobs.

```bash
#!/bin/bash
#SBATCH -J 'slurmArray'  ### Job Name
#SBATCH --nodes=1        ### No. of Nodes
#SBATCH --ntasks=1       ### No. of Tasks
#SBATCH -p short         ### Submit the job to Partition (Optional)
#SBATCH -o outLog_%A_%a   ### Output Log File (Optional)
#SBATCH -e errLog_%A_%a   ### Error Log File (Optional but suggest to have it)
#SBATCH -t 00:10:00       ### Job Execution Time
#SBATCH --array=0-3      ### Mail to you (Optional)
#SBATCH --mail-user=usernam@ucsb.edu
#SBATCH --mail-type ALL  ### Mail send you when the job starts and end (Optional)
```
Slurm Job Array Submission script

- The `A_%a` construct in the output and error file names is used to generate unique output and error files based on the master job ID (`A`) and the array-tasks ID (`a`).
- Job Array indices can be specified as array index values, a range of index values, and an optional step size.

```bash
# Submit a job array with index values between 0 and 15
#SBATCH --array=0-15

# Submit a job array with index values of 1, 3, 9, and 15
#SBATCH --array=1, 3, 9, 15

# Submit a job array with index values between 1 and 16 with a step size of 2
#SBATCH --array=1-16:2
```
#!/bin/bash
#SBATCH -J 'slurmArray'
#SBATCH --nodes=1
#SBATCH --ntasks=1
#SBATCH -p short
#SBATCH -o outLog_%A_%a
#SBATCH -e errLog_%A_%a
#SBATCH -t 00:10:00
#SBATCH –array=0-3

echo "SLURM_JOB_ID: " $SLURM_JOBID
echo "SLURM_ARRAY_JOB_ID: " $SLURM_ARRAY_JOB_ID
echo "SLURM_ARRAY_TASK_ID: " $SLURM_ARRAY_TASK_ID
echo "SLURM_ARRAY_TASK_COUNT: " $SLURM_ARRAY_TASK_COUNT
echo "SLURM_ARRAY_TASK_MAX: " $SLURM_ARRAY_TASK_MAX
echo "SLURM_ARRAY_TASK_MIN: " $SLURM_ARRAY_TASK_MIN
Dependency Jobs

- You can schedule jobs depending on the termination status of previously scheduled jobs. This way, you can concatenate your jobs into a pipeline or expand to more complicated dependencies.
- For example, job1.s is a submission script you plan to submit a batch job:

```bash
#!/bin/bash
#SBATCH -J 'JobDep1'
#SBATCH --nodes=1
#SBATCH --ntasks=1
#SBATCH -p short
#SBATCH -o outLog_%x_%j
#SBATCH -e errLog_%x_%j
#SBATCH -t 00:10:00
#SBATCH --mail-user=userdata@ucsb.edu
#SBATCH --mail-type ALL

# Run Bash Command
echo "***** My first Program *****"
echo "***** Prepare the Data *****"
echo "***** Done for Preparation *****"
echo "Time: " $(date +"%T")
```

### Job Name
### No. of Nodes
### No. of Tasks
### Submit the job to Partition (Optional)
### Output Log File (Optional)
### Error Log File (Optional but suggest to have it)
### Job Execution Time
### Mail to you (Optional)
### Mail send you when the job starts and end (Optional)
Dependency Jobs

- Submit the job script to the Slurm job scheduler from the POD login node:
  
  ```
  $ sbatch job.s
  Submitted batch job 1234567
  ```

- You can submit another job that is put on the waiting list of the queue.

  ```
  $ sbatch -dependency=aftercorr:1234567 job2.s
  ```

- This command indicates that `job2.s` will be put in the queue after the job ID `1234567` is terminated for any reason. The dependency option flag can be after, afterany, aftercorr, afterok, and afternotok.

- The following command would submit 2 jobs with respect to their dependencies.

  ```
  # First Job
  jobID_1=$(sbatch job1.s | cut -f 4 -d ' ')
  
  # Second Job - this job depends on the first job
  sbatch --dependency=aftercorr:$jobID_1 job2.s
  ```
<table>
<thead>
<tr>
<th>after</th>
<th>This job is execution after the specified jobs have begun execution</th>
</tr>
</thead>
<tbody>
<tr>
<td>afterany</td>
<td>This job can begin execution after the specified jobs have been terminated</td>
</tr>
<tr>
<td>aftercorr</td>
<td>A task of this job array can begin execution after the corresponding task ID in the specified job has completed successfully</td>
</tr>
<tr>
<td>afternotok</td>
<td>This job can begin execution after the specified jobs have terminated in some failed state</td>
</tr>
<tr>
<td>afterok</td>
<td>This job can begin execution after the specified jobs have been successfully executed</td>
</tr>
<tr>
<td>singleton</td>
<td>This job can begin execution after any previously launched jobs sharing the same job name and the user has terminated</td>
</tr>
</tbody>
</table>
Slurm Job Dependency Submission script

Slurm job script file: job1.s

```bash
#!/bin/bash
#SBATCH -J 'JobDep1'
#SBATCH --nodes=1
#SBATCH --ntasks=1
#SBATCH -p short
#SBATCH -o outLog_%x_%j
#SBATCH -e errLog_%x_%j
#SBATCH -t 00:10:00
#SBATCH --mail-user=usernam@ucsb.edu
#SBATCH --mail-type ALL

# Run Bash Command
echo "***** My first Program *****"
echo "***** Prepare the Data *****"
echo "***** Done for Parparation *****"
echo "Time: " $(date +"%T")
```
Slurm Job Dependency Submission script

Slurm job script file: job2.s

#!/bin/bash
#SBATCH -J 'JobDep2'
#SBATCH --nodes=1
#SBATCH --ntasks=1
#SBATCH -p short
#SBATCH -o outLog_%x_%j
#SBATCH -e errLog_%x_%j
#SBATCH -t 00:10:00
#SBATCH --mail-user=usernam@ucsb.edu
#SBATCH --mail-type ALL

# Run Bash Command
echo ***** Start the Program *****
echo ***** Code1 is Running *****
echo ***** Code2 is Running *****
echo ***** End the Program *****
echo "Time: " $(date +"%T")
Slurm Job Dependency Submission script

Slurm job script file: job3.s

```bash
#!/bin/bash
#SBATCH -J 'JobDep3'
#SBATCH --nodes=1
#SBATCH --ntasks=1
#SBATCH -p short
#SBATCH -o outLog_%x_%j
#SBATCH -e errLog_%x_%j
#SBATCH -t 00:10:00
#SBATCH --mail-user=usernam@ucsb.edu
#SBATCH --mail-type ALL

# Run Bash Command
echo "***** The Last Step *****"
echo "***** Analyze the Data *****"
echo "***** Done for analyzing data *****"
echo "Time: " $(date +"%T")
```
Slurm Job Dependency Submission script

batch script file: depJOB.s

#!/bin/bash

# First Job
jobID_1=$(sbatch job1.s | cut -f 4 -d ' ')

# Second Job - this job depends on the first job
jobID_2=$(sbatch --dependency=aftercorr:$jobID_1 job2.s | cut -f 4 -d ' ')

# Third Job - this job also depends on the second job
sbatch --dependency=aftercorr:$jobID_2 job3.s

- Execute the batch job script from the POD login node:

  $ sh depJOB.s
  Submitted batch job 1234567
Running Interactive Job

- Interactive computing refers to software which accepts input from the user as it runs. **Interactive computing** involves **real-time** user inputs to perform tasks on a set of compute node(s) including:
  - Coe development, real-time data exploration, etc.
  - Used when applications have large data sets or are too large to download to local device, or too large to compute on the local device
  - Actions performed on remote compute nodes as a result of user input or program out.

- To request an interactive computing node with 4 cores for 4 hours:
  
  ```bash
  $ srun -N 1 -n 4 -p batch --time=4:00:00 --pty bash -i
  ```

- To request an interactive computing GPU node for 4 hours:
  
  ```bash
  $ srun -N 1 -n 1 -p gpu --gres=gpu:1 --time=4:00:00 --pty bash -i
  ```
Why Run Jupyter Notebook/Lab, VS Code on the cluster?

- Computational resource requirement (GPU, multiple Cores, and etc.)
- Large memory requirement for your data
- Convenience to analyze your large scale data on the cluster
- Scaling up to long runtimes
Set Up Your Jupyter Notebook on the POD/Braid2

- Get to a compute node from the login node
  
  $ srun -N 1 -n 1 -p gpu --gres=gpu:1 --time=04:00:00 --pty bash -i

  [jay@pod-login1 ~]$  
  [jay@node122 ~]$

- Make sure your conda environment is activated
  
  (base) [jay@node122 ~]$

- Activate the specific conda environment
  
  $ conda activate pytorch112_gpu116
  
  (base) [jay@node122 ~]$
  $ conda activate pytorch112_gpu116
  (pytorch112_gpu116) [jay@node122 ~]$
Set Up Your Jupyter Notebook on the POD/Braid2

- Make sure the jupyter has been installed in the conda environment

```
$ conda list jupyter
# packages in environment at /home/jay/Software/anaconda3/envs/pytorch112_gpu116:

# Name     Version    Build    Channel
jupyter-client  8.3.1      pypi_0  pypi
jupyter-core    5.3.2      pypi_0  pypi
jupyter-events  0.7.0      pypi_0  pypi
jupyter-lsp     2.2.0      pypi_0  pypi
jupyter-server  2.7.3      pypi_0  pypi
jupyter-server-terminals 0.4.4      pypi_0  pypi
jupyterlab      4.0.6      pypi_0  pypi
jupyterlab-pygments 0.2.2      pypi_0  pypi
jupyterlab-server 2.25.0     pypi_0  pypi
```

- Get the ip from the host

```
$ hostname -i
10.1.50.122
```

- Launch the Jupyter notebook from the server

```
$ jupyter-notebook --no-browser --port=8888 --ip=10.1.50.122
To access the server, open this file in a browser:
file:///home/jay/.local/share/jupyter/runtime/jpsserver-8888-open.html
Or copy and paste one of these URLs:
http://10.1.50.122:8888/tree?token=bf11d6512a520a13deb981d6c627d791198e25218536a840
http://127.0.0.1:8888/tree?token=bf11d6512a520a13deb981d6c627d791198e25218536a840
```

Set Up Your Jupyter Notebook on the POD/Braid2

- Open a new terminal in order to access the Jupyter notebook from your remote machine over ssh
  
  ```
  $ ssh -N -L 8888:10.1.50.122:8888 your_user_name@pod.cnsi.ucsb.edu
  ```

- Open a browser window, copy the
  http://127.0.0.1:8888/tree?token=44b5cf8a93ea5edf5e70f202e81480e07aef19690bcd2c22 and pate it to the browser.

- After you finish your job, don’t forget to release your resource.
  $ scancel your_job_id
Set Up Your Jupyter Notebook on the Braid

- Get to a compute node from the login node
  
  $ qsub -l -l nodes=1:ppn=2 -l walltime=02:00:00

  ```
  (base) $ bash-4.1$ qsub -I -l nodes=1:ppn=4 -l walltime=02:00:00
  qsub: waiting for job 5343731.braid.cnsi.ucsb.edu to start
  qsub: job 5343731.braid.cnsi.ucsb.edu ready
  ```

- Make sure your conda environment is activated

  ```
  (base) $ bash-4.1$
  ```

- Get the ip from the host

  $ hostname -i

  ```
  (base) $ bash-4.1$ hostname -i
  10.0.90.50
  ```
Set Up Your Jupyter Notebook on the Braid

- Make sure the jupyter has been installed in the conda environment

$ conda list jupyter

<table>
<thead>
<tr>
<th>Package</th>
<th>Version</th>
<th>Channel</th>
<th>Conda-Forge</th>
</tr>
</thead>
<tbody>
<tr>
<td>jupyter</td>
<td>1.0.0</td>
<td>pyhd8ed1ab_10</td>
<td>conda-forge</td>
</tr>
<tr>
<td>jupyter-lsp</td>
<td>2.2.2</td>
<td>pyhd8ed1ab_0</td>
<td>conda-forge</td>
</tr>
<tr>
<td>jupyter_client</td>
<td>8.6.0</td>
<td>pyhd8ed1ab_0</td>
<td>conda-forge</td>
</tr>
<tr>
<td>jupyter_console</td>
<td>6.6.3</td>
<td>pyhd8ed1ab_0</td>
<td>conda-forge</td>
</tr>
<tr>
<td>jupyter_core</td>
<td>5.7.1</td>
<td>py310hff52083_0</td>
<td>conda-forge</td>
</tr>
<tr>
<td>jupyter_events</td>
<td>0.9.0</td>
<td>pyhd8ed1ab_0</td>
<td>conda-forge</td>
</tr>
<tr>
<td>jupyter_server</td>
<td>2.12.5</td>
<td>pyhd8ed1ab_0</td>
<td>conda-forge</td>
</tr>
<tr>
<td>iupyer server terminals</td>
<td>0.5.1</td>
<td>ovhd8ed1ab 0</td>
<td>conda-forge</td>
</tr>
</tbody>
</table>

- Launch the Jupyter notebook from the server

$ jupyter notebook --no-browser --port=8888 --ip=10.0.90.50

To access the server, open this file in a browser:

file:///home2/jay/.local/share/jupyter/runtime/jpserver-20452-open.html

Or copy and paste one of these URLs:

http://10.0.90.50:8888/tree?token=b73f105eaedf5b950f9d799ece39154918961769e3c3349f
http://127.0.0.1:8888/tree?token=b73f105eaedf5b950f9d799ece39154918961769e3c3349f
Set Up Your Jupyter Notebook on the Braid

- Open a new terminal in order to access the Jupyter notebook from your local machine over ssh
  
  ```
  $ ssh -oHostKeyAlgorithms=+ssh-rsa -N -L 8888:10.0.90.50:8888 your_username@braid.cnsi.ucsb.edu
  
  (base) EEUC-YT61Y2PL:$ jaychi$ ssh -oHostKeyAlgorithms=+ssh-rsa -N -L 8888 jay@braid.cnsi.ucsb.edu
  jay@braid.cnsi.ucsb.edu's password:
  ```

- Open a browser window, copy the
  
  http://127.0.0.1:8888/tree?token=b73f105eafd5b950f9d799ece39154918961769e3c3349f and paste it to the browser.
Connect Visual Studio Code to POD

- According to the Wikipedia, “Visual Studio Code (VS Code) is a source code editor that support a variety of programming languages, including C, C#, C++, Fortran, Go, Java, JavaScript, Node.js, Python, Rust, and Julia.”

- GitHub Copilot is a code completion tool developed by GitHub and OpenAI that assists users of Visual Studio Code integrated development environments (IDEs) by autocompleting code.

- Get to a compute node from the login node

  ```bash
  $ srun -N 1 -n 1 -p gpu --gres=gpu:1 --time=04:00:00 --pty bash -i
  ```

  ```bash
  [jay@pod-login1 ~]$ srun -N 1 -n 1 -p gpu --gres=gpu:1 --time=04:00:00 --pty bash -i
  ```
Connect Visual Studio Code to POD

- Connect VS Code locally to the Computing Node in HPC
  - Open VS Code command palette
  - Install Remote - SSH

- Configuring SSH
  - Open SSH config file
  - Add the following config detail
Connect Visual Studio Code to POD

- Open VS Code command palette
  - Remote-SSH: Connect to Host

- Choose the computing node

- Disconnect to the HPC

- After you finish your job, don’t forget to release your resource.
  $ scancel your_job_id
Google Colab

- **What is Google Colab?**
  - Google Colab (Colaboratory) allows you to write and execute Python and R in your browser with
    - No need to install packages
    - GPU access
    - Sharing with your partners

- **Tutorial link**
  - [https://reurl.cc/Epg3M0](https://reurl.cc/Epg3M0)
Getting Started to use Colab
Getting Started to use Colab

```python
import numpy as np

arrA = np.array([[1., 2., 3.], [2., 3., 4.]])
print('Array A:
', arrA)
print('The shape of Array is: ', arrA.shape)
print('If GPU is available: ', torch.cuda.is_available())
```

Array A:
```
[[1. 2. 3.]
 [2. 3. 4.]]
```
The shape of Array is: (2, 3)
If GPU is available: False

Executing the Code Block: Shift + return

```
# This is my first Colab
## 1.1 Introduction the Colab
### 1.1.1 Introduction to Python
### 1.1.2 Introduction to Torch

This is my first Colab
1.1 Introduction the Colab
1.1.1 Introduction to Python
1.1.2 Introduction to Torch
```
# Changing Runtime Type

## Notebook settings

**Runtime type**
- Python 3

**Hardware accelerator**
- None
- GPU
- TPU

## Runtime commands
- Run all
- Run before
- Run the focused cell
- Run selection
- Run after
- Interrupt execution
- Restart runtime
- Restart and run all
- Disconnect and delete runtime

## Additional options
- Manage sessions
- View resources
- View runtime logs
Run Jupyter Notebook/Lab on the SDSC Expanse

- Connect to the Expanse Portal: https://portal.expanse.sdsc.edu/

Expanse User Guide

Technical Summary

Expanse is a dedicated Advanced Cyberinfrastructure Coordination Ecosystem: Services and Support (ACCESS) cluster designed by Dell and SDSC delivering 5.15 peak petaflops, and will offer Composable Systems and Cloud Bursting.

Expanse’s standard compute nodes are each powered by two 64-core AMD EPYC 7742 processors and contain 256 GB of DDR4 memory, while each GPU node contains four NVIDIA V100s (32 GB SMX2) connected via NVLINK and dual 20-core Intel Xeon 6248 CPUs. Expanse also has four TB large memory nodes.

Expanse is organized into 13 SDSC Scalable Compute Units (SSCUs), comprising 728 standard nodes, 54 GPU nodes and 4 large memory nodes. Every Expanse node has access to a 12 PB Lustre parallel file system (provided by Aceon Computing) and a 7 PB Ceph Object Store system. Expanse uses the Bright Computing HPC Cluster management system and the SLurm workload manager for job scheduling.
Run Jupyter Notebook/Lab on the SDSC Expanse

**Jupyter Session**

- **Account:**
- **Partition (Please choose the gpus, gpus-shared, or gpus-preempt as the partition if using gpus):**
  - shared
- **Time limit (hr):**
  - 30
- **Number of cores:**
  - 1
- **Memory required per node (GB):**
  - 2
- **GPUs (optional):**
  - 0

**Satellite Reverse Proxy Service**

**SDSC Expanse**

- **Job State:** Mapped

**Environment**

- Singularity Image File Location: Use your own or to include from existing container library
  - /cm/shared/apps/containers/singularity/pthor/c/jupyter-latest.sif
- Environment modules to be loaded (e.g., to use latest version of system Anaconda) include
- Conda Environment (Enter your own conda environment if any):
National Supercomputer Resources: ACCESS

- Advanced Cyberinfrastructure Coordination Ecosystem: Services & Support (ACCESS)

- ACCESS is an advanced computing and data resource supported by the National Science Foundation (NSF).

- ACCESS Services include Allocations, Support, Operation and Metrics, along with a Coordination Office

- Access website: https://access-ci.org/
National Supercomputer Resources: ACCESS

Four Allocation Opportunities to suit a variety of needs (credit thresholds):

- **Explore (400,000)**
  - Best-suited for endeavors with light resource requirements
  - Grad students can be PIs

- **Discover (1,500,000)**
  - Minimal effort to start production research activities
  - Potential best-fit for Campus Champion Allocations

- **Accelerate (3,000,000)**
  - More substantial resource requirements
  - Multi-grand research, Gateways, etc.

- **Maximize (No upper limit)**
  - For large-scale research project with extreme resource needs
  - Will largely resemble XRAC process
Allocation Eligibility

- Available to any research or educator as US academic, non-profit research, or educational institution.
- Can be in any official position including adjunct or instructional.
- Postdoctoral researchers can be a PI of any project type.
- Graduate students can lead an “Explore” ACCESS allocation under their advisor’s guidance.
- NSF Graduate Fellows and Honorable mentions can apply for “Discover” allocations.
- Ref: https://allocations.access-ci.org/access-allocations-policies#eligibility
## Comparison Table

<table>
<thead>
<tr>
<th>Opportunity</th>
<th>Explore</th>
<th>Discover</th>
<th>Accelerate</th>
<th>Maximize</th>
</tr>
</thead>
<tbody>
<tr>
<td>Purpose</td>
<td>Resource evaluation, grad student projects, small classes and training events, benchmarking, code development and porting, similar small-scale uses.</td>
<td>Grants with modest resource needs, Campus Champions, large classes and training events, NSF graduate fellowships, benchmarking and code testing at scale, gateway development.</td>
<td>Mid-scale resource needs, consolidating multi-grant programs, collaborative projects, preparation for Maximize ACCESS requests, gateways with growing communities.</td>
<td>Large-scale research projects.</td>
</tr>
<tr>
<td>Allocation credit threshold</td>
<td>Small</td>
<td>Medium</td>
<td>Large</td>
<td>No upper limit</td>
</tr>
<tr>
<td>Allocation duration</td>
<td>Supporting grant duration or 12 months</td>
<td>Supporting grant duration or 12 months</td>
<td>Supporting grant duration or 12 months</td>
<td>12 months</td>
</tr>
<tr>
<td>Requests accepted</td>
<td>Continuously</td>
<td>Continuously</td>
<td>Continuously</td>
<td>Every 6 months</td>
</tr>
<tr>
<td>Multiple requests allowed</td>
<td>Multiple requests allowed</td>
<td>Multiple requests allowed</td>
<td>Multiple requests allowed</td>
<td>1 allowed (some exceptions)</td>
</tr>
<tr>
<td>Requirements and review process</td>
<td>Overview</td>
<td>1-page proposal</td>
<td>3-page proposal (max. length)</td>
<td>10-page proposal (max. length)</td>
</tr>
<tr>
<td>Confirmation of eligibility and suitability of requested resources</td>
<td>Confirmation of eligibility and suitability of requested resources</td>
<td>Panel merit review</td>
<td>Panel merit review</td>
<td></td>
</tr>
</tbody>
</table>

Ref: [https://allocations.access-ci.org/prepare-requests-overview](https://allocations.access-ci.org/prepare-requests-overview)
National Supercomputer Resources: ACCESS

Researchers and educators can gain access to advanced computing, software, and data resources to accomplish their research goals, making research possible for the diverse community by participating in merit reviews or allocations.

Resource providers are at the center of the ACCESS Allocation process. Submissions are made available for a specific allocation opportunity, and data resources to accomplish their research goals.

Reviewers provide a valuable service to ACCESS, the NSF, and the computing community by participating in merit reviews or allocations.

We hope you'll get involved! Let's get started.

Explore ACCESS
Explore ACCESS allocations are intended for purposes that require small resource amounts. Researchers can try out resources or run benchmarks. Instructors can provide access for small-scale classroom activities, research software engineers can develop or port codes, and so on. Graduate students can conduct thesis or dissertation work.

Discover ACCESS
Discover ACCESS projects are intended to fill the needs of many modest-scale research activities or other resource needs. The goal of this opportunity is to allow many researchers to request allocations with a minimum amount of effort so they can complete their work. To submit a request, you will need to submit a one-page description of the project to address the review criteria. You can also ask for an advisory review from the community to guide you to appropriate resources.

Accelerate ACCESS
Accelerate ACCESS projects support activities that require more substantial resource amounts to pursue their research objectives. Researchers are expected to have reasonably well-defined plans for their resource use and to submit a 3-page project description for merit review. Reviewers will look more closely at how your resource usage plan addresses the review criteria.

Submissions open: 2022-12-15 – 2023-01-15

For projects with resource needs beyond those provided by an Accelerate ACCESS project, a Maximize ACCESS request is required. ACCESS has an upper limit on the size of allocations that can be requested or awarded at this level, but resource providers may have limits on allocation amount resources.

Maximize ACCESS – March 2023

Submit a Maximize ACCESS - March 2023 Request

Submit a Discover ACCESS Request

Submit an Explore ACCESS Request
Resource Providers (PRs)

- ACCESS consists of a set of Resource Providers (PRs) that offer a wide range of computational resources including systems such as high-performance computing (HPC) clusters, virtualization (cloud-style) clusters, high throughput computing (HTC) clusters, massive storage clusters, large memory clusters, and composable clusters.

- ACES (Texas A&M)
- Anvil (Purdue)
- Bridges-2 (PSC)
- DARWIN (Delaware)
- Delta (NCSA)
- Expanse (SDSC)
- FASTER (Texas A&M)
- Jetstream2 (IU)
- OOKAMI (Stonybrook)
- KyRIC (Kentucky)
- Rockfish (JHU)
- Stampede-2 (TACC)
- RANCH (TACC)
- Open Science Grid (OSG)
- Open Storage Network (OSN)
National Supercomputer Resources: ACCESS

Exchange Calculator

Number of units on this resource:

- 10,000 ACCESS Credits

Equals this many units on this resource:

- 186 SDSC Expanse GPU

Purdue Amvl CPU
Purdue Amvl GPU
SDSC Expanse GPU
SDSC Expanse GPU Projects Storage

Resource Type: Compute
Resource Description: Expanse GPU will be a Dell integrated cluster, NVIDIA V100 GPUs with NVLink, interconnected with Mellanox HDR InfiniBand in a hybrid fat-tree topology. There are a total of 62 nodes with four V100 SMX2 GPUs per node (with NVLink connectivity). There are two 20-core Xeon 6248 CPUs per node. Full-duplex bandwidth will be available at rack level (62 CPU nodes, 8 GPU nodes) with HDR100 connectivity to each node. HDR200 switches are used at the rack level and there will be 3:1 oversubscription cross-rack. In addition, Expanse also has four 2 TB large memory nodes. The system will also feature 12PB of Lustre based performance storage (140GB/s aggregated), and 7PB of Ceph based object storage.

Recommended Use: GPUs are a specialized resource that performs well for certain classes of algorithms and applications. Recommend to be used for accelerating simulation codes optimized to take advantage of GPUs (using CUDA, OpenACC). There is a large and growing base of community codes that have been optimized for GPUs including those in molecular dynamics, and machine learning. GPU-enabled applications on Expanse will include: AMBER, Gromacs, BEAST, OpenMM, NAMD, TensorFlow, and PyTorch.

Organization: San Diego Supercomputer Center
Units: GPU Hours
Description: SDSC Expanse Projects Storage

Overview
Available resources
Exchange calculator

Requests
Allocations
Prepare requests
Use credits
Updates
Policies
FAQs

Looking for research or classroom objectives? Explore the ACCESS marketplace, making research possible. Become a part of the national research community that ACCESS serves. View and review the largest allocation requests.
SDSC HPC for UC

- Request HPC@UC at [https://www.sdsc.edu/support/hpc_uc_apply-exp.html](https://www.sdsc.edu/support/hpc_uc_apply-exp.html)
- Up to 500K core-hours of computing, associated data storage, and access to SDSC expertise to assist their research team.
- Awards are active for one year. NO supplements, renewals or Extensions
- Applicants must not have an active ACCESS award
- Developed to support onboarding to ACCESS and large, formal allocation requests
- SDSC staff will assist in developing these allocation applications
- Applications are reviewed on an ongoing basis. Applicants will be notified within 10 business days of the review decision.
- Ref: [https://www.sdsc.edu/support/hpc_uc_apply-exp.html](https://www.sdsc.edu/support/hpc_uc_apply-exp.html)
<table>
<thead>
<tr>
<th>Resource Type:</th>
<th>Compute</th>
</tr>
</thead>
<tbody>
<tr>
<td>Resource Description:</td>
<td>Jetstream2 is a user-friendly cloud environment designed to give researchers and students access to computing and data analysis resources on demand as well as for gateway and other infrastructure projects. Jetstream2 is a hybrid-cloud platform that provides flexible, on-demand, programmable cyberinfrastructure tools ranging from interactive virtual machine services to a variety of infrastructure and orchestration services for research and education. The primary resource is a standard CPU resource consisting of AMD Milan 7713 CPUs with 128 cores per node and 512gb RAM per node connected by 100gbps ethernet to the spine.</td>
</tr>
<tr>
<td>Recommended Use:</td>
<td>For the researcher needing virtual machine services on demand as well as for software creators and researchers needing to create their own customized virtual machine environments. Additional use cases are for research-supporting infrastructure services that need to be &quot;always on&quot; as well as science gateway services and for education support, providing virtual machines for students.</td>
</tr>
<tr>
<td>Organization:</td>
<td>Indiana University</td>
</tr>
<tr>
<td>Units:</td>
<td>SUs</td>
</tr>
<tr>
<td>Description:</td>
<td>1 SU = 1 Jetstream2 vCPU-hour. VM sizes and cost per hour are available <a href="https://docs.jetstream-cloud.org/general/vm">https://docs.jetstream-cloud.org/general/vm</a> sizes/</td>
</tr>
</tbody>
</table>
Jetstream2 is a user-friendly cloud computing environment for researchers and educators running on OpenStack and featuring Exosphere as the primary user interface. It is built on the successes of Jetstream 1 and continues the main features of that system while extending to a broader range of hardware and services, including GPUs, large memory nodes, virtual clustering, programmable cyberinfrastructure with OpenStack Heat and Terraform, and many other features. It is designed to provide both infrastructure for gateways and other "always on" services as well as giving researchers access to interactive computing and data analysis resources on demand.

For a more in-depth description please see the System Overview.

Jetstream2 Status

Overall JS2 system status: Operational

Please visit https://jetstream.status.io/ for detailed system status information and planned maintenance announcements. Also see, Jetstream2 system status and information for additional information on our outages and maintenance mailing list and community chat.

Accessing Jetstream2

Access to Jetstream2 is available solely through Advanced Cyberinfrastructure Coordination Ecosystem: Services & Support (ACCESS) allocations. You must be on a valid allocation or the PI of a valid allocation to have access to Jetstream2.

Ref:
https://docs.jetstream-cloud.org/
Cloud Computing: Amazon Web Services (AWS)

- If you choose to use AWS, it is recommended to take advantage of the Campus Cloud Landing Zone (LZ) for AWS. A UCSB purchases order is required to request an Campus Cloud account (https://ucsb.github.io/campus-cloud-docs/getting-started/#procurement).

  Important: You may need the help of a PI or Department Purchasing person to create a Purchase Order which is necessary to request an account in the Campus Cloud.
Amazon Elastic Compute Cloud (Amazon EC2)

- **Use Case:**
  - Run cloud-native and enterprise applications
  - Scale for HPC applications
  - Train and deploy ML applications

- **EC2 Instance Types**
  - General Purpose
  - Compute Optimized
  - Memory Optimization
  - Accelerated Computing
  - Storage Optimized

- **More Information**
  - Amazon EC2: [https://aws.amazon.com/ec2/](https://aws.amazon.com/ec2/)
  - Amazon EC2 Pricing Estimation: [https://aws.amazon.com/ec2/pricing/on-demand/](https://aws.amazon.com/ec2/pricing/on-demand/)
  - [https://instances.vantage.sh/](https://instances.vantage.sh/)
If you like to use AWS to be your cloud computing platform, RONIN removes the enormous complexity of AWS offerings and provides an easy-to-use self-service platform.

UCSB provides RONIN information support if you like to use AWS to do your computing research via the RONIN platform.

Contact with Bill Doering: billd@ucsb.edu
Ronin Platform: Control Your AWS Cost
Acknowledgements - [https://csc.cnsi.ucsb.edu/publications](https://csc.cnsi.ucsb.edu/publications)

Please acknowledge the CSC in publications and presentations if you are using our facility’s computational resources (including staff involvement) in your research.

“We acknowledge support from the Center for Scientific Computing from the CNSI, MRL: an NSF MRSEC (DMR-2308708) and NSF CNS-1725797.”

For users of GPU nodes, please add the grant number NSF OAC-1925717
Questions and Thought

● What else content should we cover?
● Other ideas for a workshop?
  ○ Running Parallel Python / Matlab / R on the Cluster, Mathematica, Singularity/Docker Container, etc.

● More Information:

https://csc.cnsi.ucsb.edu/