ACCESS | Advancing Innovation

Anvil 101

New User Tutorial

The Anvil Team, Purdue Research Computing

NSF

PURDUE UNIVERSITY | Information Technology

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Acknowledgement

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Full Agenda

- Anvil system architecture including node types, storage, interconnects, and networking.
- Getting started with accounts and allocations
- Compilation and programing environment on Anvil
- Running Jobs on Anvil
- Data management and transfer on Anvil
- Q&A

Agenda

1. Anvil overview

- Introduction to Anvil
- Hardware
- Anvil group and consulting

About Anvil

- **Category I: A national composable advanced computational resource for the future of science and engineering**
- **By the Purdue research computing team. Full access started February, 2022**
- **NSF award #2005632; 5 years of operations; allocated via NSF ACCESS**

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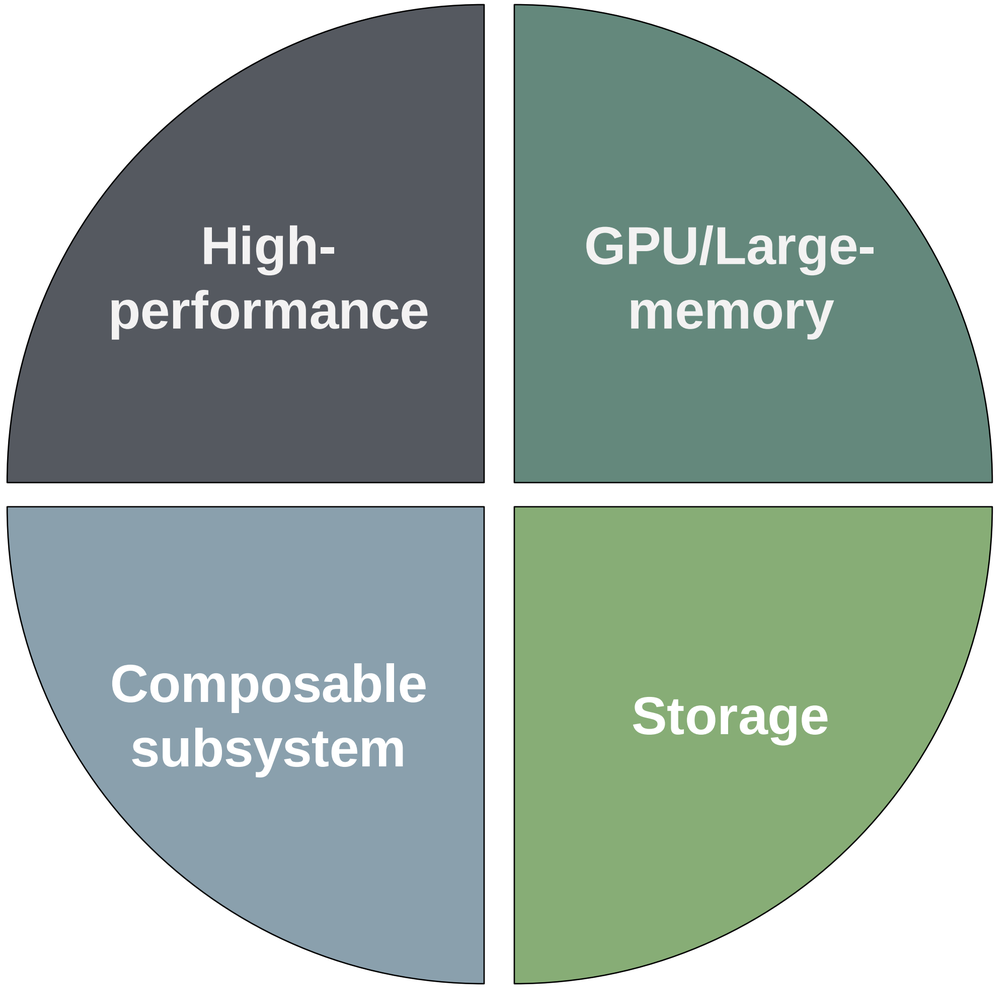
System Resources

- **1000** compute nodes
- **128** core AMD 3rd Gen EPYC 7763 processors
- **5.3** PF peak performance



- **16** nodes with **4** NVIDIA A100 GPUs each
- **32** large memory nodes with **1** TB of RAM

- **8** large memory & storage nodes
- Kubernetes – Rancher for DevOps

- Multi-tier storage (including object storage)
- **10** PB of parallel filesystem, and **3** PB of all-flash storage
- Globus data transfer

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Service & Support

Quick turnaround via ACCESS support tickets

[support.access-ci.org/user/login?destination=/open-a-ticket]

Support team

[comprising domain experts from multiple disciplines]

Advanced user support

[data science consulting, HPC performance optimization, science gateway development]

Multimodal Training Delivery

[live lessons, online tutorials, video lessons]

Agenda

2. Getting started

- Get anvil account and allocation
- Logging in
- Check account usage

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2. Getting started

- **Get anvil account and allocation**
- **Logging in**
- **Check account usage**

Obtaining an Account

As an ACCESS computing resource, Anvil is accessible to ACCESS users who are given an allocation on the system. To obtain an account, users may submit a proposal through:

ACCESS Allocation Request System: https://allocations.access-ci.org/

Sign up for an ACCESS account (if you don't have one already) at https://allocations.access-ci.org

Prepare an allocation request with details of your proposed computational workflows (science, software needs), resource requirements, and a short CV. See the individual "Preparing Your … Request" pages for details on what documents are required:

https://allocations.access-ci.org/prepare-requests-overview.

Obtaining an Allocation

How do I get onto Anvil through ACCESS?

Allocation	Credit Threshold
Explore ACCESS	400,000
Discover ACCESS	1,500,000
Accelerate ACCESS	3,000,000
Maximize ACCESS	Not awarded in credits.

Obtaining an Allocation

When your request is approved, you only get ACCESS **credits** awarded. You still need to go through the step of exchanging these credits for time on Anvil.

You need not use up all your credits and may also use part of your credits for time on other ACCESS resources.

Exchange calculator (**https://allocations.access-ci.org/exchange_calculator**)

You will also need to go to the allocations page and add any users you would like to have access to these resources.

Note that they will need to sign up for ACCESS accounts as well before you can add them.

For other questions you may have, take a look at the FAQs on the ACCESS page here:

(**https://allocations.access-ci.org/ramps-policies-faqs**)

Obtaining an Allocation

When your ACCESS allocation is approved, you will receive an email from ACCESS.

After you transfer your credit to Anvil, it takes a bit of time for ACCESS to send the information to Anvil.

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2. Getting started

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Logging in via SSO Hub

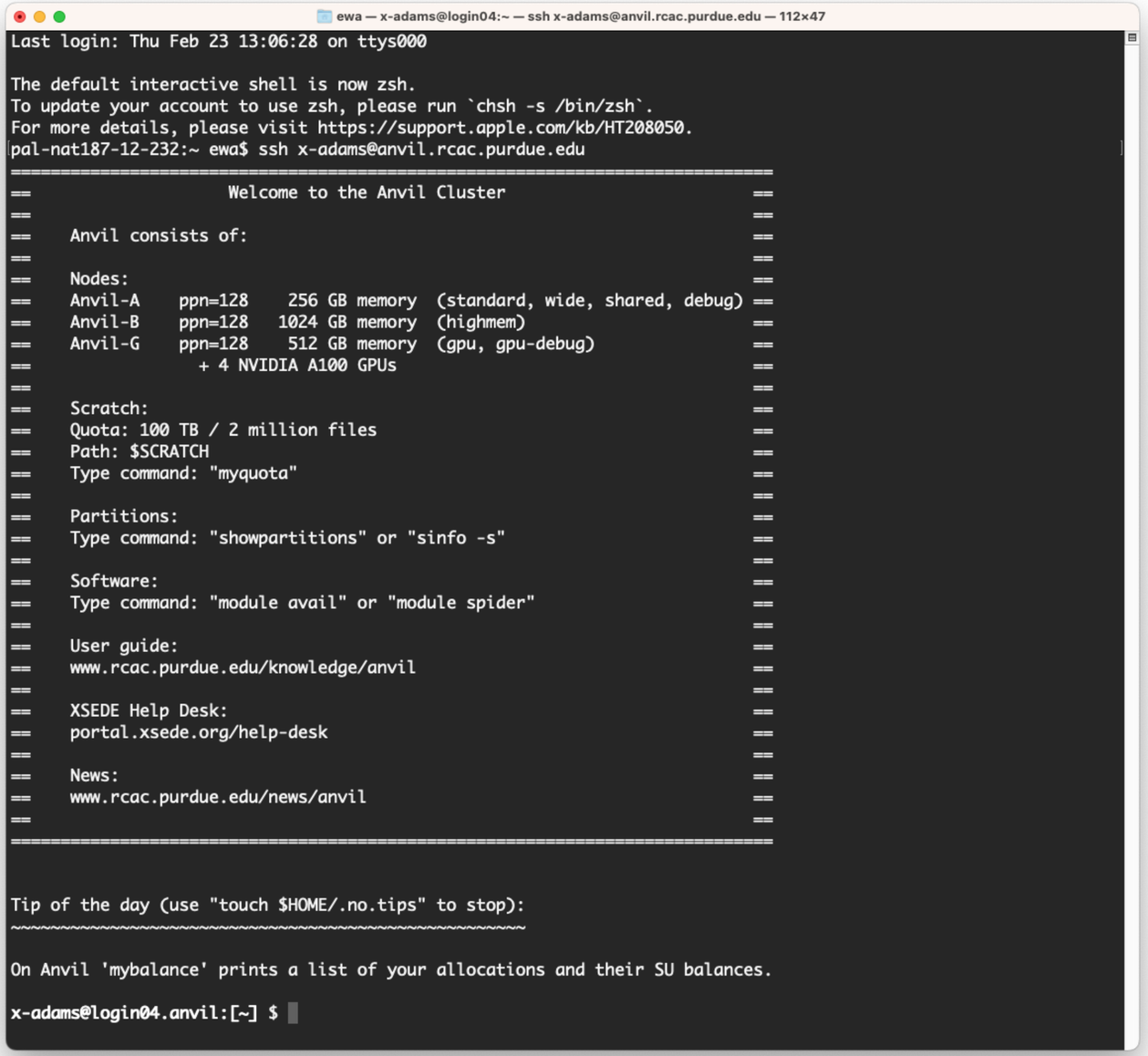
Anvil accepts standard SSH connections with **public keys-based** authentication to ***anvil.rcac.purdue.edu*** using your Anvil username:

```
localhost$ ssh my-x-anvil-username anvil.rcac.purdue.edu
```

Please note:

- Your Anvil username is not the same as your ACCESS portal username. Anvil usernames look like x-ACCESSusername or similar, starting with an x-.

- Password-based authentication is not supported on Anvil (in favor of **SSH keys**). There is *NO* "Anvil password", and your ACCESS password will not be accepted by Anvil's SSH either.


ewa — x-adams@login04:~ — ssh x-adams@anvil.rcac.purdue.edu — 112×47
Last login: Thu Feb 23 13:06:28 on ttys000
The default interactive shell is now zsh.
To update your account to use zsh, please run `chsh -s /bin/zsh`.
For more details, please visit https://support.apple.com/kb/HT208050.
pal-nat187-12-232:~ ewa$ ssh x-adams@anvil.rcac.purdue.edu
Welcome to the Anvil Cluster
Anvil consists of:
Nodes:
Anvil-A ppn=128 256 GB memory (standard, wide, shared, debug)
Anvil-B ppn=128 1024 GB memory (highmem)
Anvil-G ppn=128 512 GB memory (gpu, gpu-debug)
+ 4 NVIDIA A100 GPUs
Scratch:
Quota: 100 TB / 2 million files
Path: $SCRATCH
Type command: "myquota"
Partitions:
Type command: "showpartitions" or "sinfo -s"
Software:
Type command: "module avail" or "module spider"
User guide:
www.rcac.purdue.edu/knowledge/anvil
XSEDE Help Desk:
portal.xsede.org/help-desk
News:
www.rcac.purdue.edu/news/anvil
Tip of the day (use "touch $HOME/.no.tips" to stop):
On Anvil 'mybalance' prints a list of your allocations and their SU balances.
x-adams@login04.anvil:[~] $

Logging in via SSH

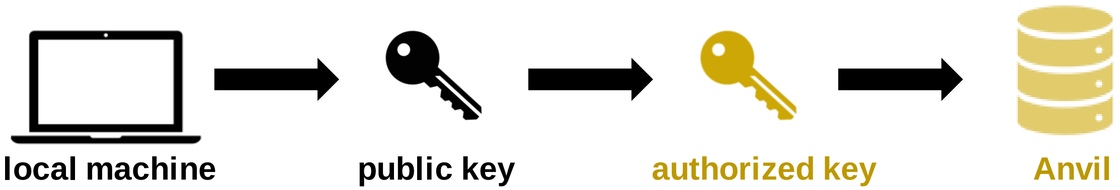
Anvil accepts standard SSH connections with **public keys-based** authentication to *anvil.rcac.purdue.edu* using your Anvil username:

```
localhost$ ssh -l my-x-anvil-username anvil.rcac.purdue.edu
```

Your Anvil username is **not** the same as your ACCESS Portal username. Anvil usernames look like x-ACCESSusername or similar, starting with an x-.

Password-based authentication is not supported on Anvil (in favor of SSH keys). There is no "Anvil password", and your ACCESS User Portal password will not be accepted by Anvil's SSH either.

Please see Appendix or **Anvil user guide** (www.rcac.purdue.edu/knowledge/anvil/access/login/sshkeys) for more detail about **SSH keys**.

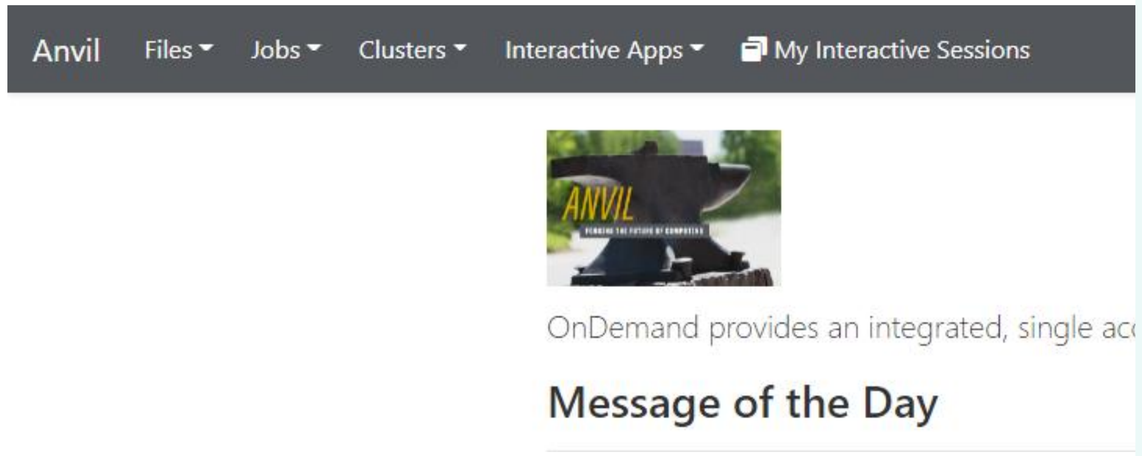


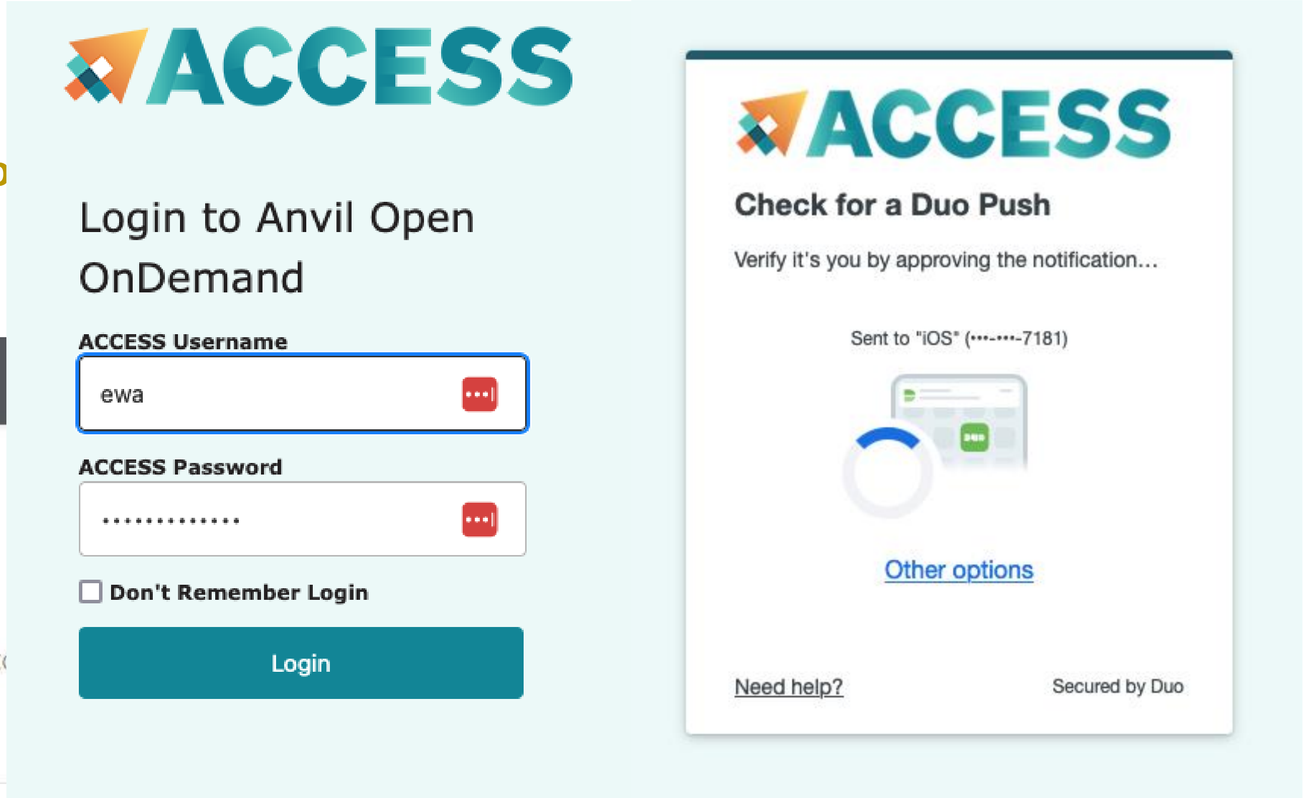
Open OnDemand

Open OnDemand allows one to interact with HPC resources through a web browser and easily manage files, submit jobs, and interact with graphical applications directly in a browser, all with no software to install.

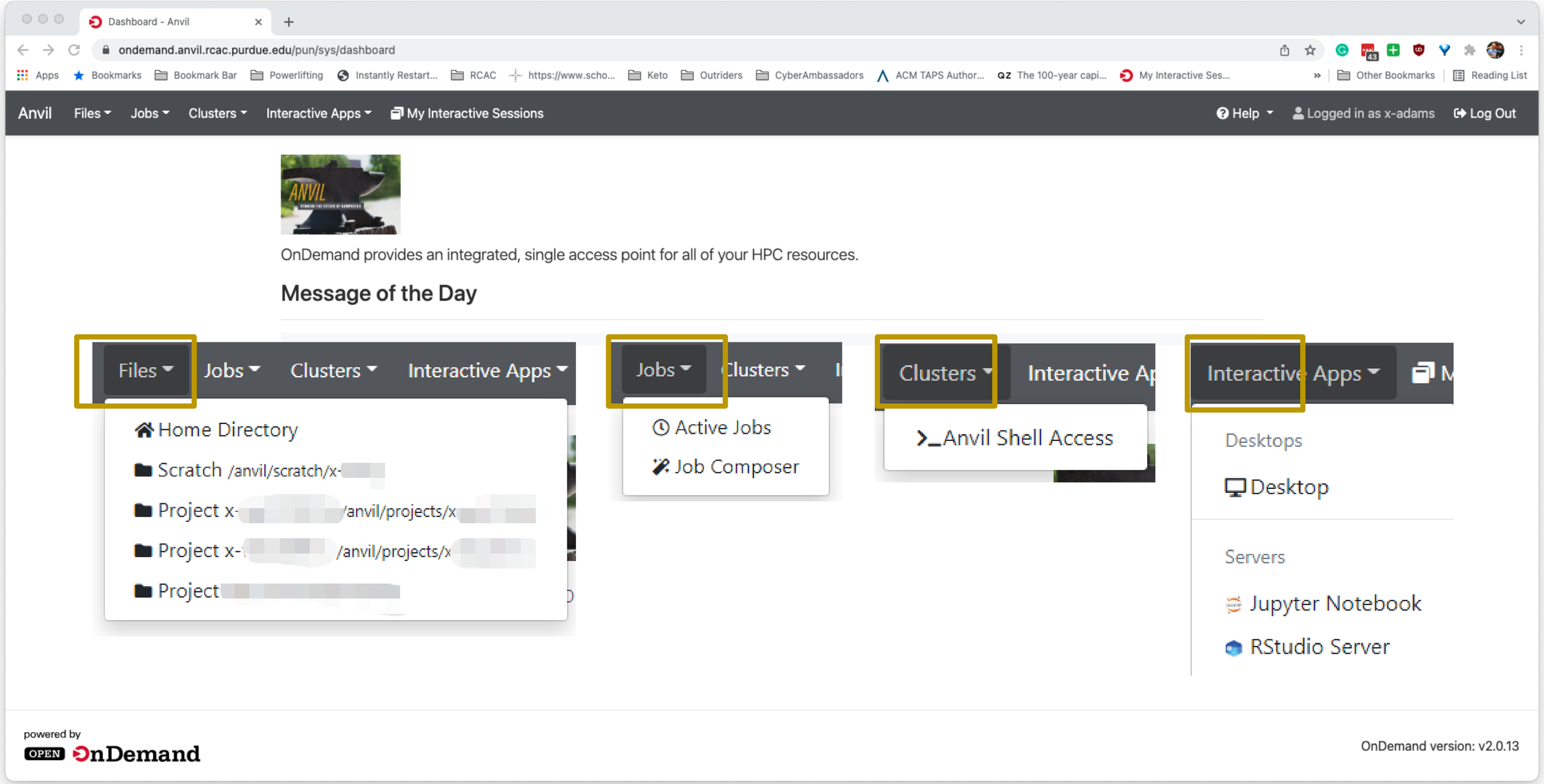
Navigate to ***https://ondemand.anvil.rcac.purdue.edu***

Log in using your **ACCESS portal username and passwo**





More training section about Open OnDemand will be given by Anvil team in the future.


Dashboard - Anvil
ondemand.anvil.rcac.purdue.edu/pun/sys/dashboard
Anvil
Files
Jobs
Clusters
Interactive Apps
My Interactive Sessions
Help
Logged in as x-adams
Log Out
OnDemand provides an integrated, single access point for all of your HPC resources.
Message of the Day
Home Directory
Scratch /anvil/scratch/x-
Project x-
/anvil/projects/x
Project x-
/anvil/projects/x
Project
Active Jobs
Job Composer
Anvil Shell Access
Desktops
Desktop
Servers
Jupyter Notebook
RStudio Server
powered by
OPEN OnDemand
OnDemand version: v2.0.13

Agenda

2. Getting started

- Get anvil account and allocation
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- **Check account usage**

Check Allocation Usage

To keep track of the usage of the allocation by your project team, you can use ***mybalance***:

```
[x-anvilusername@login01:~]$ mybalance
```

Allocation Account	Type	SU Limit	SU Usage (account)	SU Usage (user)	SU Balance
xxxxxx-cpu	CPU	1000.0	95.7	3.0	904.3
xxxxxx-gpu	GPU	1000.0	43.5	1.5	956.5

You can also check the allocation usage through **ACCESS User Portal**:

https://allocations.access-ci.org/allocations/summary

You should see at least one allocation.

CPU and GPU nodes use are count separately, so there are using different allocation accounts.

Check Allocation Usage

x-adams@login05:~ ⌥⌘1

```
x-adams@login05.anvil:[~] $ mybalance

Allocation      Type    SU Limit    SU Usage   SU Usage  SU Balance
Account                            (account)    (user)
=============  ====  ==========  ========== ==========  ==========
asc170016       CPU     50000.0     12645.4        1.4     37354.6
asc170016-gpu   GPU      2500.0        25.4        0.0      2474.6
tra220012       CPU      2000.0         0.0        0.0      2000.0

x-adams@login05.anvil:[~] $
```

Agenda

3. Compilation and programing environment

- Module system
- Provide software and software installation policy
- Compiling source code (examples and explanation)

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- **Module system**
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Modules

- Module commands allow you to add applications and libraries to your environment.
- This allows us to simultaneously and safely provide several versions of the same software.
- Anvil team makes recommendations for both CPU and GPU stack regarding the CUDA version, compiler, math library, and MPI library. If you have no specific requirements, you can simply load the recommended set by:

```
$ module load modtree/cpu # for CPU
$ module load modtree/gpu # for GPU
```

Modules

- Lmod is a hierarchical module system, a module can only be loaded after loading the necessary compilers and MPI libraries that it depends on. A list of all available modules can be found by:

```
$ module spider
```

- The module spider command can also be used to search for specific module names.

```
$ module spider intel # all modules with names containing 'intel'
```

- To unload a module

```
$ module unload mymodulename
```

Modules

- To unload all loaded modules and reset everything to original state.

```
$ module purge
```

- To see all available modules that are compatible with current loaded modules

```
$ module avail
```

- To display information about a specified module, including environment changes, dependencies, software version and path.

```
$ module show mymodulename
```

- Show all modules currently loaded in my environment:

```
$ module list
```

Example: Modules

$ module list # Show all modules currently loaded in my environment

Currently Loaded Modules:

This default environment can be loaded by *$ module load modtree/cpu*

1) gmp/6.2.1 2) mpfr/4.0.2 3) mpc/1.1.0 4) zlib/1.2.11 5) gcc/11.2.0 6) libfabric/1.12.0 7) numactl/2.0.14 8) openmpi/4.0.6 9) modtree/cpu

$ module purge # To unload all loaded modules and reset everything to original state

$ module list

No modules loaded

Example: Modules

```
$ module load modtree/cpu          # To load the default CPU environment recommended by the Anvil team

$ module list

Currently Loaded Modules:

  1) gmp/6.2.1   2) mpfr/4.0.2   3) mpc/1.1.0   4) zlib/1.2.11   5) gcc/11.2.0   6) libfabric/1.12.0   7) numactl/2.0.14   8) openmpi/4.0.6   9) modtree/cpu

$ module unload openmpi/4.0.6      # To unload the openmpi/4.0.6  module

$ module list

Currently Loaded Modules:

  1) gmp/6.2.1   2) mpfr/4.0.2   3) mpc/1.1.0   4) zlib/1.2.11   5) gcc/11.2.0   6) modtree/cpu
```

When unload *openmpi* module, two more dependent modules are removed.

Example: Modules

```
$ module spider openmpi                  # Report all the versions for the modules that match “openmpi ”
----------------------------------------------------------------------------------------------------------------------------------------------------------
openmpi:
----------------------------------------------------------------------------------------------------------------------------------------------------------
Versions:
       openmpi/3.1.6
       openmpi/4.0.6 …


$ module spider openmpi/4.0.6          # Report detailed information on a particular module version openmpi/4.0.6
----------------------------------------------------------------------------------------------------------------------------------------------------------
openmpi: openmpi/4.0.6
----------------------------------------------------------------------------------------------------------------------------------------------------------
  You will need to load all module(s) on any one of the lines below before the "openmpi/4.0.6" module is available to load.
    aocc/3.1.0      gcc/10.2.0      gcc/11.2.0      gcc/8.4.1      intel/19.0.5.281
  Help:
    An open source Message Passing Interface implementation. The Open MPI Project is an open source Message Passing
Interface implementation that
    is developed and maintained by a consortium of academic, research, and industry partners. Open MPI is therefore able to
combine the expertise …
```

Agenda

3. Compilation and programing environment

- Module system
- **Provide software and software installation policy**
- Compiling source code (examples and explanation)

Provide Software

Programming Libraries & Compilers	• Various popular programming languages, GNU, Intel and AOCC compilers, message passing libraries • Workflow, data management and analysis tools • Debugging and profiling tools
Scientific Applications	• General purpose mathematics and statistics modeling tools, visualization tools • Broad application base with installs and modules from various science and engineering domains
Containers and Datasets	• Support for Singularity containerization and execution (e.g. NGC, BioContainers) • Efficient access to various databases (e.g., NCBI)

Provide Software: https://purduercac-applications.readthedocs.io/en/latest/

Need additional software? Please see the **Software Installation Request Policy**.

Agenda

3. Compilation and programing environment

- Module system
- Provide software and software installation policy
- **Compiling source code (examples and explanation)**

Supported Compilers

CPU nodes

Compilers: GNU, Intel, AOCC (AMD)

MPI implementations: OpenMPI, Intel MPI (IMPI) and MVAPICH2

All compilers installed on Anvil include OpenMP functionality for C, C++, and Fortran

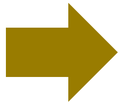
GPU nodes

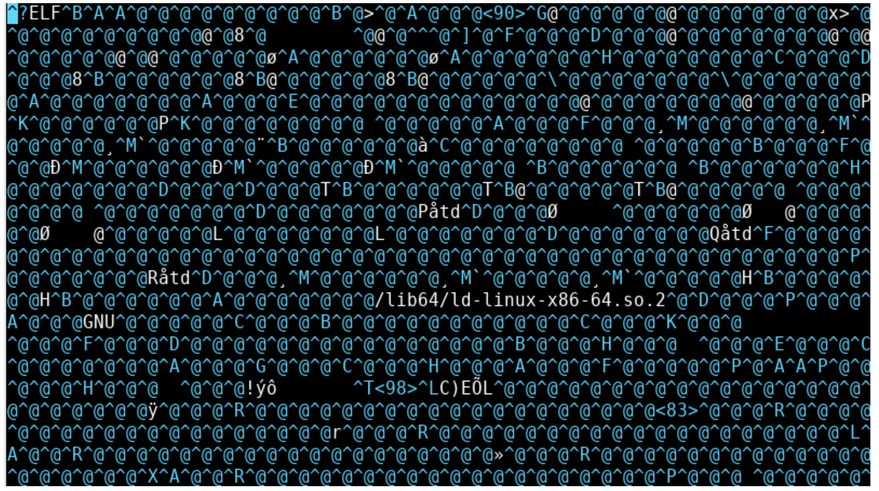
- The GPU nodes on Anvil support CUDA and OpenCL
- **OpenACC** functionality are support by:
  - **PGI** compilers through the ***nvhpc*** modules
  - **GNU** compiler through ***gcc/11.2.0-openacc*** module
- Some GPU codes may require compiled on the GPU nodes through an interactive session.

Example: Compiling Serial C++ Code

```cpp
//  C++

#include <iostream>
#include <unistd.h>

using namespace std;

int main () {
    int len=30;
    char name[30];
    gethostname(name,len);      // get run-host name
    cout << "Runhost:" << name << "    hello, world\n" << endl;
    return 0;
}
```

Source code: serial_hello.cpp





Machine code: serial

```
$ module list
Currently Loaded Modules:
  1) gmp/6.2.1   2) mpfr/4.0.2   3) mpc/1.1.0   4) zlib/1.2.11   5) gcc/11.2.0   6) libfabric/1.12.0   7) numactl/2.0.14   8) openmpi/4.0.6   9) modtree/cpu

$ g++ serial_hello.cpp -o serial          # Complie the c++ code with GNU compiler

$ ls
serial_hello.cpp     serial               # Executable files generated

$ ./serial

Runhost:a600.anvil.rcac.purdue.edu   hello, world
```

Compiling Serial Programs

The following table illustrates how to compile your serial program:			
Language	**Intel Compiler**	**GNU Compiler**	**AOCC Compiler**
Fortran 77	$ ifort myprogram.f -o myprogram	$ gfortran myprogram.f -o myprogram	$ flang program.f -o program
Fortran 90	$ ifort myprogram.f90 -o myprogram	$ gfortran myprogram.f90 -o myprogram	$ flang program.f90 -o program
Fortran 95	$ ifort myprogram.f90 -o myprogram	$ gfortran myprogram.f95 -o myprogram	$ flang program.f90 -o program
C	$ icc myprogram.c -o myprogram	$ gcc myprogram.c -o myprogram	$ clang program.c -o program
C++	$ icc myprogram.cpp -o myprogram	$ g++ myprogram.cpp -o myprogram	$ clang++ program.C -o program

*Intel compiler does not recognize the suffix ".f95". You may use ".f90" to stand for any Fortran code regardless of version as it is a free-formatted form

Compiling MPI Programs

The following table illustrates how to compile your MPI program. Any compiler flags accepted by Intel ifort/icc compilers are compatible with their respective MPI compiler.		
Language	**Intel Compiler with Intel MPI (IMPI)**	**Intel/GNU/AOCC Compiler with OpenMPI/MVAPICH2**
Fortran 77	$ mpiifort myprogram.f -o myprogram	$ mpif77 myprogram.f -o myprogram
Fortran 90	$ mpiifort myprogram.f90 -o myprogram	$ mpif90 myprogram.f90 -o myprogram
Fortran 95	$ mpiifort myprogram.f90 -o myprogram	$ mpif90 myprogram.f90 -o myprogram
C	$ mpiicc myprogram.c -o myprogram	$ mpicc myprogram.c -o myprogram
C++	$ mpiicc myprogram.C -o myprogram	$ mpicxx myprogram.C -o myprogram

*Intel compiler does not recognize the suffix ".f95". You may use ".f90" to stand for any Fortran code regardless of version as it is a free-formatted form

Compiling OpenMP Programs

The following table illustrates how to compile your shared-memory program. Any compiler flags accepted by Intel ifort/icc compilers are compatible with OpenMP.

Language	Intel Compiler	GNU Compiler	AOCC Compiler
Fortran 77	$ ifort -openmp myprogram.f -o myprogram	$ gfortran -fopenmp myprogram.f -o myprogram	$ flang -fopenmp myprogram.f -o myprogram
Fortran 90	$ ifort -openmp myprogram.f90 -o myprogram	$ gfortran -fopenmp myprogram.f90 -o myprogram	$ flang -fopenmp myprogram.f90 -o myprogram
Fortran 95	$ ifort -openmp myprogram.f90 -o myprogram	$ gfortran -fopenmp myprogram.f90 -o myprogram	$ flang -fopenmp myprogram.f90 -o myprogram
C	$ icc -openmp myprogramram.c -o myprogram	$ gcc -fopenmp myprogram.c -o myprogram	$ clang -fopenmp myprogram.c -o myprogram
C++	$ icc -openmp myprogram.cpp -o myprogram	$ g++ -fopenmp myprogram.cpp -o myprogram	$ clang++ -fopenmp myprogram.cpp -o myprogram

*Intel compiler does not recognize the suffix ".f95". You may use ".f90" to stand for any Fortran code regardless of version as it is a free-formatted form

Compiling Hybrid Programs

The following tables illustrate how to compile your hybrid (MPI/OpenMP) program. Any compiler flags accepted by Intel ifort/icc compilers are compatible with their respective MPI compiler.		
Language	**Intel Compiler with Intel MPI(IMPI)**	**Intel/GNU/AOCC Compiler with OpenMPI/MVAPICH2**
Fortran 77	$ mpiifort -qopenmp myprogram.f -o myprogram	$ mpif77 -fopenmp myprogram.f -o myprogram
Fortran 90	$ mpiifort -qopenmp myprogram.f90 -o myprogram	$ mpif90 -fopenmp myprogram.f90 -o myprogram
Fortran 95	$ mpiifort -qopenmp myprogram.f90 -o myprogram	$ mpif90 -fopenmp myprogram.f90 -o myprogram
C	$ mpiicc -qopenmp myprogram.c -o myprogram	$ mpicc -fopenmp myprogram.c -o myprogram
C++	$ mpiicpc -qopenmp myprogram.C -o myprogram	$ mpicxx -fopenmp myprogram.C -o myprogram

*Intel compiler does not recognize the suffix ".f95". You may use ".f90" to stand for any Fortran code regardless of version as it is a free-formatted form

Compiling NVIDIA GPU Programs

Both login and GPU-enabled compute nodes have the CUDA tools and libraries for compiling CUDA programs.

But if code require CUDA drive, you need to submit an interactive job to get to the GPU nodes. The ***gpu-debug*** queue is ideal for this case.

```
$ module load modtree/gpu

$ nvcc gpu_hello.cu -o gpu_hello

./gpu_hello

No GPU specified, using first GPUhello, world
```

Agenda

4. Running jobs

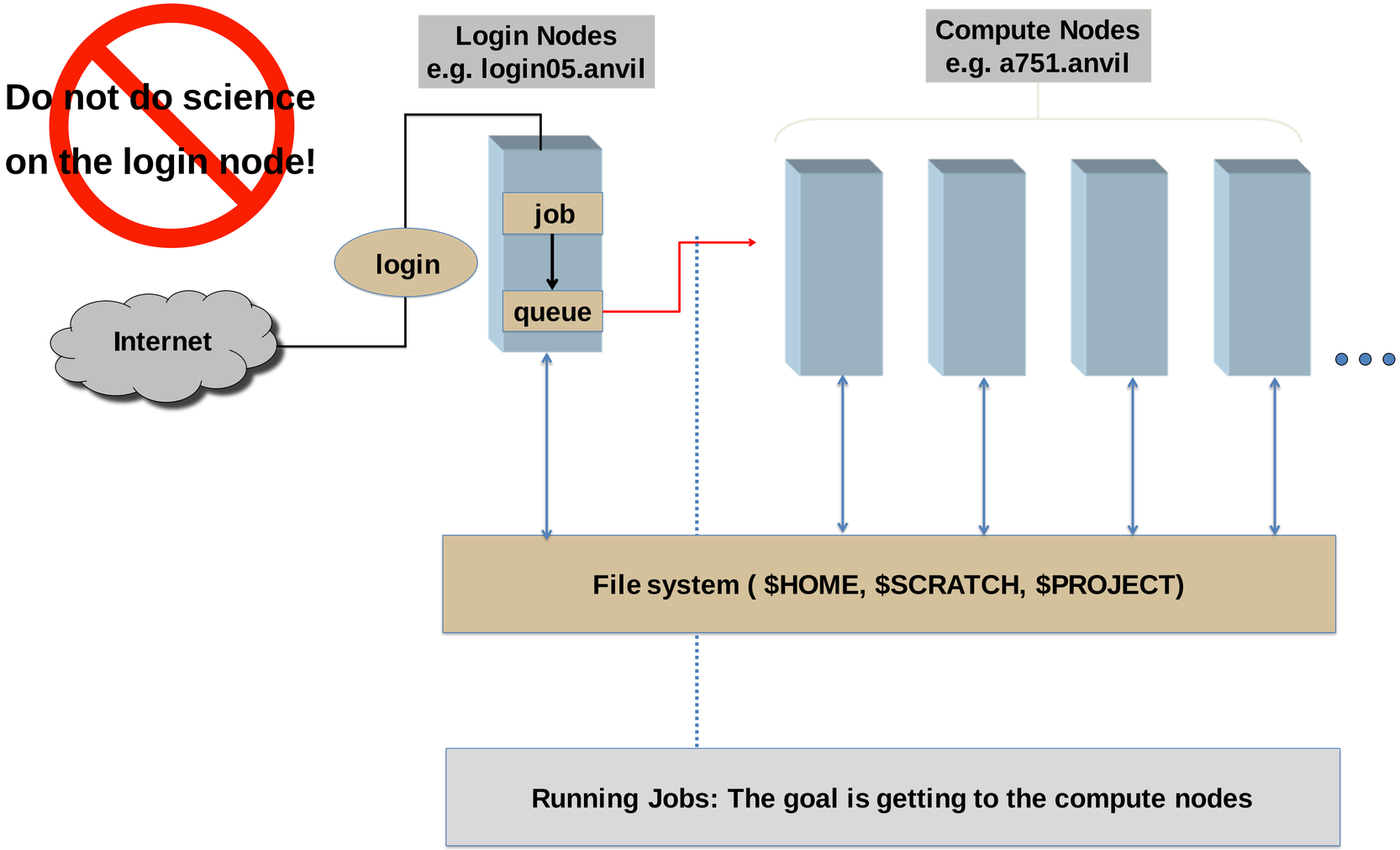
- Accessing to compute node
- Interactive jobs
- Job accounting
- Available queues
- Batch jobs & Examples

Agenda

4. Running jobs

- **Accessing to compute node**
- Interactive jobs
- Batch jobs & Examples
- Job accounting
- Available queues

LOGIN NODE VS COMPUTE NODE



Agenda

4. Running jobs

- Access to compute node
- **Interactive jobs**
- Batch jobs & Examples
- Job Accounting
- Available queues

Interactive Computing

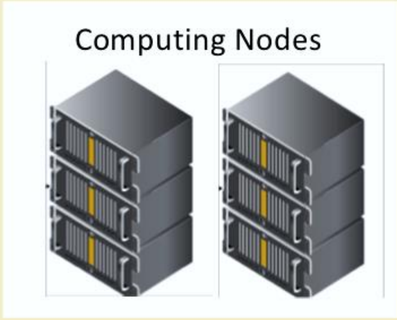
Interactive job: a job that occurs interactively with end users

Run simulations

Acquire simulation results

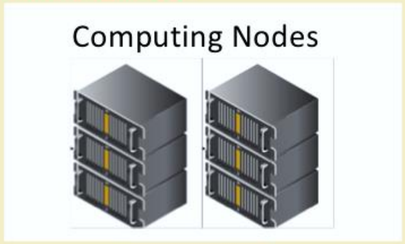
Process input data

Acquire output data



Batch job: a job that does not need user interactions

Job queue



Interactive Job

- You can use the ***sinteractive*** command to run your job in an interactive session.
- ***sinteractive*** accepts most of the same resource requests as ***sbatch***
- To quit your interactive job: ***exit*** or ***Ctrl-D***

```
$ sinteractive -N 2 -n 256 -A myallocation -t 00:30:00

salloc: Granted job allocation 198543

salloc: Waiting for resource configuration

salloc: Nodes a[478-479] are ready for job
```

This example asked for 2 nodes.

128 cores on each node.

The time limit is 30 mins.

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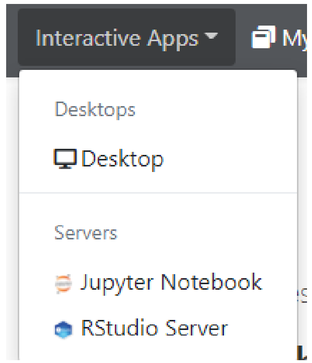
Interactive Computing

Gateway

Remote Desktop

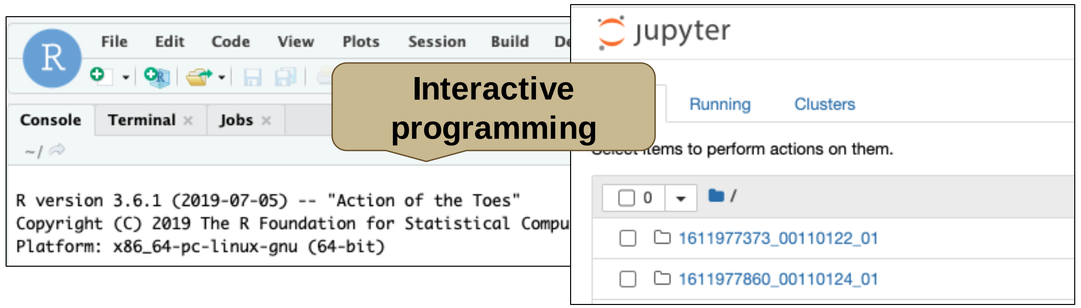
Low Barrier & Familiar Access to Compute

Quicker develop / test / debug cycle



Run GUI apps as job: Matlab, Fluent, Windows VM

Job manager and composer



Interactive programming

Interactive scientific applications

- Interactive SLURM job
- Jupyter Lab (Interactive Slurm job)
- Jupyter Notebook (Interactive Slurm job)
- MATLAB (interactive SLURM job)
- Rstudio (interactive SLURM job)
- VMD (Interactive Slurm job)

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Agenda

4. Running jobs

- Access to compute node
- Interactive jobs
- **Batch jobs & Examples**
- Job Accounting
- Available queues

Batch Script example: Serial Job in Shared Queue

```
#!/bin/bash
# FILENAME:  myjobsubmissionfile

#SBATCH -A myallocation          # Allocation name
#SBATCH --nodes=1                # Total # of nodes (must be 1 for serial job)
#SBATCH --ntasks=1               # Total # of tasks (should be 1 for serial job)
#SBATCH --time=1:30:00           # Total run time limit (hh:mm:ss)
#SBATCH -J myjobname             # Job name
#SBATCH -o myjob.o%j             # Name of stdout output file
#SBATCH -e myjob.e%j             # Name of stderr error file
#SBATCH -p shared                # Queue (partition) name
#SBATCH --mail-user=useremailaddress

# Manage processing environment, load compilers and applications.
module purge
module load compilername
module load applicationname
module list

# Launch serial code
./myexecutablefiles
```

Common Slurm Commands

- Submit jobs

```
$ sbatch mysubmissionfile

Submitted batch job 188
```

- Kill a job

```
$ scancel myjobid
```

- Check job status

```
$ squeue -u myusername (or squeue --me)

  JOBID   PARTITION   NAME    USER       ST   TIME   NODES
  188     wholenode   job1    myusername R    0:14   2
  189     wholenode   job2    myusername PD   0:00   1
```

R -- running

PD -- pending

Common Slurm Commands

- Check queued or running job information

```
$ scontrol show job 189

JobId=189 JobName=myjobname

     UserId=myusername GroupId=mygroup MCS_label=N/A

     Priority=103076 Nice=0 Account=myacct QOS=normal

     JobState=RUNNING Reason=None Dependency=(null)

     Requeue=1 Restarts=0 BatchFlag=0 Reboot=0 ExitCode=0

     RunTime=00:01:28 TimeLimit=00:30:00 TimeMin=N/A

     SubmitTime=2021-10-04T14:59:52 EligibleTime=2021-10-04T14:59:52

     AccrueTime=Unknown

    StartTime=2021-10-04T14:59:52 EndTime=2021-10-04T15:29:52 Deadline=N/A

...
```

JobState: if the job is Pending, Running, Completed, or Held.

RunTime & **TimeLimit:** how long the job has run and maximum run time.

SubmitTime: when the job was submitted to the cluster.

WorkDir: the job's working directory.

StdOut & **Stderr:** locations of stdout and stderr of the job.

Reason: why a PENDING job isn't running.

Common Slurm Commands

- Check historic (completed) job information

```
$ jobinfo 189

Name          : interactive
User          : hong400
Account       : rcac
Partition     : wholenode
Nodes         : a010
Cores         : 1
GPUs          : 0
State         : TIMEOUT
ExitCode      : 0:0
Submit        : 2021-10-04T14:59:52
Start         : 2021-10-04T14:59:52
End           : 2021-10-04T15:30:20
Waited        : 00:00:00
…
```

Example: Submit a batch job

1. cd sbatch-test # go to the sbatch-test folder

2. ls

hello.py myjobsubmitscript

3. sbatch myjobsubmitscript # submit a sbatch job

Submitted batch job XXXXXX

4. squeue -u myusername or squeue –me # check job status under myusername

Example: Submit a batch job

5. scontrol show job XXXXXX # check queued or running job information with my jobID

6. scancel XXXXXX # kill the job with my jobID

7. jobinfo XXXXXX # check historic (completed) job information with my jobID

8. vi myjob.oXXXXXX # check job output file

9. vi myjob.eXXXXXX # check job error file

MPI Job in Wholenode Queue

```
#!/bin/bash
# FILENAME:  myjobsubmissionfile

#SBATCH -A myallocation     # Allocation name
#SBATCH --nodes=2           # Total # of nodes
#SBATCH --ntasks=256        # Total # of tasks
#SBATCH --time=1:30:00      # Total run time limit (hh:mm:ss)
#SBATCH -p wholenode        # Queue (partition) name

# Manage processing environment, load compilers and applications.
module purge
module load compilername
module load mpilibrary
module load applicationname
module list

# Launch MPI code
mpirun -np $SLURM_NTASKS myexecutablefiles
```

OpenMP Job in Wholenode Queue

```
#!/bin/bash
# FILENAME:  myjobsubmissionfile

#SBATCH -A myallocation        # Allocation name
#SBATCH --nodes=1              # Total # of nodes (must be 1 for OpenMP job)
#SBATCH --ntasks=1             # Total # of tasks
#SBATCH --cpus-per-task=128    # cpu-cores per task (default value is 1, >1 for multi-threaded tasks)
#SBATCH --time=1:30:00         # Total run time limit (hh:mm:ss)
#SBATCH -p wholenode           # Queue (partition) name

# Manage processing environment, load compilers and applications.
module purge
module load compilername
module load applicationname
module list

# Set thread count (default value is 1).
export OMP_NUM_THREADS=$SLURM_CPUS_PER_TASK

# Launch OpenMP code
./myexecutablefiles
```

When running OpenMP programs, all threads must be on the same compute node to take advantage of shared memory. The threads cannot communicate between nodes.

Hybrid Job in Wholenode Queue

```
#!/bin/bash
# FILENAME:  myjobsubmissionfile

#SBATCH -A myallocation          # Allocation name
#SBATCH --nodes=2                # Total # of nodes
#SBATCH --ntasks-per-node=2      # Total # of MPI tasks per node
#SBATCH --cpus-per-task=64       # cpu-cores per task (default value is 1, >1 for multi-threaded tasks)
#SBATCH --time=1:30:00           # Total run time limit (hh:mm:ss)
#SBATCH -p wholenode             # Queue (partition) name

# Manage processing environment, load compilers and applications.
module purge
module load compilername
module load mpilibrary
module load applicationname
module list

# Set thread count (default value is 1).
export OMP_NUM_THREADS=$SLURM_CPUS_PER_TASK

# Launch MPI code
mpirun -np $SLURM_NTASKS myexecutablefiles
```

This example asks for 4 MPI tasks

2 MPI tasks per node

Each with 64 OpenMP threads

Total of 256 CPU-cores

GPU job in GPU queue

```
#!/bin/bash
# FILENAME:  myjobsubmissionfile

#SBATCH -A myGPUallocation  # Allocation name for GPU
#SBATCH --nodes=1           # Total # of nodes (must be 1 for serial job)
#SBATCH --ntasks=1          # Total # of tasks
#SBATCH --gpus-per-node=1   # Number of GPUs per node
#SBATCH --time=1:30:00      # Total run time limit (hh:mm:ss)
#SBATCH -p gpu              # Queue (partition) name
#SBATCH --mail-user=useremailaddress
#SBATCH --mail-type=all     # Send email to above address at begin and end of job

# Manage processing environment, load compilers and applications.
module purge
module load modtree/gpu
module load applicationname
module list

# Launch GPU code
./myexecutablefiles
```

When running on multiple GPUs with MPI, you need to ensure one MPI rank per GPU.

Make sure to use ***gpus-per-node=1***. Otherwise, your job may not run properly.

You can use ***sfeatures*** command to see the detailed hardware overview.

NGC GPU Container Job in GPU Queue

What is NGC?

- Nvidia GPU Cloud (NGC) is a GPU-accelerated cloud platform optimized for deep learning and scientific computing.
- Anvil team provides pre-downloaded NGC containers as convenient modules, so that you can use NGC containers as non-containerized versions of each application. More information can be found at **Anvil NGC containers**: https://www.rcac.purdue.edu/knowledge/anvil/run/examples/slurm/ngc

On Anvil, type the command below to see the lists of NGC containers we deployed:

```
$ module load modtree/gpu
$ module load ngc
$ module avail
---------------------------------------------------------------------------------------------------------------------------------------------------------- /opt/spack/ngc ----------------------------------------------------------------------------------------------------------------------------------------------------------
   autodock/2020.06                 namd/2.13-multinode              pytorch/20.11-py3                rapidsai/0.17                    tensorflow/20.06-tf2-py3
   gamess/17.09-r2-libcchem         namd/2.13-singlenode      (D)    pytorch/20.12-py3                rapidsai/21.06                   tensorflow/20.11-tf1-py3
   gromacs/2018.2                   namd/3.0-alpha3-singlenode       pytorch/21.06-py3                rapidsai/21.10            (D)    tensorflow/20.11-tf2-py3
   gromacs/2020.2                   nvhpc/20.7                       pytorch/21.09-py3         (D)    relion/2.1.b1                    tensorflow/20.12-tf1-py3
   gromacs/2021                     nvhpc/20.9                       qmcpack/v3.5.0                   relion/3.1.0                     tensorflow/20.12-tf2-py3
   gromacs/2021.3            (D)    nvhpc/20.11                      quantum_espresso/v6.6a1          relion/3.1.2                     tensorflow/21.06-tf1-py3
   julia/v1.5.0                     nvhpc/21.5                       quantum_espresso/v6.7     (D)    relion/3.1.3              (D)    tensorflow/21.06-tf2-py3
   julia/v2.4.2                     nvhpc/21.9                (D)    rapidsai/0.12                    tensorflow/20.02-tf1-py3         tensorflow/21.09-tf1-py3
   lammps/10Feb2021                 paraview/5.9.0                   rapidsai/0.13                    tensorflow/20.02-tf2-py3         tensorflow/21.09-tf2-py3 (D)
   lammps/15Jun2020                 pytorch/20.02-py3                rapidsai/0.14                    tensorflow/20.03-tf1-py3         torchani/2021.04
   lammps/24Oct2018                 pytorch/20.03-py3                rapidsai/0.15                    tensorflow/20.03-tf2-py3
   lammps/29Oct2020                 pytorch/20.06-py3                rapidsai/0.16                    tensorflow/20.06-tf1-py3
```

NGC GPU Container Job in GPU Queue

```
#!/bin/bash
# FILENAME:  myjobsubmissionfile

#SBATCH -A myGPUallocation  # Allocation name for GPU
#SBATCH --nodes=1           # Total # of nodes (must be 1 for serial job)
#SBATCH --ntasks=1          # Total # of tasks
#SBATCH --gpus-per-node=1   # Number of GPUs per node
#SBATCH --time=1:30:00      # Total run time limit (hh:mm:ss)
#SBATCH -p gpu              # Queue (partition) name

# Manage processing environment, load compilers and applications.
module purge
module load modtree/gpu
module load ngc
module load applicationname
module list

# Launch GPU code
./myexecutablefiles
```

When running on multiple GPUs with MPI, you need to ensure one MPI rank per GPU.

Agenda

4. Running jobs

- Access to compute node
- Interactive jobs
- Batch jobs & Examples
- **Job Accounting**
- Available queues

Job Accounting

- For **CPU** jobs, the charge unit is **Service Unit (SU)**, i.e. 1 CPU using ≤ ~2G memory for 1 hour, based on the actual resources tied up by your job.

  Example: a 4 cores + 2 hours job:

  - Submitted to **shared** queues job
    - if mem ≤ ~8G, charge = 4 cores x 2 hours = **8 SU**
    - if mem = 9G, charge = 5 cores x 2 hours = **10 SU**
  - Submitted to **node-exclusive** job, all **128** cores will be charged, even if only 4 cores are used, charge = 128 cores x 2 hours = **256 SU**

  Jobs submitted to the **large memory nodes** will be charged **4 SU per core** (4x wholenode charge).

- For **GPU** jobs, 1 SU is 1 GPU using ≤ ~64G memory for 1 hour. 4 GPU on a node. All GPU nodes are **shared**.
- Filesystem storage is not charged.

Agenda

4. Running jobs

- Access to compute node
- Interactive jobs
- Batch jobs & Examples
- Job Accounting
- **Available queues**

Slurm Partitions (Queues)

Anvil Production Queues							
Queue Name	Node Type	Max Nodes per Job	Max Cores per Job	Max Duration	Max running Jobs in Queue	Max running + submitted Jobs in Queue	Charging factor
debug	regular	2 nodes	256 cores	2 hrs	1	2	1
gpu-debug	gpu	1 node	2 gpus	0.5 hrs	1	2	1
DEFAULT **wholenode**	regular	16 nodes	2,048 cores	96 hrs	64	128	1
wide	regular	56 nodes	7,168 cores	12 hrs	5	10	1
shared	regular	1 node	128 cores	96 hrs	6400 cores		1
highmem	large-memory	1 node	128 cores	48 hrs	2	4	4
gpu	gpu			48 hrs	8 gpus		1

* For **gpu** queue: max of 12 GPU per job and max of 32 GPU in use by a single group.

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Slurm Partitions (Queues)

$ showpartitions

Partition statistics for cluster anvil at Tue Jun 21 11:02:14 EDT 2022

Partition		#Nodes		#CPU_cores		Cores_pending		Job_Nodes		MaxJobTime	Cores	Mem/Node
Name	State	Total	Idle	Total	Idle	Resorc	Other	Min	Max	Day-hr:mn	/node	(GB)
wholenode:*	up	750	637	96000	81536	0	897	1	infin	infinite	128	257
~~standard~~	~~up~~	~~750~~	~~637~~	~~96000~~	~~81536~~	~~0~~	~~20676~~	~~1~~	~~infin~~	~~infinite~~	~~128~~	~~257~~
shared	up	250	245	32000	31551	0	0	1	infin	infinite	128	257
wide	up	750	637	96000	81536	0	0	1	infin	infinite	128	257
highmem	up	32	32	4096	4096	0	0	1	infin	infinite	128	1031
debug	up	17	17	2176	2176	0	0	1	infin	infinite	128	257
gpu	up	16	8	2048	1911	0	96	1	infin	infinite	128	515
gpu-debug	up	16	8	2048	1911	0	0	1	infin	infinite	128	515

* wholenode is the default partition.

standard partition will be removed soon.

Agenda

5. Data management and transfer

- File system
- Scp, Rsync, SFTP, Globus
- Lost file recovery

Agenda

5. Data management and transfer

- **File system**
- Scp, Rsync, SFTP, Globus
- Lost file recovery

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File Systems

Anvil File Systems					
File System	**Mount Point**	**Quota**	**Snapshots**	**Purpose**	**Purge policy**
Anvil ZFS	/home **$HOME**	25 GB	Full schedule*	Home directories: area for storing personal software, scripts, compiling, editing, etc.	Not purged
Anvil ZFS	/apps	N/A	Weekly*	Applications	
Anvil GPFS	/anvil	N/A	No		
Anvil GPFS	/anvil/scratch **$SCRATCH**	100 TB	No	User scratch: area for job I/O activity, temporary storage	Files older than 30-day (access time) will be purged
Anvil GPFS	/anvil/projects **$PROJECT or $WORK**	5 TB	Full schedule*	Per allocation: area for shared data in a project, common datasets and software installation	Not purged while allocation is active. Removed 90 days after allocation expiration
Anvil GPFS	/anvil/datasets	N/A	Weekly*	Common data sets (not allocated to users)	
Versity	N/A (Globus)	20 TB	No	Tape storage per allocation	

* Full schedule keeps nightly snapshots for 7 days, weekly snapshots for 3 weeks, and monthly snapshots for 2 months.

File Systems

To check the quota of different file systems, type ***myquota*** at the command line.

```
x-anvilusername@login03.anvil:[~] $ myquota

Type       Location             Size          Limit      Use       Files    Limit    Use

=============================================================================

home       x-anvilusername   261.5MB     25.0GB     1%          -          -          -

scratch    anvil                 6.3GB       100.0TB    0.01%     3k       1,048k   0.36%

projects   accountname1      37.2GB       5.0TB       0.73%     403k     1,048k   39%

projects   accountname2      135.8GB     5.0TB       3%         20k      1,048k   2%
```

Agenda

5. Data management and transfer

- File system
- **Scp, Rsync, SFTP, Globus**
- Lost file recovery

Transferring Files

Users can transfer files between Anvil and Linux-based systems or Mac or windows terminal using either ***scp*** or ***rsync*** or ***SFTP***.

- **SCP** (Secure CoPy) is a simple way of transferring files between two machines that use the SSH protocol.

  NOTE: SSH Keys is ***required*** for SCP.

  Following is an example of transferring a ***test.txt*** file from Anvil home directory to local machine, make sure to use your anvil user name **x-anvilusername**:

```
localhost> scp x-anvilusername@anvil.rcac.purdue.edu:/home/x-anvilusername/test.txt .

Warning: Permanently added the xxxxxxx host key for IP address 'xxx.xxx.xxx.xxx' to the list of known hosts.

test.txt                                      100%    0     0.0KB/s   00:00
```

Transferring Files

Users can transfer files between Anvil and Linux-based systems or Mac or windows terminal using either ***scp*** or ***rsync*** or ***SFTP***.

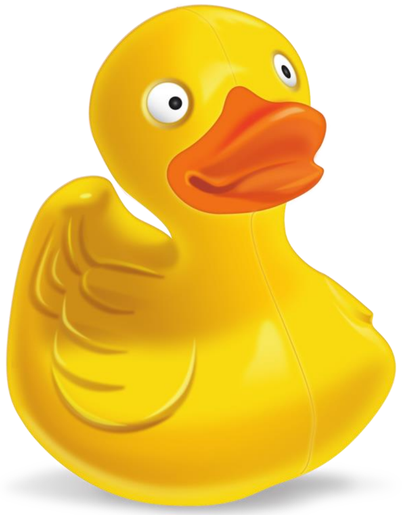
- **Rsync**, or Remote Sync lets you transfer files and directories to local and remote destinations. It allows to copy only the changes from the source and offers customization, use for mirroring, performing backups, or migrating data between different filesystems.

  NOTE: SSH Keys is ***required*** for Rsync. Also make sure to use your anvil user name **x-anvilusername**:

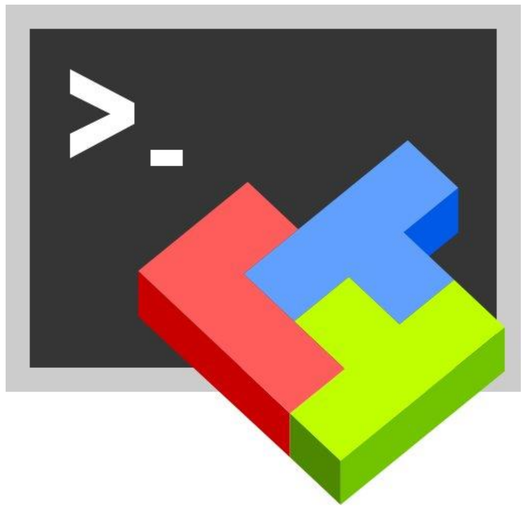
Transferring Files

- **SFTP** (Secure File Transfer Protocol) is available as graphical file transfer programs and as a command-line program. **SFTP** has more features than **SCP** and allows for other operations on remote files, remote directory listing, and resuming interrupted transfers.

- More details can be found at **Anvil File Transfer-SFTP:** www.rcac.purdue.edu/knowledge/anvil/storage/transfer/sftp



Cyberduck for Mac OS X



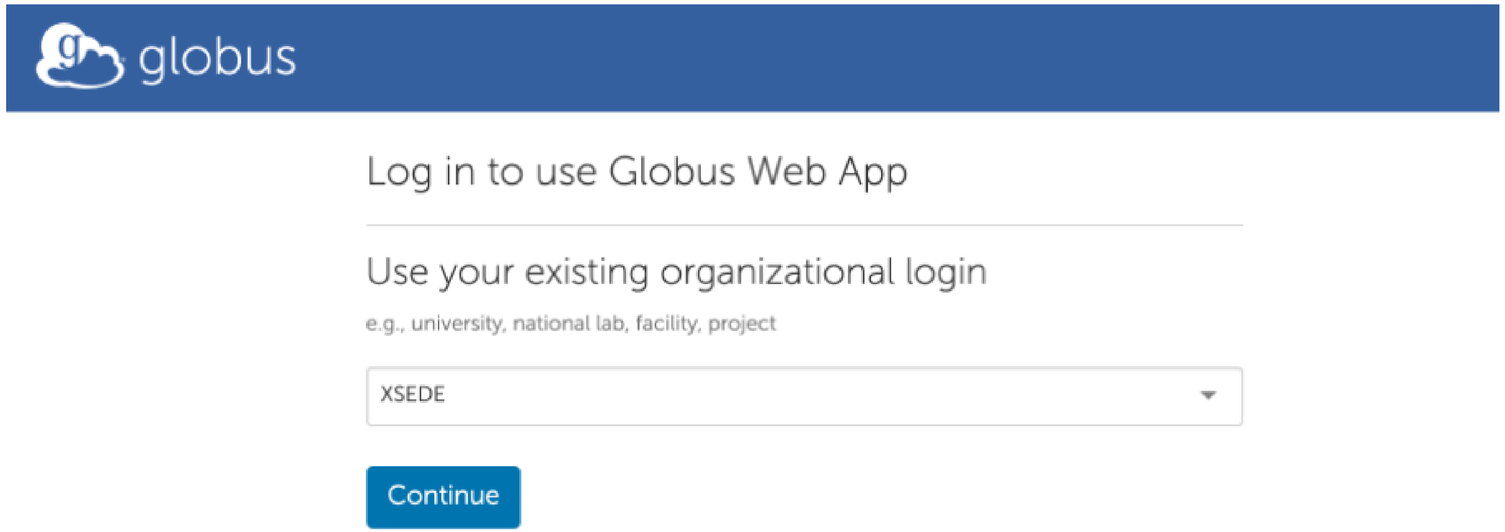
MobaXterm for Microsoft Windows

Transferring Files

- **Globus** is also a powerful and easy to use file transfer. It works between any XSEDE and non-XSEDE sites running Globus, and it connects any of these research systems to personal systems.

  You may use Globus to connect to your home, scratch, and project storage directories on Anvil. Since Globus is web-based, it works on any operating system connected to the internet.

  More details can be found at **XSEDE Data Transfer & Management:** https://portal.xsede.org/data-management



Agenda

5. Data management and transfer

- File system
- Scp, Rsync, SFTP, Globus
- **Lost file recovery**

Lost File Recovery

- Your ***$HOME*** and ***$PROJECT*** directories on Anvil are protected. A series of snapshots are taken every night after midnight. Each snapshot provides the state of your files at the time.

- These snapshots are kept for a limited time at various intervals. Please refer to **Anvil File Systems:** www.rcac.purdue.edu/knowledge/anvil/storage/filesystems for more detail.

- Only files saved during an overnight snapshot are recoverable. If you lose a file the same day you created it, the file is not recoverable.

- Snapshots are **not** a substitute for regular backups. For additional security, you might consider off-site back up important data (e.g. use Globus to transfer to your institution, etc)

Lost File Recovery

- If you know when you lost the file, you can use the ***flost*** command.
- The default location ***flost*** looks at is $HOME directory. For other location (e.g. in $PROJECT), you need to specify where the lost file was with ***-w*** argument.
- If you do not know the date, you may try entering different dates to ***flost***.
- Or you may manually browse the snapshots in ***/home/.zfs/snapshot*** folder for **$HOME** directory or ***/anvil/projects/.snapshots*** folder for $**PROJECT** directory.

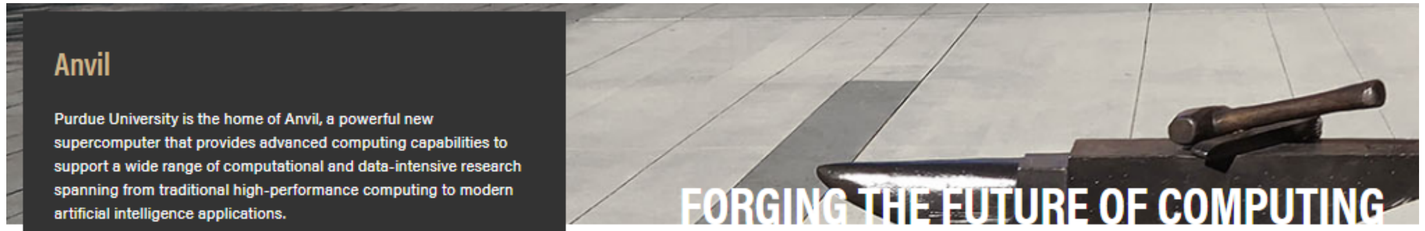
Agenda

6. Helpful tips

Helpful Tools

The Anvil cluster provides a list of useful auxiliary tools:

The following table provides a list of auxiliary tools:	
Tools	**Use**
myquota	Check the quota of different file systems
flost	A utility to recover files from snapshots
showpartitions	Display all Slurm partitions and their current usage
myscratch	Show the path to your scratch directory
jobinfo	Collates job information from the *sstat*, *sacct* and *squeue* SLURM commands to give a uniform interface for both current and historical jobs
sfeatures	Show the list of available constraint feature names for different node types.
myproject	print the location of my project directory
mybalance	Check the allocation usage of your project team



News & Events

Anvil Maintenance
June 2, 2022 8:00am - 6:00pm EDT

Archive

Overview

Anvil, built through a $10 million system acquisition from the National Science Foundation (NSF), and provides resources to the NSF's Extreme Science and Engineering Discovery Environment (XSEDE), which serves tens of thousands of researchers across the U.S., and in which Purdue has been a partner for the past nine years. Anvil entered production in February 2022 and will serve researchers for five years. Additional funding from the NSF will support Anvil's operations and user support.

The name "Anvil" reflects the Purdue Boilermakers' strength and workmanlike focus on producing results, and the Anvil supercomputer will enable important discoveries across many different areas of science and engineering. Anvil also will serve as an experiential learning laboratory for students to gain real-world experience using computing for their science, and for student interns to work with the Anvil team for construction and operation. We will be training the research computing practitioners of the future. Learn more about Anvil's mission in the Anvil press release.

Anvil is funded under NSF award number 2005632. Carol Song is the principal investigator and project director. Preston Smith, executive director of Research Computing, Xiao Zhu, computational scientist and senior research scientist, and Rajesh Kalyanam, data scientist, software engineer, and research scientist, are all co-PIs on the project.

www.rcac.purdue.edu/anvil

Documentation

ARCHITECTURE
Look over the specs and architecture to get an idea of what Anvil can do.

GETTING STARTED
Learn how to set up an account and connect to the system.

SUBMITTING JOBS
Learn how to submit jobs, check status, and output.

SOFTWARE
See the initial list of pre-installed software.

DATA MANAGEMENT
Learn about our file system and the ways to transfer files.

POLICIES & TIPS & FAQS
Know what to expect and what we expect from you.

THANK YOU!

Contact Us

For user support please submit a ticket at **Help Desk**, by selecting the appropriate Anvil resource to have it routed to us.