Delta User Guide

The Delta documentation has moved to https://docs.ncsa.illinois.edu/systems/delta/. Please update any bookmarks you may have. Click in the link above if you are not automatically redirected in 5 seconds.

Figures: Delta System (storage and compute)

Delta is supported by the National Science Foundation under Grant No. OAC-2005572.

Any opinions, findings, and conclusions or recommendations expressed in this material are those of the author(s) and do not necessarily reflect the views of the National Science Foundation.

***Delta* is now accepting proposals.**

Status Updates and Notices

Delta is in production.

System status, planned outages, and maintenance info:

current outages - https://support.access-ci.org/outages

infrastructure news - https://operations.access-ci.org/infrastructure_news.

Delta Affinity Group site with links to news, slack channel for users : https://support.access-ci.org/affinity-groups/delta.

key: light grey font is work in progress

Items in light grey font are in progress and coming soon. Example software or feature not yet implemented.

Introduction

Delta is a dedicated, ACCESS-allocated resource allocated resource designed by HPE and NCSA, delivering a highly capable GPU-focused compute environment for GPU and CPU workloads. Besides offering a mix of standard and reduced precision GPU resources, *Delta* also offers GPU-dense nodes with both NVIDIA and AMD GPUs. *Delta* provides high performance node-local SSD scratch filesystems, as well as both standard Lustre and relaxed-POSIX parallel filesystems spanning the entire resource.

Delta's CPU nodes are each powered by two 64-core AMD EPYC 7763 ("Milan") processors, with 256 GB of DDR4 memory. The *Delta* GPU resource has four node types: one with 4 NVIDIA A100 GPUs (40 GB HBM2 RAM each) connected via NVLINK and 1 64-core AMD EPYC 7763 ("Milan") processor, the second with 4 NVIDIA A40 GPUs (48 GB GDDR6 RAM) connected via PCIe 4.0 and 1 64-core AMD EPYC 7763 ("Milan") processor, the third with 8 NVIDIA A100 GPUs in a dual socket AMD EPYC 7763 (128-cores per node) node with 2 TB of DDR4 RAM and NVLINK, and the fourth with 8 AMD MI100 GPUs (32GB HBM2 RAM each) in a dual socket AMD EPYC 7763 (128-cores per node) node with 2 TB of DDR4 RAM and PCIe 4.0.

Delta has 124 standard CPU nodes, 100 4-way A100-based GPU nodes, 100 4-way A40-based GPU nodes, 5 8-way A100-based GPU nodes, and 1 8-way MI100-based GPU node. Every *Delta* node has high-performance node-local SSD storage (740 GB for CPU nodes, 1.5 TB for GPU nodes), and is connected to the 7 PB Lustre parallel filesystem via the high-speed interconnect. The *Delta* resource uses the SLURM workload manager for job scheduling.

Delta supports the ACCESS core software stack, including remote login, remote computation, data movement, science workflow support, and science gateway support toolkits.

Top of Page

Account Administration

- For ACCESS projects please use the ACCESS user portal for project and account management.
- Non-ACCESS Account and Project administration, such as adding a someone to a project, is handled by NCSA Identity and NCSA group management tools. For more information, please see the NCSA Allocation and Account Management documentation page.

Configuring Your Account

- Bash is the default shell, submit a support request to change your default shell
- Environment variables: ACCESS CUE, SLURM batch
- Using Modules

Allocation Policies

- ACCESS awarded projects and allocations should receive periodic messages regarding approaching project expiration.
  - ACCESS projects are marked for inactivation once it has no valid resource allocation on the system.
  - Current ACCESS policy is for user access to be removed for users who are not a member of any active project on Delta.
- Illinois awarded projects and allocations currently do not receive periodic messages regarding approaching project expiration.
  - Manual notifications are being provided as needed.
  - The Delta Project office is working on a process for notifications, project and account inactivation based on expiration dates.
- There is a 30-day grace-period for expired Delta projects to allow for data management access only..

Allocation Supplements and Extensions

Requests for resource allocation supplements (compute, GPU, or storage) and extensions can be made via the appropriate XRAS website.

- ACCESS allocation PIs can go to the ACCESS Manage Allocations page for instructions.
- NCSA allocation PIs can find instructions for requesting supplements and extensions at the Delta Allocations page.

System Architecture

Delta is designed to help applications transition from CPU-only to GPU or hybrid CPU-GPU codes. Delta has some important architectural features to facilitate new discovery and insight:

- A single processor architecture (AMD) across all node types: CPU and GPU

- Support for NVIDIA A100 MIG GPU partitioning allowing for fractional use of the A100s if your workload isn't able to exploit an entire A100 efficiently
- Ray tracing hardware support from the NVIDIA A40 GPUs
- Nine large memory (2 TB) nodes
- A low latency and high bandwidth HPE/Cray Slingshot interconnect between compute nodes
- Lustre for home, projects and scratch file systems
- support for relaxed and non-posix IO
- Shared-node jobs and the single core and single MIG GPU slice
- Resources for persistent services in support of Gateways, Open OnDemand, and Data Transport nodes.
- Unique AMD MI-100 resource

Top of Page

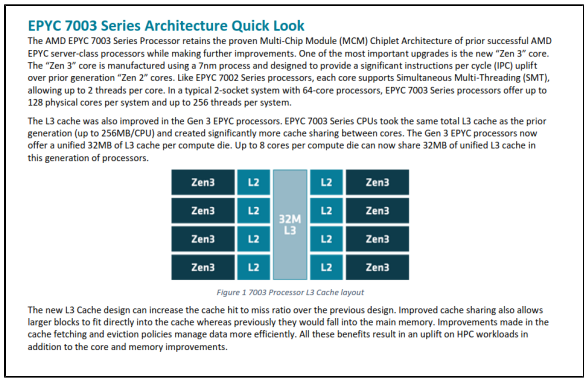
Model Compute Nodes

The Delta compute ecosystem is composed of five node types:

1. Dual-socket CPU-only compute nodes
2. Single socket 4-way NVIDIA A100 GPU compute nodes
3. Single socket 4-way NVIDIA A40 GPU compute nodes
4. Dual-socket 8-way NVIDIA A100 GPU compute nodes
5. Single socket 8-way AMD MI100 GPU compute nodes

The CPU-only and 4-way GPU nodes have 256 GB of RAM per node while the 8-way GPU nodes have 2 TB of RAM. The CPU-only node has 0.74 TB of local storage while all GPU nodes have 1.5 TB of local storage.

Each socket contains an AMD 7763 processor: https://www.amd.com/system/files/documents/amd-epyc-7003-sb-hpc-esi-vps.pdf Consistent with AMD's advice for HPC nodes and our own testing all Delta nodes have Simultaneous Multi Treading (SMT) turned off.



EPYC 7003 Series Architecture Quick Look

The AMD EPYC 7003 Series Processor retains the proven Multi-Chip Module (MCM) Chiplet Architecture of prior successful AMD EPYC server-class processors while making further improvements. One of the most important upgrades is the new "Zen 3" core. The "Zen 3" core is manufactured using a 7nm process and designed to provide a significant instructions per cycle (IPC) uplift over prior generation "Zen 2" cores. Like EPYC 7002 Series processors, each core supports Simultaneous Multi-Threading (SMT), allowing up to 2 threads per core. In a typical 2-socket system with 64-core processors, EPYC 7003 Series processors offer up to 128 physical cores per system and up to 256 threads per system.

The L3 cache was also improved in the Gen 3 EPYC processors. EPYC 7003 Series CPUs took the same total L3 cache as the prior generation (up to 256MB/CPU) and created significantly more cache sharing between cores. The Gen 3 EPYC processors now offer a unified 32MB of L3 cache per compute die. Up to 8 cores per compute die can now share 32MB of unified L3 cache in this generation of processors.

Figure 1 7003 Processor L3 Cache layout

The new L3 Cache design can increase the cache hit to miss ratio over the previous design. Improved cache sharing also allows larger blocks to fit directly into the cache whereas previously they would fall into the main memory. Improvements made in the cache fetching and eviction policies manage data more efficiently. All these benefits result in an uplift on HPC workloads in addition to the core and memory improvements.

Table. CPU Compute Node Specifications

Specification	Value
Number of nodes	132
CPU	AMD EPYC 7763 "Milan" (PCIe Gen4)
Sockets per node	2
Cores per socket	64
Cores per node	128
Hardware threads per core	1 (SMT off)
Hardware threads per node	128
Clock rate (GHz)	~ 2.45
RAM (GB)	256
Cache (KB) L1/L2/L3	64/512/32768
Local storage (TB)	0.74 TB

The AMD CPUs are set for 4 NUMA domains per socket (NPS=4).

Table. 4-way NVIDIA A40 GPU Compute Node Specifications

Specification	Value
Number of nodes	100
GPU	NVIDIA A40 (Vendor page)
GPUs per node	4
GPU Memory (GB)	48 DDR6 with ECC
CPU	AMD Milan
CPU sockets per node	1
Cores per socket	64
Cores per node	64
Hardware threads per core	1 (SMT off)
Hardware threads per node	64
Clock rate (GHz)	~ 2.45
RAM (GB)	256
Cache (KB) L1/L2/L3	64/512/32768
Local storage (TB)	1.5 TB

The AMD CPUs are set for 4 NUMA domains per socket (NPS=4).
The A40 GPUs are connected via PCIe Gen4 and have the following affinitization to NUMA nodes on the CPU. Note that the relationship between GPU index and NUMA domain are inverse.

Table. 4-way NVIDIA A40 Mapping and GPU-CPU Affinitization

	GPU0	GPU1	GPU2	GPU3	HSN	CPU Affinity	NUMA Affinity
GPU0	X	SYS	SYS	SYS	SYS	48-63	3
GPU1	SYS	X	SYS	SYS	SYS	32-47	2
GPU2	SYS	SYS	X	SYS	SYS	16-31	1
GPU3	SYS	SYS	SYS	X	PHB	0-15	0
HSN	SYS	SYS	SYS	PHB	X		

Table Legend

X = Self
SYS = Connection traversing PCIe as well as the SMP interconnect between NUMA nodes (e.g., QPI/UPI)
NODE = Connection traversing PCIe as well as the interconnect between PCIe Host Bridges within a NUMA node
PHB = Connection traversing PCIe as well as a PCIe Host Bridge (typically the CPU)
NV# = Connection traversing a bonded set of # NVLinks

Table. 4-way NVIDIA A100 GPU Compute Node Specifications

Specification	Value
Number of nodes	100
GPU	NVIDIA A100 (Vendor page)
GPUs per node	4
GPU Memory (GB)	40
CPU	AMD Milan
CPU sockets per node	1

Cores per socket	64
Cores per node	64
Hardware threads per core	1 (SMT off)
Hardware threads per node	64
Clock rate (GHz)	~ 2.45
RAM (GB)	256
Cache (KB) L1/L2/L3	64/512/32768
Local storage (TB)	1.5 TB

The AMD CPUs are set for 4 NUMA domains per socket (NPS=4).

Table. 4-way NVIDIA A100 Mapping and GPU-CPU Affinitization

	GPU0	GPU1	GPU2	GPU3	HSN	CPU Affinity	NUMA Affinity
GPU0	X	NV4	NV4	NV4	SYS	48-63	3
GPU1	NV4	X	NV4	NV4	SYS	32-47	2
GPU2	NV4	NV4	X	NV4	SYS	16-31	1
GPU3	NV4	NV4	NV4	X	PHB	0-15	0
HSN	SYS	SYS	SYS	PHB	X		

Table Legend

X = Self
SYS = Connection traversing PCIe as well as the SMP interconnect between NUMA nodes (e.g., QPI/UPI)
NODE = Connection traversing PCIe as well as the interconnect between PCIe Host Bridges within a NUMA node
PHB = Connection traversing PCIe as well as a PCIe Host Bridge (typically the CPU)
NV# = Connection traversing a bonded set of # NVLinks

Table. 8-way NVIDIA A100 GPU Large Memory Compute Node Specifications

Specification	Value
Number of nodes	6
GPU	NVIDIA A100 (Vendor page)
GPUs per node	8
GPU Memory (GB)	40
CPU	AMD Milan
CPU sockets per node	2
Cores per socket	64
Cores per node	128
Hardware threads per core	1 (SMT off)
Hardware threads per node	128
Clock rate (GHz)	~ 2.45
RAM (GB)	2,048
Cache (KB) L1/L2/L3	64/512/32768
Local storage (TB)	1.5 TB

The AMD CPUs are set for 4 NUMA domains per socket (NPS=4).

Table. 8-way NVIDIA A100 Mapping and GPU-CPU Affinitization

	GPU0	GPU1	GPU2	GPU3	GPU4	GPU5	GPU6	GPU7	HSN	CPU Affinity	NUMA Affinity
GPU0	X	NV12	NV12	NV12	NV12	NV12	NV12	NV12	SYS	48-63	3
GPU1	NV12	X	NV12	NV12	NV12	NV12	NV12	NV12	SYS	48-63	3
GPU2	NV12	NV12	X	NV12	NV12	NV12	NV12	NV12	SYS	16-31	1
GPU3	NV12	NV12	NV12	X	NV12	NV12	NV12	NV12	SYS	16-31	1
GPU4	NV12	NV12	NV12	NV12	X	NV12	NV12	NV12	SYS	112-127	7
GPU5	NV12	NV12	NV12	NV12	NV12	X	NV12	NV12	SYS	112-127	7
GPU6	NV12	NV12	NV12	NV12	NV12	NV12	X	NV12	SYS	80-95	5
GPU7	NV12	NV12	NV12	NV12	NV12	NV12	NV12	X	SYS	80-95	5
HSN	SYS	SYS	SYS	SYS	SYS	SYS	SYS	SYS	X		

Table Legend

X = Self
SYS = Connection traversing PCIe as well as the SMP interconnect between NUMA nodes (e.g., QPI/UPI)
NODE = Connection traversing PCIe as well as the interconnect between PCIe Host Bridges within a NUMA node
PHB = Connection traversing PCIe as well as a PCIe Host Bridge (typically the CPU)
NV# = Connection traversing a bonded set of # NVLinks

Table. 8-way AMD MI100 GPU Large Memory Compute Node Specifications

Specification	Value
Number of nodes	1
GPU	AMD MI100 (Vendor page)
GPUs per node	8
GPU Memory (GB)	32
CPU	AMD Milan
CPU sockets per node	2
Cores per socket	64
Cores per node	128
Hardware threads per core	1 (SMT off)
Hardware threads per node	128
Clock rate (GHz)	~ 2.45
RAM (GB)	2,048
Cache (KB) L1/L2/L3	64/512/32768
Local storage (TB)	1.5 TB

Top of Page

Login Nodes

Login nodes provide interactive support for code compilation.

Specialized Nodes

Delta will support data transfer nodes (serving the "NCSA Delta" Globus collection) and nodes in support of other services.

Network

Delta is connected to the NPCF core router & exit infrastructure via two 100Gbps connections, NCSA's 400Gbps+ of WAN connectivity carry traffic to/from users on an optimal peering.

Delta resources are inter-connected with HPE/Cray's 100Gbps/200Gbps SlingShot interconnect.

File Systems

Note: Users of Delta have access to 3 file systems at the time of system launch, a fourth relaxed-POSIX file system will be made available at a later date.

Delta
The Delta storage infrastructure provides users with their HOME and SCRATCH areas. These file systems are mounted across all Delta nodes and are accessible on the Delta DTN Endpoints. The aggregate performance of this subsystem is 70GB/s and it has 6PB of usable space. These file systems run Lustre via DDN's ExaScaler 6 stack (Lustre 2.14 based).

Hardware:
DDN SFA7990XE (Quantity: 3), each unit contains

- One additional SS9012 enclosure
- 168 x 16TB SAS Drives
- 7 x 1.92TB SAS SSDs

The HOME file system has 4 OSTs and is set with a default stripe size of 1.

The SCRATCH file system has 8 OSTs and has Lustre Progressive File Layout (PFL) enabled which automatically restripes a file as the file grows. The thresholds for PFL striping for SCRATCH are

File size	stripe count
0-32M	1 OST
32M-512M	4 OST
512M+	8 OST

Best Practices

- To reduce the load on the file system metadata services, the ls option for context dependent font coloring, **--color**, is disabled by default.

Future Hardware:
An additional pool of NVME flash from DDN has been installed in early summer 2022. This flash is initially deployed as a tier for "hot" data in scratch. This subsystem will have an aggregate performance of 500GB/s and will have 3PB of raw capacity. As noted above this subsystem will transition to an independent relaxed POSIX namespace file system, communications on that timeline will be announced as updates are available.

Taiga
Taiga is NCSA's global file system which provides users with their $WORK area. This file system is mounted across all Delta systems at /taiga (note that Taiga is used to provision the Delta /projects file system from /taiga/nsf/delta) and is accessible on both the *Delta* and *Taiga* DTN endpoints. For NCSA & Illinois researchers, *Taiga* is also mounted across NCSA's *HAL, HOLL-I, and Radiant* compute environments. This storage subsystem has an aggregate performance of 110GB/s and 1PB of its capacity allocated to users of the *Delta* system. /taiga is a Lustre file system running DDN's Exascaler 6 Lustre stack. See the Taiga and Granite NCSA wiki site for more information.

Hardware:
DDN SFA400NVXE (Quantity: 2), each unit contains

- 4 x SS9012 enclosures
- NVME for metadata and small files

DDN SFA18XE (Quantity: 1), each unit contains

- 10 x SS9012 enclosures
- NVME for for metadata and small files

$WORK and $SCRATCH

A "module reset" in a job script will populate $WORK and $SCRATCH environment variables automatically, or you may set them as WORK=/projects/<account>/$USER , SCRATCH= /scratch/<account>/$USER .

File System	Quota	Snapshots	Purged	Key Features
HOME (/u)	**50GB.** 600,000 files per user.	No/TBA	No	Area for software, scripts, job files, etc. **NOT** intended as a source /destination for I/O during jobs
WORK (/projects)	**500 GB**. Up to 1-25 TB by allocation request. Large requests may have a monetary fee.	No/TBA	No	Area for shared data for a project, common data sets, software, results, etc.
SCRATCH (/scratch)	**1000 GB**. Up to 1-100 TB by allocation request.	No	No	Area for computation, largest allocations, where I/O from jobs should occur
/tmp	**0.74 (CPU) or 1.50 TB (GPU)** shared or dedicated depending on node usage by job (s), no quotas in place	No	After each job	Locally attached disk for fast small file IO.

quota usage

The **quota** command allows you to view your use of the file systems and use by your projects. Below is a sample output for a person "user" who is in two projects: aaaa, and bbbb. The home directory quota does not depend on which project group the file is written with.

quota command

```
<user>@dt-login01 ~]$ quota
Quota usage for user <user>:
--------------------------------------------------------------------------------
----------------
| Directory Path | User | User | User  | User | User   | User |
|                | Block| Soft | Hard  | File | Soft   | Hard |
|                | Used | Quota| Limit | Used | Quota  | Limit|
--------------------------------------------------------------------------------
-----------
| /u/<user>      | 20k  | 50G  | 27.5G | 5    | 600000 | 660000 |
--------------------------------------------------------------------------------
-----------
Quota usage for groups user <user> is a member of:
--------------------------------------------------------------------------------
----------
| Directory Path | Group | Group | Group | Group | Group  | Group |
|                | Block | Soft  | Hard  | File  | Soft   | Hard  |
|                | Used  | Quota | Limit | Used  | Quota  | Limit |
--------------------------------------------------------------------------------
----------------
| /projects/aaaa | 8k    | 500G  | 550G  | 2     | 300000 | 330000 |
| /projects/bbbb | 24k   | 500G  | 550G  | 6     | 300000 | 330000 |
| /scratch/aaaa  | 8k    | 552G  | 607.2G| 2     | 500000 | 550000 |
| /scratch/bbbb  | 24k   | 9.766T| 10.74T| 6     | 500000 | 550000 |
--------------------------------------------------------------------------------
---------------
```

File System Dependency Specification for Jobs

We request that jobs specify file system or systems being used in order for us to respond to resource availability issues. We assume that all jobs depend on the HOME file system.

Table of Slurm Feature/constraint labels

File system	Feature/constraint label	Note
WORK (/projects)	projects	
SCRACH (/scratch)	scratch	
IME (/ime)	ime	depends on scratch

TAIGA (/taiga)	taiga	

The Slurm constraint specifier and slurm Feature attribute for jobs are used to add file system dependencies to a job.

Slurm Feature Specification

For already submitted and pending (PD) jobs, please use the Slurm Feature attribute as follows:

```
$ scontrol update job=JOBID Features="feature1&feature2"
```

For example, to add scratch and ime Features to an already submitted job:

```
$ scontrol update job=713210 Features="scratch&ime"
```

To verify the setting:

```
$ scontrol show job 713210 | grep Feature
   Features=scratch&ime DelayBoot=00:00:00
```

Slurm constraint Specification

To add Slurm job constraint attributes when submitting a job with sbatch (or with srun as a command line argument) use the following:

```
#SBATCH --constraint="constraint1&constraint2.."
```

For example, to add scratch and ime constraints to when submitting a job:

```
#SBATCH --constraint="scratch&ime"
```

To verify the setting:

```
$ scontrol show job 713267 | grep Feature
   Features=scratch&ime DelayBoot=00:00:00
```

Top of Page

Accessing the System

Direct Access

Direct access to the Delta login nodes is via ssh using your NCSA username, password and NCS Duo MFA. Please see NCSA Allocation and Account Management page for links to NCSA Identity and NCSA Duo services. The login nodes provide access to the CPU and GPU resources on Delta.

login node hostname	example usage with ssh
dt-login01.delta.ncsa.illinois.edu	`ssh -Y username@dt-login01.delta.ncsa.illinois.edu` `( -Y allows X11 forwarding from linux hosts )`
dt-login02.delta.ncsa.illinois.edu	`ssh -l username dt-login02.delta.ncsa.illinois.edu` `( -l username alt. syntax for user@host )`

login.delta.ncsa.illinois.edu (round robin DNS name for the set of login nodes)	`ssh username@login.delta.ncsa.illinois.edu`

Please see NCSA Allocation and Account Management for the steps to change your NCSA password for direct access and set up NCSA DUO. For ACCESS awarded projects, to find your local NCSA username please go your ACCESS Profile page and scroll to the bottom for the **Resource Provider Site Usernames** table. Please contact help@ncsa.illinois.edu for assistance if you do not know your NCSA username.

Use of ssh-key pairs is disabled for general use. Please contact NCSA Help at help@ncsa.illinois.edu for key-pair use by Gateway allocations.

maintaining persistent sessions: tmux

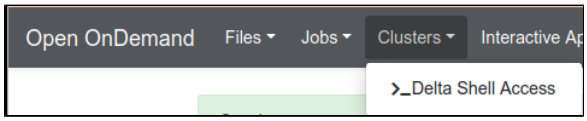
tmux is available on the login nodes to maintain persistent sessions. See the tmux man page for more information. Use the targeted login hostnames (dt-login01 or dt-login02) to attach to the login node where you started tmux after making note of the hostname. Avoid the round-robin hostname when using tmux.

ssh keyboard-interactive

```
For command line ssh clients, make sure to use the following settings
if you have trouble logging in to delta:

ssh -o PreferredAuthentications=keyboard-interactive,password
```

An OpenOnDemand shell interface is available at: https://openondemand.delta.ncsa.illinois.edu/pun/sys/shell/ssh/dt-login02



Top of Page

Citizenship

You share Delta with thousands of other users , and what you do on the system affects others. Exercise good citizenship to ensure that your activity does not adversely impact the system and the research community with whom you share it. Here are some rules of thumb:

- Don't run production jobs on the login nodes (very short time debug tests are fine)
- Don't stress filesystems with known-harmful access patterns (many thousands of small files in a single directory)
- submit an informative help-desk ticket including loaded modules (module list) and stdout/stderr messages

Managing and Transferring Files

File Systems

Each user has a home directory, $HOME, located at /u/$USER.

For example, a user (with username auser) who has an allocated project with a local project serial code **abcd** will see the following entries in their `$HOME` and entries in the project and scratch file systems. To determine the mapping of ACCESS project to local project please use the `accounts` command.

Directory access changes can be made using the `facl` command. Contact help@ncsa.illinois.edu if you need assistance with enabling access to specific users and projects.

```
$ ls -ld /u/$USER
drwxrwx---+ 12 root root 12345 Feb 21 11:54 /u/$USER

$ ls -ld /projects/abcd
drwxrws---+  45 root   delta_abcd      4096 Feb 21 11:54 /projects/abcd

$ ls -l /projects/abcd
total 0
drwxrws---+ 2 auser delta_abcd 6 Feb 21 11:54 auser
drwxrws---+ 2 buser delta_abcd 6 Feb 21 11:54 buser
...

$ ls -ld /scratch/abcd
drwxrws---+  45 root   delta_abcd      4096 Feb 21 11:54 /scratch/abcd

$ ls -l /scratch/abcd
total 0
drwxrws---+ 2 auser delta_abcd 6 Feb 21 11:54 auser
drwxrws---+ 2 buser delta_abcd 6 Feb 21 11:54 buser
...
```

To avoid issues when file systems become unstable or non-responsive, we recommend not putting symbolic links from $HOME to the project and scratch spaces.

/tmp on compute nodes (job duration)

The high performance ssd storage (740GB cpu, 1.5TB gpu) is available in /tmp (*unique to each node and job–not a shared filesystem*) and may contain less than the expected free space if the node(s) are running multiple jobs. Codes that need to perform i/o to many small files should target /tmp on each node of the job and save results to other filesystems before the job ends.

Transferring your Files

To transfer files to and from the Delta system :

GUI apps need to support DUO 2-factor authentication

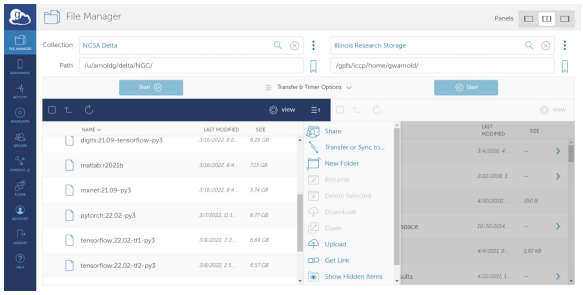
Many GUI applications that support ssh/scp/sftp will work with DUO. A good first step is to use the interactive (not stored/saved) password option with those apps. The interactive login should present you with the 1st password prompt (your kerberos password) followed by the 2nd password prompt for DUO (push to device or passcode from DUO app).

- scp - to be used for small to modest transfers to avoid impacting the usability of the Delta login node (*login.delta.ncsa.illinois.edu*).
- rsync - to be used for small to modest transfers to avoid impacting the usability of the Delta login node.
    - This page on Campus Cluster (which is a **different** system than Delta) has examples of using these text-mode file transfer methods (but **do not** follow the examples directly, because they refer to nodes on Campus Cluster itself): https://campuscluster.illinois.edu/resources/docs/storage-and-data-guide/
- Globus - to be used for large data transfers.

    Upgrade your Globus Connect Personal

    Upgrade to at least version 3.2.0 before Dec 12, 2022. See: https://docs.globus.org/ca-update-2022/#notice

    - Use the Delta collection "**NCSA Delta**".



- Please see the following documentation on using Globus
  - https://docs.globus.org/how-to/get-started/

Sharing Files with Collaborators

Top of Page

Building Software

The Delta programming environment supports the GNU, AMD (AOCC), Intel and NVIDIA HPC compilers. Support for the HPE/Cray Programming environment is forthcoming.

Modules provide access to the compiler + MPI environment.

The default environment includes the GCC 11.2.0 compiler + OpenMPI with support for cuda and gdrcopy. nvcc is in the cuda module and is loaded by default.

AMD recommended compiler flags for GNU, AOCC, and Intel compilers for Milan processors can be found in the AMD Compiler Options Quick Reference Guide for Epyc 7xx3 processors.

Serial

To build (compile and link) a serial program in Fortran, C, and C++:

gcc	aocc	nvhpc
gfortran *myprog*.f gcc *myprog*.c g++ *myprog*.cc	flang *myprog*.f clang *myprog*.c clang *myprog*.cc	nvfortran *myprog*.f nvc *myprog*.c nvc++ *myprog*.cc

MPI

To build (compile and link) a MPI program in Fortran, C, and C++:

MPI Implementation	modulefiles for MPI/Compiler	Build Commands

OpenMPI (Home Page / Documentation)	`aocc/3.2.0 openmpi`
	
	`gcc/11.2.0 openmpi`
	
	`nvhpc/22.2 openmpi`
	
	`intel-oneapi-compilers/2022.0.2 openmpi`
		Fortran 77: mpif77 *myprog*.f
		Fortran 90: mpif90 *myprog*.f90
		C: mpicc *myprog*.c
		C++: mpic++ *myprog*.cc

OpenMP

To build an OpenMP program, use the -fopenmp / -mp option:

gcc	aocc	nvhpc
gfortran -fopenmp *myprog*.f gcc -fopenmp *myprog*.c g++ -fopenmp *myprog*.cc	flang -fopenmp *myprog*.f clang -fopenmp *myprog*.c clang -fopenmp *myprog*.cc	nvfortran -mp *myprog*.f nvc -mp *myprog*.c nvc++ -mp *myprog*.cc

Hybrid MPI/OpenMP

To build an MPI/OpenMP hybrid program, use the -fopenmp / -mp option with the MPI compiling commands:

GCC		PGI/NVHPC
mpif77 -fopenmp *myprog*.f mpif90 -fopenmp *myprog*.f90 mpicc -fopenmp *myprog*.c mpic++ -fopenmp *myprog*.cc		mpif77 -mp *myprog*.f mpif90 -mp *myprog*.f90 mpicc -mp *myprog*.c mpic++ -mp *myprog*.cc

Cray xthi.c sample code

Document - XC Series User Application Placement Guide CLE6..0UP01 S-2496 | HPE Support

This code can be compiled using the methods show above. The code appears in some of the batch script examples below to demonstrate core placement options.

xthi.c

```
#define _GNU_SOURCE

#include <stdio.h>
#include <unistd.h>
#include <string.h>
#include <sched.h>
#include <mpi.h>
#include <omp.h>

/* Borrowed from util-linux-2.13-pre7/schedutils/taskset.c */
static char *cpuset_to_cstr(cpu_set_t *mask, char *str)
{
  char *ptr = str;
  int i, j, entry_made = 0;
  for (i = 0; i < CPU_SETSIZE; i++) {
    if (CPU_ISSET(i, mask)) {
      int run = 0;
      entry_made = 1;
      for (j = i + 1; j < CPU_SETSIZE; j++) {
        if (CPU_ISSET(j, mask)) run++;
        else break;
      }
      if (!run)
        sprintf(ptr, "%d,", i);
      else if (run == 1) {
        sprintf(ptr, "%d,%d,", i, i + 1);
        i++;
      } else {
        sprintf(ptr, "%d-%d,", i, i + run);
        i += run;
      }
      while (*ptr != 0) ptr++;
    }
  }
  ptr -= entry_made;
  *ptr = 0;
  return(str);
}

int main(int argc, char *argv[])
{
  int rank, thread;
  cpu_set_t coremask;
  char clbuf[7 * CPU_SETSIZE], hnbuf[64];

  MPI_Init(&argc, &argv);
  MPI_Comm_rank(MPI_COMM_WORLD, &rank);
  memset(clbuf, 0, sizeof(clbuf));
  memset(hnbuf, 0, sizeof(hnbuf));
  (void)gethostname(hnbuf, sizeof(hnbuf));
  #pragma omp parallel private(thread, coremask, clbuf)
  {
    thread = omp_get_thread_num();
    (void)sched_getaffinity(0, sizeof(coremask), &coremask);
    cpuset_to_cstr(&coremask, clbuf);
    #pragma omp barrier
    printf("Hello from rank %d, thread %d, on %s. (core affinity = %s)\n",
            rank, thread, hnbuf, clbuf);
  }
  MPI_Finalize();
  return(0);
}
```

A version of xthi is also available from ORNL

```
% git clone https://github.com/olcf/XC30-Training/blob/master/affinity
/Xthi.c
```

OpenACC

To build an OpenACC program, use the -acc option and the -mp option for multi-threaded:

NON-MULTITHREADED		MULTITHREADED
nvfortran -acc *myprog*.f nvc -acc *myprog*.c nvc++ -acc *myprog*.cc		nvfortran -acc -mp *myprog*.f nvc -acc -mp *myprog*.c nvc++ -acc -mp *myprog*.cc

CUDA

Cuda compilers (nvcc) are included in the cuda module which is loaded by default under modtree /gpu. For the cuda fortran compiler and other Nvidia development tools, load the "nvhpc" module.

nv* commands when nvhpc is loaded

```
[arnoldg@dt-login03 namd]$ nv
nvaccelerror             nvidia-bug-report.sh     nvlink
nvaccelinfo              nvidia-cuda-mps-control  nv-nsight-cu
nvc                      nvidia-cuda-mps-server   nv-nsight-cu-cli
nvc++                    nvidia-debugdump         nvprepro
nvcc                     nvidia-modprobe          nvprof
nvcpuid                  nvidia-persistenced      nvprune
nvcudainit               nvidia-powerd            nvsize
nvdecode                 nvidia-settings          nvunzip
nvdisasm                 nvidia-sleep.sh          nvvp
nvextract                nvidia-smi               nvzip
nvfortran                nvidia-xconfig
```

See also: https://developer.nvidia.com/hpc-sdk

HIP / ROCM (AMD MI100)

To access the development environment for the gpuMI100x8 partition, start a job on the node with srun or sbatch. Then set your PATH to prefix /opt/rocm/bin where the HIP and ROCM tools are installed. A sample batch script to obtain an xterm is shown along with setting the path on the compute node:

interactive xterm batch script for slurm

```
#!/bin/bash -x

MYACCOUNT=$1
GPUS=--gpus-per-node=1
PARTITION=gpuMI100x8-interactive
srun --tasks-per-node=1 --nodes=1 --cpus-per-task=4 \
  --mem=16g \
  --partition=$PARTITION \
  --time=00:30:00 \
  --account=$MYACCOUNT \
  $GPUS --x11 \
  xterm
```

AMD HIP development environment on gpud01

```
[arnoldg@gpud01 bin]$ export PATH=/opt/rocm/bin:$PATH
[arnoldg@gpud01 bin]$ hipcc
No Arguments passed, exiting ...
[arnoldg@gpud01 bin]$
```

See also: https://developer.amd.com/resources/rocm-learning-center/fundamentals-of-hip-programming/ , https://rocmdocs.amd.com/en/latest/

Top of Page

Software

Delta software is provisioned, when possible, using spack to produce modules for use via the lmod based module system. Select NVIDIA NGC containers are made available (see the container section below) and are periodically updated from the NVIDIA NGC site. An automated list of available software can be found on the ACCESS website.

modules/lmod

Delta provides two sets of modules and a variety of compilers in each set. The default environment is **modtree/gpu** which loads a recent version of gnu compilers , the openmpi implementation of MPI, and cuda. The environment with gpu support will build binaries that run on both the gpu nodes (with cuda) and cpu nodes (potentially with warning messages because those nodes lack cuda drivers). For situations where the same version of software is to be deployed on both gpu and cpu nodes but with separate builds, the **modtree/cpu** environment provides the same default compiler and MPI but without cuda. Use module spider package_name to search for software in lmod and see the steps to load it for your environment.

module (lmod) command	example

module list
 	
(display the currently loaded modules)
	`$ module list`
	
	`Currently Loaded Modules:`
	`  1) gcc/11.2.0  3) openmpi/4.1.2  5) modtree/gpu`
	`  2) ucx/1.11.2  4) cuda/11.6.1`

module load <package_name>
 	
(loads a package or metamodule such as modtree/gpu or netcdf-c)
	`$ module load modtree/cpu`
	
	`Due to MODULEPATH changes, the following have been reloaded:`
	`  1) gcc/11.2.0  2) openmpi/4.1.2  3) ucx/1.11.2`
	
	`The following have been reloaded with a version change:`
	`  1) modtree/gpu => modtree/cpu`

module spider <package_name> (finds modules and displays the ways to load them) module -r spider "regular expression"	$ module spider openblas ---------- openblas: openblas/0.3.20 ---------- You will need to load all module(s) on any one of the lines below before the "openblas/0.3.20" module is available to load. aocc/3.2.0 gcc/11.2.0 Help: OpenBLAS: An optimized BLAS library $ module -r spider "^r$" ---------- r: ---------- Versions: r/4.1.3 ...

see also: User Guide for Lmod

Please open a service request ticket by sending email to help@ncsa.illinois.edu for help with software not currently installed on the Delta system. For single user or single project use cases the preference is for the user to use the spack software package manager to install software locally against the system spack installation as documented <here>. Delta support staff are available to provide limited assistance. For general installation requests the Delta project office will review requests for broad use and installation effort.

Python

submitting python issues

When submitting support issues for python, please provide the following and understand that Delta support staff time is a finite resource while python developments (new software and modules) are growing at nearly infinite velocity.

- python version or environment used (describe fully, with the commands needed to reproduce)
- error output or log from what went wrong (screenshots are more difficult to work with than text data, we don't run trained inference on screenshots attached to Jira)
- pertinent URLs describing what you were following/attempting (if applicable), note that URL recipes specific to vendors may be difficult to reproduce when not using their cloud resources (Ex: Google colab)

On Delta, you may install your own python software stacks as needed. There are a couple choices when customizing your python setup. You may use any of these methods with any of the python versions or instances described below (or you may install your own python versions):

1. venv (python virtual environment)
    a. can name environments (metadata) and have multiple environments per python version or instance
2. conda environments
    a. similar to venv but with more flexibility , see this comparison (1/2 way down the page)
3. pip3 : pip3 install --user <python_package>
    a. useful when you need just 1 python environment per python version. CAUTION: Python modules installed this way into your $HOME/.local/ will match on python

versions and this can create incompatibilities between containers or python venv or conda environments when they have a common python version number.

A couple examples using all of the above are shown at this site covering scikit-learn-intelex (an Intel accelerated scikit learn subset library for x86_64 architecture) : https://github.com/intel/scikit-learn-intelex/blob/master/INSTALL.md

NGC containers for gpu nodes

The Nvidia NGC containers on Delta provide optimized python frameworks built for Delta's A100 and A40 gpus. Delta staff recommend using an NGC container when possible with the gpu nodes (or use the anaconda3_gpu module described later).

The default gcc (latest version) programming environment for either modtree/cpu or modtree/gpu contains:

Anaconda

anaconda3_cpu

Use python from the anaconda3_cpu module if you need some of the modules provided by Anaconda in your python workflow. See the "managing environments" section of the Conda getting started guide to learn how to customize Conda for your workflow and add extra python modules to your environment. *We recommend starting with anaconda3_cpu for modtree/cpu and the cpu nodes, do not use this module with gpus, use anaconda3_gpu instead. The Delta team frequently updates anaconda3_* to track the latest packages.*

anaconda and containers

If you use anaconda with NGC containers, take care to use the python from the container and not the python from anaconda or one of its environments. The container's python should be 1st in $PATH. You may --bind the anaconda directory or other paths into the container so that you can start your conda environments, but with the container's python (/usr/bin/python).

older versions of python and modules

https://repo.anaconda.com/archive/ contains previous Anaconda versions. The bundles are not small, but using one from Anaconda would ensure that you get software that was built to work together at a point in time. If you require an older version of a python lib/module, we suggest looking back in time at the Anaconda site.

```
$ module load modtree/cpu
$ module load gcc anaconda3_cpu
$ which conda
/sw/external/python/anaconda3_cpu/conda
$ module list Currently Loaded Modules:
  1) cue-login-env/1.0   6) libfabric/1.14.0     11) ucx/1.11.2
  2) default             7) lustre/2.14.0_ddn23  12) openmpi/4.1.2
  3) gcc/11.2.0          8) openssh/8.0p1        13) modtree/cpu
  4) knem/1.1.4          9) pmix/3.2.3           14) anaconda3_cpu/4.13.0
  5) libevent/2.1.8     10) rdma-core/32.0
```

List of modules in anaconda3_cpu

The current list of modules available in anaconda3_cpu is shown via "conda list", including tensorflow, pytorch, etc:

anaconda3_cpu modules: conda list

```
# packages in environment at /sw/external/python/anaconda3_cpu: #
Name                    Version                   Build  Channel
_ipyw_jlab_nb_ext_conf    0.1.0           py39h06a4308_1
_libgcc_mutex             0.1                       main
_openmp_mutex             4.5                      1_gnu
absl-py                   1.1.0                   pypi_0    pypi
aiobotocore               2.3.3                   pypi_0    pypi
aiohttp                   3.8.1           py39h7f8727e_1
```

```
aioitertools              0.10.0                   pypi_0    pypi
aiosignal                 1.2.0              pyhd3eb1b0_0
alabaster                 0.7.12             pyhd3eb1b0_0
anaconda                  2022.05                  py39_0
anaconda-client           1.9.0            py39h06a4308_0
anaconda-navigator        2.1.4            py39h06a4308_0
anaconda-project          0.10.2             pyhd3eb1b0_0
anyio                     3.5.0            py39h06a4308_0
appdirs                   1.4.4              pyhd3eb1b0_0
argon2-cffi               21.3.0             pyhd3eb1b0_0
argon2-cffi-bindings      21.2.0           py39h7f8727e_0
arrow                     1.2.2              pyhd3eb1b0_0
astroid                   2.6.6            py39h06a4308_0
astropy                   5.0.4            py39hce1f21e_0
asttokens                 2.0.5              pyhd3eb1b0_0
astunparse                1.6.3                    pypi_0    pypi
async-timeout             4.0.1              pyhd3eb1b0_0
atomicwrites              1.4.0                     py_0
attrs                     21.4.0             pyhd3eb1b0_0
automat                   20.2.0                    py_0
autopep8                  1.6.0              pyhd3eb1b0_0
awscli                    1.25.14                  pypi_0    pypi
babel                     2.9.1              pyhd3eb1b0_0
backcall                  0.2.0              pyhd3eb1b0_0
backports                 1.1                pyhd3eb1b0_0
backports.functools_lru_cache 1.6.4              pyhd3eb1b0_0
backports.tempfile        1.0                pyhd3eb1b0_1
backports.weakref         1.0.post1                 py_1
bcrypt                    3.2.0            py39he8ac12f_0
beautifulsoup4            4.11.1           py39h06a4308_0
binaryornot               0.4.4              pyhd3eb1b0_1
bitarray                  2.4.1            py39h7f8727e_0
bkcharts                  0.2              py39h06a4308_0
black                     19.10b0                   py_0
blas                      1.0                        mkl
bleach                    4.1.0              pyhd3eb1b0_0
blosc                     1.21.0               h8c45485_0
bokeh                     2.4.2            py39h06a4308_0
boto3                     1.21.32            pyhd3eb1b0_0
botocore                  1.24.21                  pypi_0    pypi
bottleneck                1.3.4            py39hce1f21e_0
brotli                    1.0.9                he6710b0_2
brotlipy                  0.7.0          py39h27cfd23_1003
brunsli                   0.1                  h2531618_0
bzip2                     1.0.8                h7b6447c_0
c-ares                    1.18.1               h7f8727e_0
ca-certificates           2022.3.29            h06a4308_1
cachetools                4.2.2              pyhd3eb1b0_0
certifi                   2021.10.8         py39h06a4308_2
cffi                      1.15.0           py39hd667e15_1
cfitsio                   3.470                hf0d0db6_6
chardet                   4.0.0          py39h06a4308_1003
charls                    2.2.0                h2531618_0
charset-normalizer        2.0.4              pyhd3eb1b0_0
click                     8.0.4            py39h06a4308_0
cloudpickle               2.0.0              pyhd3eb1b0_0
clyent                    1.2.2            py39h06a4308_1
colorama                  0.4.4              pyhd3eb1b0_0
colorcet                  2.0.6              pyhd3eb1b0_0
conda                     4.13.0           py39h06a4308_0
conda-build               3.21.8           py39h06a4308_2
conda-content-trust       0.1.1              pyhd3eb1b0_0
conda-env                 2.6.0                        1
conda-pack                0.6.0              pyhd3eb1b0_0
conda-package-handling    1.8.1            py39h7f8727e_0
conda-repo-cli            1.0.4              pyhd3eb1b0_0
conda-token               0.3.0              pyhd3eb1b0_0
conda-verify              3.4.2                     py_1
constantly                15.1.0             pyh2b92418_0
cookiecutter              1.7.3              pyhd3eb1b0_0
cpuonly                   2.0                          0    pytorch-
```

```
nightly
cryptography              3.4.8           py39hd23ed53_0
cssselect                 1.1.0             pyhd3eb1b0_0
curl                      7.82.0              h7f8727e_0
cycler                    0.11.0            pyhd3eb1b0_0
cython                    0.29.28         py39h295c915_0
cytoolz                   0.11.0          py39h27cfd23_0
daal4py                   2021.5.0        py39h78b71dc_0
dal                       2021.5.1          h06a4308_803
dask                      2022.2.1          pyhd3eb1b0_0
dask-core                 2022.2.1          pyhd3eb1b0_0
dataclasses               0.8               pyh6d0b6a4_7
datashader                0.13.0            pyhd3eb1b0_1
datashape                 0.5.4           py39h06a4308_1
dbus                      1.13.18             hb2f20db_0
debugpy                   1.5.1           py39h295c915_0
decorator                 5.1.1             pyhd3eb1b0_0
defusedxml                0.7.1             pyhd3eb1b0_0
diff-match-patch          20200713          pyhd3eb1b0_0
dill                      0.3.5.1                 pypi_0    pypi
distributed               2022.2.1          pyhd3eb1b0_0
docutils                  0.16                    pypi_0    pypi
entrypoints               0.4             py39h06a4308_0
et_xmlfile                1.1.0           py39h06a4308_0
etils                     0.7.1                   pypi_0    pypi
executing                 0.8.3             pyhd3eb1b0_0
expat                     2.4.4               h295c915_0
ffmpeg                    4.2.2               h20bf706_0
filelock                  3.6.0             pyhd3eb1b0_0
flake8                    3.9.2             pyhd3eb1b0_0
flask                     1.1.2             pyhd3eb1b0_0
flatbuffers               1.12                    pypi_0    pypi
fontconfig                2.13.1              h6c09931_0
fonttools                 4.25.0            pyhd3eb1b0_0
freetype                  2.11.0              h70c0345_0
frozenlist                1.2.0           py39h7f8727e_0
fsspec                    2022.5.0                pypi_0    pypi
funcx                     1.0.2                   pypi_0    pypi
funcx-common              0.0.15                  pypi_0    pypi
future                    0.18.2          py39h06a4308_1
gast                      0.4.0                   pypi_0    pypi
gensim                    4.1.2           py39h295c915_0
giflib                    5.2.1               h7b6447c_0
glib                      2.69.1              h4ff587b_1
glob2                     0.7               pyhd3eb1b0_0
globus-cli                3.8.0                   pypi_0    pypi
globus-sdk                3.11.0                  pypi_0    pypi
gmp                       6.2.1               h2531618_2
gmpy2                     2.1.2           py39heeb90bb_0
gnutls                    3.6.15              he1e5248_0
google-api-core           1.25.1            pyhd3eb1b0_0
google-auth               1.33.0            pyhd3eb1b0_0
google-auth-oauthlib      0.4.6                   pypi_0    pypi
google-cloud-core         1.7.1             pyhd3eb1b0_0
google-cloud-storage      1.31.0                    py_0
google-crc32c             1.1.2           py39h27cfd23_0
google-pasta              0.2.0                   pypi_0    pypi
google-resumable-media    1.3.1             pyhd3eb1b0_1
googleapis-common-protos  1.53.0          py39h06a4308_0
greenlet                  1.1.1           py39h295c915_0
grpcio                    1.42.0          py39hce63b2e_0
gst-plugins-base          1.14.0              h8213a91_2
gstreamer                 1.14.0              h28cd5cc_2
gviz-api                  1.10.0                  pypi_0    pypi
h5py                      3.6.0           py39ha0f2276_0
hdf5                      1.10.6              hb1b8bf9_0
heapdict                  1.0.1             pyhd3eb1b0_0
holoviews                 1.14.8            pyhd3eb1b0_0
hvplot                    0.7.3             pyhd3eb1b0_1
hyperlink                 21.0.0            pyhd3eb1b0_0
icu                       58.2                he6710b0_3
```

```
idna                      3.3                pyhd3eb1b0_0
imagecodecs               2021.8.26        py39h4cda21f_0
imageio                   2.9.0              pyhd3eb1b0_0
imagesize                 1.3.0              pyhd3eb1b0_0
importlib-metadata        4.11.3           py39h06a4308_0
importlib-resources       5.9.0                    pypi_0    pypi
importlib_metadata        4.11.3               hd3eb1b0_0
incremental               21.3.0             pyhd3eb1b0_0
inflection                0.5.1            py39h06a4308_0
iniconfig                 1.1.1              pyhd3eb1b0_0
intake                    0.6.5              pyhd3eb1b0_0
intel-openmp              2021.4.0          h06a4308_3561
intervaltree              3.1.0              pyhd3eb1b0_0
ipykernel                 6.9.1            py39h06a4308_0
ipython                   8.2.0            py39h06a4308_0
ipython_genutils          0.2.0              pyhd3eb1b0_1
ipywidgets                7.6.5              pyhd3eb1b0_1
isort                     5.9.3              pyhd3eb1b0_0
itemadapter               0.3.0              pyhd3eb1b0_0
itemloaders               1.0.4              pyhd3eb1b0_1
itsdangerous              2.0.1              pyhd3eb1b0_0
jax                       0.3.16                   pypi_0    pypi
jaxlib                    0.3.15                   pypi_0    pypi
jdcal                     1.4.1              pyhd3eb1b0_0
jedi                      0.18.1           py39h06a4308_1
jeepney                   0.7.1              pyhd3eb1b0_0
jinja2                    2.11.3             pyhd3eb1b0_0
jinja2-time               0.2.0              pyhd3eb1b0_3
jmespath                  0.10.0             pyhd3eb1b0_0
joblib                    1.1.0              pyhd3eb1b0_0
jpeg                      9e                   h7f8727e_0
jq                        1.6                h27cfd23_1000
json5                     0.9.6              pyhd3eb1b0_0
jsonschema                4.4.0            py39h06a4308_0
jupyter                   1.0.0            py39h06a4308_7
jupyter_client            6.1.12             pyhd3eb1b0_0
jupyter_console           6.4.0              pyhd3eb1b0_0
jupyter_core              4.9.2            py39h06a4308_0
jupyter_server            1.13.5             pyhd3eb1b0_0
jupyterlab                3.3.2              pyhd3eb1b0_0
jupyterlab_pygments       0.1.2                    py_0
jupyterlab_server         2.10.3             pyhd3eb1b0_1
jupyterlab_widgets        1.0.0              pyhd3eb1b0_1
jxrlib                    1.1                  h7b6447c_2
keras                     2.9.0                    pypi_0    pypi
keras-preprocessing       1.1.2                    pypi_0    pypi
keyring                   23.4.0           py39h06a4308_0
kiwisolver                1.3.2            py39h295c915_0
krb5                      1.19.2               hac12032_0
lame                      3.100                h7b6447c_0
lazy-object-proxy         1.6.0            py39h27cfd23_0
lcms2                     2.12                 h3be6417_0
ld_impl_linux-64          2.35.1               h7274673_9
lerc                      3.0                  h295c915_0
libaec                    1.0.4                he6710b0_1
libarchive                3.4.2                h62408e4_0
libclang                  14.0.1                   pypi_0    pypi
libcrc32c                 1.1.1                he6710b0_2
libcurl                   7.82.0               h0b77cf5_0
libdeflate                1.8                  h7f8727e_5
libedit                   3.1.20210910         h7f8727e_0
libev                     4.33                 h7f8727e_1
libffi                    3.3                  he6710b0_2
libgcc-ng                 9.3.0               h5101ec6_17
libgfortran-ng            7.5.0                ha8ba4b0_17
libgfortran4              7.5.0                ha8ba4b0_17
libgomp                   9.3.0               h5101ec6_17
libidn2                   2.3.2                h7f8727e_0
liblief                   0.11.5               h295c915_1
libllvm11                 11.1.0               h3826bc1_1
libnghttp2                1.46.0               hce63b2e_0
```

```
libopus                   1.3.1              h7b6447c_0
libpng                    1.6.37             hbc83047_0
libprotobuf               3.19.1             h4ff587b_0
libsodium                 1.0.18             h7b6447c_0
libspatialindex           1.9.3              h2531618_0
libssh2                   1.10.0             h8f2d780_0
libstdcxx-ng              9.3.0             hd4cf53a_17
libtasn1                  4.16.0             h27cfd23_0
libtiff                   4.2.0              h85742a9_0
libunistring              0.9.10             h27cfd23_0
libuuid                   1.0.3              h7f8727e_2
libvpx                    1.7.0              h439df22_0
libwebp                   1.2.2              h55f646e_0
libwebp-base              1.2.2              h7f8727e_0
libxcb                    1.14               h7b6447c_0
libxml2                   2.9.12             h03d6c58_0
libxslt                   1.1.34             hc22bd24_0
libzopfli                 1.0.3              he6710b0_0
llvmlite                  0.38.0          py39h4ff587b_0
locket                    0.2.1           py39h06a4308_2
lxml                      4.8.0           py39h1f438cf_0
lz4-c                     1.9.3              h295c915_1
lzo                       2.10               h7b6447c_2
markdown                  3.3.4           py39h06a4308_0
markupsafe                2.0.1           py39h27cfd23_0
matplotlib                3.5.1           py39h06a4308_1
matplotlib-base           3.5.1           py39ha18d171_1
matplotlib-inline         0.1.2             pyhd3eb1b0_2
mccabe                    0.6.1           py39h06a4308_1
mistune                   0.8.4          py39h27cfd23_1000
mkl                       2021.4.0           h06a4308_640
mkl-service               2.4.0           py39h7f8727e_0
mkl_fft                   1.3.1           py39hd3c417c_0
mkl_random                1.2.2           py39h51133e4_0
mock                      4.0.3             pyhd3eb1b0_0
mpc                       1.1.0              h10f8cd9_1
mpfr                      4.0.2              hb69a4c5_1
mpi                       1.0                      mpich
mpich                     3.3.2              hc856adb_0
mpmath                    1.2.1           py39h06a4308_0
msgpack-python            1.0.2           py39hff7bd54_1
multidict                 5.2.0           py39h7f8727e_2
multipledispatch          0.6.0           py39h06a4308_0
munkres                   1.1.4                    py_0
mypy_extensions           0.4.3           py39h06a4308_1
navigator-updater         0.2.1                   py39_1
nbclassic                 0.3.5             pyhd3eb1b0_0
nbclient                  0.5.13          py39h06a4308_0
nbconvert                 6.4.4           py39h06a4308_0
nbformat                  5.3.0           py39h06a4308_0
ncurses                   6.3                h7f8727e_2
nest-asyncio              1.5.5           py39h06a4308_0
nettle                    3.7.3              hbbd107a_1
networkx                  2.7.1             pyhd3eb1b0_0
nltk                      3.7               pyhd3eb1b0_0
nose                      1.3.7          pyhd3eb1b0_1008
notebook                  6.4.8           py39h06a4308_0
numba                     0.55.1          py39h51133e4_0
numexpr                   2.8.1           py39h6abb31d_0
numpy                     1.21.5          py39he7a7128_1
numpy-base                1.21.5          py39hf524024_1
numpydoc                  1.2               pyhd3eb1b0_0
oauthlib                  3.2.0                   pypi_0    pypi
olefile                   0.46              pyhd3eb1b0_0
oniguruma                 6.9.7.1             h27cfd23_0
openh264                  2.1.1               h4ff587b_0
openjpeg                  2.4.0               h3ad879b_0
openpyxl                  3.0.9             pyhd3eb1b0_0
openssl                   1.1.1n              h7f8727e_0
opt-einsum                3.3.0                   pypi_0    pypi
packaging                 21.3              pyhd3eb1b0_0
```

```
pandas                    1.4.2            py39h295c915_0
pandocfilters             1.5.0              pyhd3eb1b0_0
panel                     0.13.0           py39h06a4308_0
param                     1.12.0             pyhd3eb1b0_0
parsel                    1.6.0            py39h06a4308_0
parso                     0.8.3              pyhd3eb1b0_0
partd                     1.2.0              pyhd3eb1b0_1
patchelf                  0.13                 h295c915_0
pathspec                  0.7.0                      py_0
patsy                     0.5.2            py39h06a4308_1
pcre                      8.45                 h295c915_0
pep8                      1.7.1            py39h06a4308_0
pexpect                   4.8.0              pyhd3eb1b0_3
pickleshare               0.7.5           pyhd3eb1b0_1003
pillow                    9.0.1            py39h22f2fdc_0
pip                       21.2.4           py39h06a4308_0
pkginfo                   1.8.2              pyhd3eb1b0_0
plotly                    5.6.0              pyhd3eb1b0_0
pluggy                    1.0.0            py39h06a4308_1
poyo                      0.5.0              pyhd3eb1b0_0
prometheus_client         0.13.1             pyhd3eb1b0_0
prompt-toolkit            3.0.20             pyhd3eb1b0_0
prompt_toolkit            3.0.20               hd3eb1b0_0
protego                   0.1.16                     py_0
protobuf                  3.19.1           py39h295c915_0
psutil                    5.8.0            py39h27cfd23_1
ptyprocess                0.7.0              pyhd3eb1b0_2
pure_eval                 0.2.2              pyhd3eb1b0_0
py                        1.11.0             pyhd3eb1b0_0
py-lief                   0.11.5           py39h295c915_1
pyasn1                    0.4.8              pyhd3eb1b0_0
pyasn1-modules            0.2.8                      py_0
pycodestyle               2.7.0              pyhd3eb1b0_0
pycosat                   0.6.3            py39h27cfd23_0
pycparser                 2.21               pyhd3eb1b0_0
pyct                      0.4.6            py39h06a4308_0
pycurl                    7.44.1           py39h8f2d780_1
pydantic                  1.10.2                  pypi_0    pypi
pydispatcher              2.0.5            py39h06a4308_2
pydocstyle                6.1.1              pyhd3eb1b0_0
pyerfa                    2.0.0            py39h27cfd23_0
pyflakes                  2.3.1              pyhd3eb1b0_0
pygments                  2.11.2             pyhd3eb1b0_0
pyhamcrest                2.0.2              pyhd3eb1b0_2
pyjwt                     2.1.0            py39h06a4308_0
pylint                    2.9.6            py39h06a4308_1
pyls-spyder               0.4.0              pyhd3eb1b0_0
pyodbc                    4.0.32           py39h295c915_1
pyopenssl                 21.0.0             pyhd3eb1b0_1
pyparsing                 3.0.4              pyhd3eb1b0_0
pyqt                      5.9.2            py39h2531618_6
pyrsistent                0.18.0           py39heee7806_0
pysocks                   1.7.1            py39h06a4308_0
pytables                  3.6.1            py39h77479fe_1
pytest                    7.1.1            py39h06a4308_0
python                    3.9.12               h12debd9_0
python-dateutil           2.8.2              pyhd3eb1b0_0
python-fastjsonschema     2.15.1             pyhd3eb1b0_0
python-libarchive-c       2.9                pyhd3eb1b0_1
python-lsp-black          1.0.0              pyhd3eb1b0_0
python-lsp-jsonrpc        1.0.0              pyhd3eb1b0_0
python-lsp-server         1.2.4              pyhd3eb1b0_0
python-slugify            5.0.2              pyhd3eb1b0_0
python-snappy             0.6.0            py39h2531618_3
pytorch                   1.13.0.dev20220620     py3.9_cpu_0    pytorch-
nightly
pytorch-mutex             1.0                        cpu    pytorch-
nightly
pytz                      2021.3             pyhd3eb1b0_0
pyviz_comms               2.0.2              pyhd3eb1b0_0
pywavelets                1.3.0            py39h7f8727e_0
```

```
pyxdg                     0.27               pyhd3eb1b0_0
pyyaml                    5.4.1                    pypi_0    pypi
pyzmq                     22.3.0           py39h295c915_2
qdarkstyle                3.0.2              pyhd3eb1b0_0
qstylizer                 0.1.10             pyhd3eb1b0_0
qt                        5.9.7                h5867ecd_1
qtawesome                 1.0.3              pyhd3eb1b0_0
qtconsole                 5.3.0              pyhd3eb1b0_0
qtpy                      2.0.1              pyhd3eb1b0_0
queuelib                  1.5.0            py39h06a4308_0
readline                  8.1.2                h7f8727e_1
regex                     2022.3.15        py39h7f8727e_0
requests                  2.27.1             pyhd3eb1b0_0
requests-file             1.5.1              pyhd3eb1b0_0
requests-oauthlib         1.3.1                    pypi_0    pypi
ripgrep                   12.1.1                      0
rope                      0.22.0             pyhd3eb1b0_0
rsa                       4.7.2              pyhd3eb1b0_1
rtree                     0.9.7            py39h06a4308_1
ruamel_yaml               0.15.100         py39h27cfd23_0
s3fs                      2022.5.0                 pypi_0    pypi
s3transfer                0.6.0                    pypi_0    pypi
scikit-image              0.19.2           py39h51133e4_0
scikit-learn              1.0.2            py39h51133e4_1
scikit-learn-intelex      2021.5.0         py39h06a4308_0
scipy                     1.7.3            py39hc147768_0
scrapy                    2.6.1            py39h06a4308_0
seaborn                   0.11.2             pyhd3eb1b0_0
secretstorage             3.3.1            py39h06a4308_0
send2trash                1.8.0              pyhd3eb1b0_1
service_identity          18.1.0             pyhd3eb1b0_1
setuptools                61.2.0           py39h06a4308_0
sip                       4.19.13          py39h295c915_0
six                       1.16.0             pyhd3eb1b0_1
smart_open                5.1.0              pyhd3eb1b0_0
snappy                    1.1.9                h295c915_0
sniffio                   1.2.0            py39h06a4308_1
snowballstemmer           2.2.0              pyhd3eb1b0_0
sortedcollections         2.1.0              pyhd3eb1b0_0
sortedcontainers          2.4.0              pyhd3eb1b0_0
soupsieve                 2.3.1              pyhd3eb1b0_0
sphinx                    4.4.0              pyhd3eb1b0_0
sphinxcontrib-applehelp   1.0.2              pyhd3eb1b0_0
sphinxcontrib-devhelp     1.0.2              pyhd3eb1b0_0
sphinxcontrib-htmlhelp    2.0.0              pyhd3eb1b0_0
sphinxcontrib-jsmath      1.0.1              pyhd3eb1b0_0
sphinxcontrib-qthelp      1.0.3              pyhd3eb1b0_0
sphinxcontrib-serializinghtml 1.1.5             pyhd3eb1b0_0
spyder                    5.1.5            py39h06a4308_1
spyder-kernels            2.1.3            py39h06a4308_0
sqlalchemy                1.4.32           py39h7f8727e_0
sqlite                    3.38.2               hc218d9a_0
stack_data                0.2.0              pyhd3eb1b0_0
statsmodels               0.13.2           py39h7f8727e_0
sympy                     1.10.1           py39h06a4308_0
tabulate                  0.8.9            py39h06a4308_0
tbb                       2021.5.0             hd09550d_0
tbb4py                    2021.5.0         py39hd09550d_0
tblib                     1.7.0              pyhd3eb1b0_0
tenacity                  8.0.1            py39h06a4308_0
tensorboard               2.9.1                    pypi_0    pypi
tensorboard-data-server   0.6.1                    pypi_0    pypi
tensorboard-plugin-profile 2.8.0                     pypi_0    pypi
tensorboard-plugin-wit    1.8.1                    pypi_0    pypi
tensorflow                2.9.1                    pypi_0    pypi
tensorflow-estimator      2.9.0                    pypi_0    pypi
tensorflow-io-gcs-filesystem 0.26.0                   pypi_0    pypi
termcolor                 1.1.0                    pypi_0    pypi
terminado                 0.13.1           py39h06a4308_0
testpath                  0.5.0              pyhd3eb1b0_0
text-unidecode            1.3                pyhd3eb1b0_0
```

```
textdistance              4.2.1              pyhd3eb1b0_0
threadpoolctl             2.2.0              pyh0d69192_0
three-merge               0.1.1              pyhd3eb1b0_0
tifffile                  2021.7.2           pyhd3eb1b0_2
tinycss                   0.4             pyhd3eb1b0_1002
tk                        8.6.11               h1ccaba5_0
tldextract                3.2.0              pyhd3eb1b0_0
toml                      0.10.2             pyhd3eb1b0_0
tomli                     1.2.2              pyhd3eb1b0_0
toolz                     0.11.2             pyhd3eb1b0_0
torchaudio                0.13.0.dev20220621        py39_cpu    pytorch-
nightly
torchvision               0.14.0.dev20220621        py39_cpu    pytorch-
nightly
tornado                   6.1             py39h27cfd23_0
tqdm                      4.64.0          py39h06a4308_0
traitlets                 5.1.1              pyhd3eb1b0_0
twisted                   22.2.0          py39h7f8727e_0
typed-ast                 1.4.3           py39h7f8727e_1
typing-extensions         4.1.1                hd3eb1b0_0
typing_extensions         4.1.1              pyh06a4308_0
tzdata                    2022a                hda174b7_0
ujson                     5.1.0           py39h295c915_0
unidecode                 1.2.0              pyhd3eb1b0_0
unixodbc                  2.3.9                h7b6447c_0
urllib3                   1.26.9          py39h06a4308_0
w3lib                     1.21.0             pyhd3eb1b0_0
watchdog                  2.1.6           py39h06a4308_0
wcwidth                   0.2.5              pyhd3eb1b0_0
webencodings              0.5.1           py39h06a4308_1
websocket-client          0.58.0          py39h06a4308_4
websockets                10.3                    pypi_0    pypi
werkzeug                  2.0.3              pyhd3eb1b0_0
wget                      1.21.3               h0b77cf5_0
wheel                     0.37.1             pyhd3eb1b0_0
widgetsnbextension        3.5.2           py39h06a4308_0
wrapt                     1.12.1          py39he8ac12f_1
wurlitzer                 3.0.2           py39h06a4308_0
x264                      1!157.20191217       h7b6447c_0
xarray                    0.20.1             pyhd3eb1b0_1
xlrd                      2.0.1              pyhd3eb1b0_0
xlsxwriter                3.0.3              pyhd3eb1b0_0
xz                        5.2.5                h7b6447c_0
yaml                      0.2.5                h7b6447c_0
yapf                      0.31.0             pyhd3eb1b0_0
yarl                      1.6.3           py39h27cfd23_0
zeromq                    4.3.4                h2531618_0
zfp                       0.5.5                h295c915_6
zict                      2.0.0              pyhd3eb1b0_0
zipp                      3.7.0              pyhd3eb1b0_0
zlib                      1.2.12               h7f8727e_2
zope                      1.0             py39h06a4308_1
zope.interface            5.4.0           py39h7f8727e_0
zstd                      1.4.9                haebb681_0
```

Intel_AI_toolkit

The Intel AI toolkit module contains a subset of what you'll find in anaconda_cpu. It contains conda environments optimized for cpu execution: pytorch & tensorflow. We have seen up to 2x speedup when using the Intel_AI_toolkit compared to the stock anaconda_cpu. For best results, set OMP_NUM_THREADS to the number of cores you'd like to use (--cpus-per-task in slurm). See also: https://www.intel.com/content/www/us/en/developer/tools/oneapi/ai-analytics-toolkit.html .

anaconda3_gpu (for cuda) , anaconda3_mi100 (for rocm)

Similar to the setup for anaconda_cpu, we have gpu versions of anaconda3 (module load anaconda3_gpu) and have installed pytorch and tensorflow cuda aware python modules into these versions. You may use these module when working with the gpu nodes. See *conda list* after loading the module to review what is already installed. As with anaconda3_cpu, let Delta staff know if there are generally useful modules you would like us to try to install for the broader community. A sample tensorflow test script:

anaconda3_gpu tensorflow example

```
#!/bin/bash
#SBATCH --mem=64g
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=1
#SBATCH --cpus-per-task=16     # <- match to OMP_NUM_THREADS
#SBATCH --partition=gpuA100x4-interactive
#SBATCH --time=00:10:00
#SBATCH --account=YOUR_ACCOUNT-delta-gpu
#SBATCH --job-name=tf_anaconda
### GPU options ###
#SBATCH --gpus-per-node=1
#SBATCH --gpus-per-task=1
#SBATCH --gpu-bind=verbose,per_task:1
###SBATCH --gpu-bind=none     # <- or closest

module purge # drop modules and explicitly load the ones needed
             # (good job metadata and reproducibility)

module load anaconda3_gpu
module list  # job documentation and metadata

echo "job is starting on `hostname`"

which python3
conda list tensorflow
srun python3 \
  tf_gpu.py
exit
```

Jupyter notebooks

The Detla Open OnDemand portal provides an easier way to start a Jupyter notebook. Please see Open OnDemand to access the portal.

The jupyter notebook executables are in your $PATH after loading the anaconda3 module. *Don't run jupyter on the shared login nodes.* Instead, follow these steps to attach a jupyter notebook running on a compute node to your local web browser:

1) Start a jupyter job via srun and note the hostname (*you pick the port number for --port*).

srun jupyter (anaconda3_cpu on a cpu node)

```
$ srun --account=wxyz-delta-cpu --
partition=cpu-interactive \
  --time=00:30:00 --mem=32g \
  jupyter-notebook --no-browser \
  --port=8991 --ip=0.0.0.0
...
    Or copy and paste one of these URLs:
        http://cn093.delta.internal.ncsa.edu
8891/?
token=e5b500e5aef67b1471ed1842b2676e0c0ae4b5(
52656feea
     or http://127.0.0.1:8991/?
token=e5b500e5aef67b1471ed1842b2676e0c0ae4b5(
52656feea
```

Use the 2nd URL in step 3. Note the internal hostname in the cluster for step 2.

When using a container with a gpu node, run the container's jupyter-notebook:

NGC container for gpus, jupyter-notebook, bind a directory

```
# container notebook example showing how to
access a directory outside
# of $HOME ( /projects/bbka in the example )
$ srun --account=wxyz-delta-gpu --
partition=gpuA100x4-interactive \
  --time=00:30:00 --mem=64g --gpus-per-
node=1 \
  singularity run --nv --bind /projects/bbka
\
  /sw/external/NGC/pytorch:22.02-py3 jupyter-
notebook \
  --notebook-dir /projects/wxyz \
  --no-browser --port=8991 --ip=0.0.0.0
...
http://hostname:8888/?
token=73d96b99f2cfc4c3932a3433d1b8003c052081(
5411795d5
```

In step 3 to start the notebook in your browser, replace http://h tname:8888/ with http://127.0.0.1:*8991/ (the port number yo selected with --port=)*

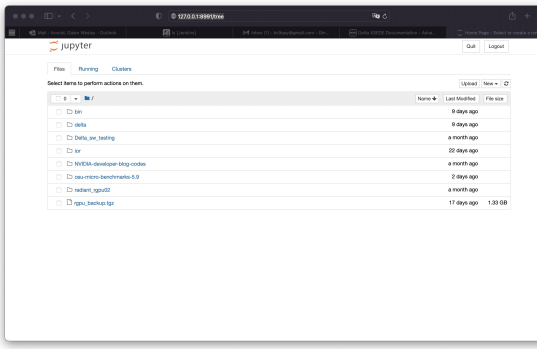
You may not see the job hostname when running with a container, find it with squeue:

squeue -u $USER

```
$ squeue -u $USER
             JOBID PARTITION     NAME
USER ST       TIME  NODES NODELIST(REASON)
            156071 gpuA100x4 singular
arnoldg  R       1:00      1 gpua045
```

Then specifu the host your job is using in the next step (gpua045 for example).

2) From your local desktop or laptop create an ssh tunnel to the compute node via a login node of delta.	**ssh tunnel for jupyter**
	`$ ssh -l my_delta_username \`
	`  -L 127.0.0.1:8991:cn093.delta.internal.ncsa.edu:8991 \`
	`  dt-login.delta.ncsa.illinois.edu`
	
	Authenticate with your login and 2-factor as usual.

3) Paste the 2nd URL (containing 127.0.0.1:*port_number* and the token string) from step 1 into your browser and you will be connected to the jupyter instance running on your compute node of Delta.	

Python (a recent or latest version)

If you do not need all of the extra modules provided by Anaconda, use the basic python installation under the gcc module. You can add modules via "pip3 install --user <modulename>", setup virtual environments, and customize as needed for your workflow but starting from a smaller installed base of python than Anaconda.

```
$ module load gcc python
$ which python
/sw/spack/delta-2022-03/apps/python/3.10.4-gcc-11.2.0-3cjjp6w/bin/python
$ module list

Currently Loaded Modules:
  1) modtree/gpu   3) gcc/11.2.0    5) ucx/1.11.2      7) python/3.10.4
  2) default       4) cuda/11.6.1   6) openmpi/4.1.2
```

This is the list of modules available in the python from "pip3 list":

python modules: pip3 list

```
Package            Version
------------------ ---------
certifi            2021.10.8
cffi               1.15.0
charset-normalizer 2.0.12
click              8.1.2
cryptography       36.0.2
globus-cli         3.4.0
globus-sdk         3.5.0
idna               3.3
jmespath           0.10.0
pip                22.0.4
pycparser          2.21
PyJWT              2.3.0
requests           2.27.1
setuptools         58.1.0
urllib3            1.26.9
```

Top of Page

Launching Applications

Top of Page

Running Jobs

Job Accounting

The charge unit for *Delta* is the Service Unit (SU). This corresponds to the equivalent use of one compute core utilizing less than or equal to 2G of memory for one hour, or 1 GPU or fractional GPU using less than the corresponding amount of memory or cores for 1 hour (see table below). *Keep in mind that your charges are based on the resources that are reserved for your job and don't necessarily reflect how the resources are used.* Charges are based on either the number of cores or the fraction of the memory requested, whichever is larger. The minimum charge for any job is 1 SU.

Node Type		Service Unit Equivalence		
		Cores	GPU Fraction	Host Memory
CPU Node		1	N/A	2 GB
GPU Node	Quad A100	16	1 A100	62.5 GB
	Quad A40	16	1 A40	62.5 GB
	8-way A100	16	1 A100	250 GB
	8-way MI100	16	1 MI100	250 GB

Please note that a weighting factor will discount the charge for the reduced-precision A40 nodes, as well as the novel AMD MI100 based node - this will be documented through the ACCESS SU converter.

Local Account Charging

Use the **`accounts`** command to list the accounts available for charging. CPU and GPU resources will have individual charge names. For example in the following, **`abcd-delta-cpu`** and **`abcd-delta-gpu`** are available for user gbauer to use for the CPU and GPU resources.

```
$ accounts
Project Summary for User 'kingda':

Project         Description                    Balance (Hours)
Deposited (Hours)
--------------  --------------------------  -----------------
------------------
bbka-delta-gpu  ncsa/delta staff allocation
5000000              5000000
bbka-delta-cpu  ncsa/delta staff allocation          100000000
100000000
```

Job Accounting Considerations

- A node-exclusive job that runs on a compute node for one hour will be charged 128 SUs (128 cores x 1 hour)
- A node-exclusive job that runs on a 4-way GPU node for one hour will be charge 4 SUs (4 GPU x 1 hour)
- A node-exclusive job that runs on a 8-way GPU node for one hour will be charge 8 SUs (8 GPU x 1 hour)

QOSGrpBillingMinutes

If you see QOSGrpBillingMinutes under the Reason column for the squeue command, as in

```
             JOBID PARTITION     NAME     USER ST       TIME  NODES
NODELIST(REASON)
           1204221       cpu    myjob     .... PD       0:00      5
(QOSGrpBillingMinutes)
```

then the resource allocation specified for the job (i.e. xyzt-delta-cpu) does not have sufficient balance to run the job based on the # of resources requested and the wallclock time. Sometimes it maybe other jobs from the same project that in the same QOSGrpBillingMinutes state are could cause other jobs using the same resource allocation that are preventing a job that would "fit" from running. The PI of the project needs to put in a supplement request using the same XRAS proposal system that was used for the current award (ACCESS or NCSA).

Reviewing job charges for a project (jobcharge)

jobcharge in /sw/user/scripts/ will show job charges by user for a project. Example usage:

jobcharge_grp.py

```
[arnoldg@dt-login03 ]$ jobcharge bbka-delta-gpu -b 10 --detail | tail -15
106  1662443  gpuMI100x8                0
nan
kingda           bash                                    2023-04-06T09:39:
01              0       0
107  1662444  gpuMI100x8               291  billing=1000,cpu=2,gres/gpu:
mi100=1,gres/gpu=1,mem=3G,node=1      kingda
bash                                   2023-04-06T09:44:11
1000       0.08
108  1662449  gpuMI100x8               614  billing=1000,cpu=2,gres/gpu:
mi100=1,gres/gpu=1,mem=3G,node=1      kingda
bash                                   2023-04-06T10:07:23
1000       0.17
109  1662477  gpuMI100x8               446  billing=1000,cpu=2,gres/gpu:
mi100=1,gres/gpu=1,mem=3G,node=1      kingda
bash                                   2023-04-06T10:15:08
1000       0.12
110  1662492  gpuMI100x8               760  billing=8000,cpu=2,gres/gpu:
mi100=8,gres/gpu=8,mem=3G,node=1      kingda
bash                                   2023-04-06T10:28:00
8000       1.69
111  1662511  gpuMI100x8-interactive  1521  billing=16000,cpu=128,gres/gpu:
mi100=8,gres/gpu=8,mem=64G,node=1  arnoldg
bash                                   Unknown
16000       6.76
_____SUMMARY_____________________
User               Charge (SU)
---------------  -------------
arnoldg                  25.76
babreu                    6.66
kingda                    2.06
rmokos                    0.96
svcdeltajenkins           0.23
Total                    35.67

[arnoldg@dt-login03 scripts]$ jobcharge bbka-delta-gpu -b 10
Output for 2023-03-27-11:25:24 through 2023-04-06-11:25:24:
User               Charge (SU)
---------------  -------------
arnoldg                  26.04
babreu                    6.66
kingda                    2.06
rmokos                    0.96
svcdeltajenkins           0.23
Total                    35.95

[arnoldg@dt-login03 ]$ jobcharge bbka-delta-gpu -h
usage: jobcharge [-h] [-m MONTH] [-y YEAR] [-b DAYSBACK] [-s STARTTIME] [-
```

```
e ENDTIME] [--detail]
                accountstring

positional arguments:
  accountstring         account name

optional arguments:
  -h, --help            show this help message and exit
  -m MONTH, --month MONTH
                        Month (1-12) Default is current month
  -y YEAR, --year YEAR  Year (20XX) default is current year
  -b DAYSBACK, --daysback DAYSBACK
                        Number of days back
  -s STARTTIME, --starttime STARTTIME
                        Start time string in format (format: %Y-%m-%d-%H:%
M:%S)
                        Example:2023-01-03-01:23:21)
  -e ENDTIME, --endtime ENDTIME
                        End time time string in format (format: %Y-%m-%d-%
H:%M:%S)
                        Example:2023-01-03-01:23:21)
  --detail              detail output, per-job [svchydroswmanage@hydrol1
scripts]$
```

Performance tools

- AMDuProf guide
- NVIDIA Nsight Systems

Accessing the Compute Nodes

Delta implements the Slurm batch environment to manage access to the compute nodes. Use the Slurm commands to run batch jobs or for interactive access to compute nodes. See: https://slurm.schedmd.com/quickstart.html for an introduction to Slurm. There are two ways to access compute nodes on Delta.

Batch jobs can be used to access compute nodes. Slurm provides a convenient direct way to submit batch jobs. See https://slurm.schedmd.com/heterogeneous_jobs.html#submitting for details. Slurm supports job arrays for easy management of a set of similar jobs, see: job_array.html.

Sample Slurm batch job scripts are provided in the Job Scripts section below.

Direct ssh access to a compute node in a running batch job from a dt-loginNN node is enabled, once the job has started.

```
$ squeue --job jobid
             JOBID PARTITION     NAME     USER ST       TIME  NODES
NODELIST(REASON)
             12345       cpu     bash   gbauer  R       0:17      1 cn001
```

Then in a terminal session:

```
$ ssh cn001
cn001.delta.internal.ncsa.edu (172.28.22.64)
  OS: RedHat 8.4   HW: HPE   CPU: 128x    RAM: 252 GB
  Site: mgmt  Role: compute
$
```

See also: Monitoring a node during a job.

Top of Page

Scheduler

For information, consult:

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

slurm quick reference guide

Partitions (Queues)

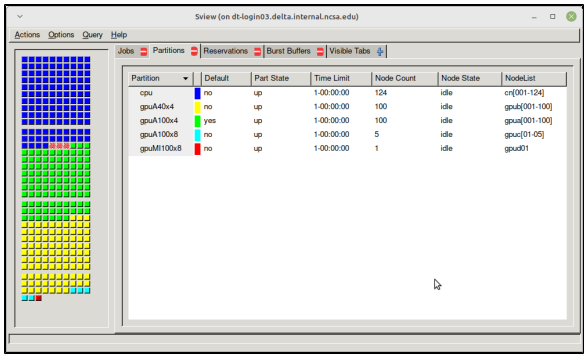
Table. Delta Production Default Partition Values

Property	Value
Default Memory per core	1000 MB
Default Wallclock time	30 minutes

Table. Delta Production Partitions/Queues

Partition/Queue	Node Type	Max Nodes per Job	Max Duration	Max Running in Queue/user*	Charge Factor
cpu	CPU	TBD	48 hr	TBD	1.0
cpu-interactive	CPU	TBD	30 min	TBD	2.0
gpuA100x4 gpuA100x4* (asterisk indicates this is the default queue, but submit jobs to gpuA100x4)	quad A100	TBD	48 hr	TBD	1.0
gpuA100x4-interactive	quad-A100	TBD	1 hr	TBD	2.0
gpuA100x8	octa-A100	TBD	48 hr	TBD	1.5
gpuA100x8-interactive	octa-A100	TBD	1 hr	TBD	3.0
gpuA40x4	quad-A40	TBD	48 hr	TBD	0.5
gpuA40x4-interactive	quad-A40	TBD	1 hr	TBD	1.0
gpuMI100x8	octa-MI100	TBD	48 hr	TBD	0.25
gpuMI100x8-interactive	octa-MI100	TBD	1 hr	TBD	0.5

sview view of slurm partitions



Node Policies

Node-sharing is the default for jobs. Node-exclusive mode can be obtained by specifying all the consumable resources for that node type or adding the following Slurm options:

```
--exclusive --mem=0
```

GPU NVIDIA MIG (GPU slicing) for the A100 will be supported at a future date.

Pre-emptive jobs will be supported at a future date.

Job Policies

The default job requeue or restart policy is set to not allow jobs to be automatically requeued or restarted (as of 12/19/2022).

To enable automatic requeue and restart of a job by slurm, please add the following slurm directive

```
--requeue
```

When a job is requeued due to an evant like a node failure, the batch script is initiated from its beginning. Job scripts need to be written to handle automatically restarting from checkpoints etc.

Interactive Sessions

Interactive sessions can be implemented in several ways depending on what is needed.

To start up a bash shell terminal on a cpu or gpu node

- single core with 16GB of memory, with one task on a cpu node

```
srun --account=account_name --partition=cpu-interactive \
  --nodes=1 --tasks=1 --tasks-per-node=1 \
  --cpus-per-task=4 --mem=16g \
  --pty bash
```

- single core with 20GB of memory, with one task on a A40 gpu node

```
srun --account=account_name --partition=gpuA40x4-interactive \
  --nodes=1 --gpus-per-node=1 --tasks=1 \
  --tasks-per-node=16 --cpus-per-task=1 --mem=20g \
  --pty bash
```

MPI interactive jobs: use salloc followed by srun

Since interactive jobs are already a child process of srun, one cannot srun (or mpirun) applications from within them. Within standard batch jobs submitted via sbatch, use srun to launch MPI codes. For true interactive MPI, use salloc in place of srun shown above, then "srun my_mpi.exe" after you get a prompt from salloc (exit to end the salloc interactive allocation).

interactive MPI, salloc and srun

```
[arnoldg@dt-login01 collective]$ cat osu_reduce.salloc
salloc --account=bbka-delta-cpu --partition=cpu-interactive \
  --nodes=2 --tasks-per-node=4 \
  --cpus-per-task=2 --mem=0

[arnoldg@dt-login01 collective]$ ./osu_reduce.salloc
salloc: Pending job allocation 1180009
salloc: job 1180009 queued and waiting for resources
salloc: job 1180009 has been allocated resources
salloc: Granted job allocation 1180009
salloc: Waiting for resource configuration
salloc: Nodes cn[009-010] are ready for job
[arnoldg@dt-login01 collective]$ srun osu_reduce

# OSU MPI Reduce Latency Test v5.9
# Size       Avg Latency(us)
4                       1.76
8                       1.70
16                      1.72
32                      1.80
64                      2.06
128                     2.00
256                     2.29
512                     2.39
1024                    2.66
2048                    3.29
4096                    4.24
8192                    2.36
16384                   3.91
32768                   6.37
65536                  10.49
131072                 26.84
262144                198.38
524288                342.45
1048576               687.78
[arnoldg@dt-login01 collective]$ exit
exit
salloc: Relinquishing job allocation 1180009
[arnoldg@dt-login01 collective]$
```

Interactive X11 Support

To run an X11 based application on a compute node in an interactive session, the use of the `--x11` switch with `srun` is needed. For example, to run a single core job that uses 1g of memory with X11 (in this case an xterm) do the following:

```
srun -A abcd-delta-cpu  --partition=cpu-interactive \
  --nodes=1 --tasks=1 --tasks-per-node=1 \
  --cpus-per-task=2 --mem=16g \
  --x11  xterm
```

File System Dependency Specification for Jobs

Please see the FileSystemDependencySpecificationforJobs section on setting job file system dependencies for jobs.

Jobs that do not specify a dependency on the WORK(/projects) and SCRATCH (/scratch) will be assumed to depend only on the HOME (/u) file system.

Sample Job Scripts

- Serial jobs on CPU nodes

serial example script

```
$ cat job.slurm
#!/bin/bash
#SBATCH --mem=16g
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=1
#SBATCH --cpus-per-task=4    # <- match to OMP_NUM_THREADS
#SBATCH --partition=cpu      # <- or one of: gpuA100x4 gpuA40x4
gpuA100x8 gpuMI100x8
#SBATCH --account=account_name
#SBATCH --job-name=myjobtest
#SBATCH --time=00:10:00      # hh:mm:ss for the job
#SBATCH --constraint="scratch"
### GPU options ###
##SBATCH --gpus-per-node=2
##SBATCH --gpu-bind=none     # <- or closest
##SBATCH --mail-user=you@yourinstitution.edu
##SBATCH --mail-type="BEGIN,END" See sbatch or srun man pages for
more email options


module reset # drop modules and explicitly load the ones needed
             # (good job metadata and reproducibility)
             # $WORK and $SCRATCH are now set
module load python  # ... or any appropriate modules
module list  # job documentation and metadata
echo "job is starting on `hostname`"
srun python3 myprog.py
```

- MPI on CPU nodes

mpi example script

```
#!/bin/bash
#SBATCH --mem=16g
#SBATCH --nodes=2
#SBATCH --ntasks-per-node=32
#SBATCH --cpus-per-task=2    # <- match to OMP_NUM_THREADS
#SBATCH --partition=cpu      # <- or one of: gpuA100x4 gpuA40x4
gpuA100x8 gpuMI100x8
#SBATCH --account=account_name
#SBATCH --job-name=mympi
#SBATCH --time=00:10:00      # hh:mm:ss for the job
#SBATCH --constraint="scratch"
### GPU options ###
##SBATCH --gpus-per-node=2
##SBATCH --gpu-bind=none     # <- or closest ##SBATCH --mail-
user=you@yourinstitution.edu
##SBATCH --mail-type="BEGIN,END" See sbatch or srun man pages for
more email options

module reset # drop modules and explicitly load the ones needed
             # (good job metadata and reproducibility)
             # $WORK and $SCRATCH are now set
module load gcc/11.2.0 openmpi  # ... or any appropriate modules
module list  # job documentation and metadata
echo "job is starting on `hostname`"
srun osu_reduce
```

- OpenMP on CPU nodes

openmp example script

```
#!/bin/bash
#SBATCH --mem=16g
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=1
#SBATCH --cpus-per-task=32   # <- match to OMP_NUM_THREADS
#SBATCH --partition=cpu      # <- or one of: gpuA100x4 gpuA40x4
gpuA100x8 gpuMI100x8
#SBATCH --account=account_name
#SBATCH --job-name=myopenmp
#SBATCH --time=00:10:00      # hh:mm:ss for the job
#SBATCH --constraint="scratch"
### GPU options ###
##SBATCH --gpus-per-node=2
##SBATCH --gpu-bind=none     # <- or closest
##SBATCH --mail-user=you@yourinstitution.edu
##SBATCH --mail-type="BEGIN,END" See sbatch or srun man pages for
more email options

module reset # drop modules and explicitly load the ones needed
             # (good job metadata and reproducibility)
             # $WORK and $SCRATCH are now set
module load gcc/11.2.0  # ... or any appropriate modules
module list  # job documentation and metadata
echo "job is starting on `hostname`"
export OMP_NUM_THREADS=32
srun stream_gcc
```

- Hybrid (MPI + OpenMP or MPI+X) on CPU nodes

mpi+x example script

```
#!/bin/bash
#SBATCH --mem=16g
#SBATCH --nodes=2
#SBATCH --ntasks-per-node=4
#SBATCH --cpus-per-task=4    # <- match to OMP_NUM_THREADS
#SBATCH --partition=cpu      # <- or one of: gpuA100x4 gpuA40x4
gpuA100x8 gpuMI100x8
#SBATCH --account=account_name
#SBATCH --job-name=mympi+x
#SBATCH --time=00:10:00      # hh:mm:ss for the job
#SBATCH --constraint="scratch"
### GPU options ###
##SBATCH --gpus-per-node=2
##SBATCH --gpu-bind=none     # <- or closest
##SBATCH --mail-user=you@yourinstitution.edu
##SBATCH --mail-type="BEGIN,END" See sbatch or srun man pages for
more email options

module reset # drop modules and explicitly load the ones needed
             # (good job metadata and reproducibility)
             # $WORK and $SCRATCH are now set
module load gcc/11.2.0 openmpi # ... or any appropriate modules
module list  # job documentation and metadata
echo "job is starting on `hostname`"
export OMP_NUM_THREADS=4
srun xthi
```

- 4 gpus together on a compute node

4 gpus on a compute node

```
#!/bin/bash
#SBATCH --job-name="a.out_symmetric"
#SBATCH --output="a.out.%j.%N.out"
#SBATCH --partition=gpuA100x4
#SBATCH --mem=208G
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=4  # could be 1 for py-torch
#SBATCH --cpus-per-task=16   # spread out to use 1 core per numa,
set to 64 if tasks is 1
#SBATCH --constraint="scratch"
#SBATCH --gpus-per-node=4
#SBATCH --gpu-bind=closest   # select a cpu close to gpu on pci bus
topology
#SBATCH --account=bbjw-delta-gpu
#SBATCH --exclusive  # dedicated node for this job
#SBATCH --no-requeue
#SBATCH -t 04:00:00

export OMP_NUM_THREADS=1  # if code is not multithreaded, otherwise
set to 8 or 16
srun -N 1 -n 4 ./a.out > myjob.out
# py-torch example, --ntasks-per-node=1 --cpus-per-task=64
# srun python3 multiple_gpu.py
```

- Parametric / Array / HTC jobs

Top of Page

Job Management

Batch jobs are submitted through a *job script* (as in the examples above) using the sbatch command. Job scripts generally start with a series of SLURM *directives* that describe requirements of the job such as number of nodes, wall time required, etc… to the batch system/scheduler (SLURM directives can also be specified as options on the sbatch command line; command line options take precedence over those in the script). The rest of the batch script consists of user commands.

The syntax for sbatch is:

sbatch [list of sbatch options] script_name

Refer to the sbatch man page for detailed information on the options.

squeue/scontrol/sinfo

Commands that display batch job and partition information .

SLURM EXAMPLE COMMAND	DESCRIPTION
squeue -a	List the status of all jobs on the system.
squeue -u $USER	List the status of all your jobs in the batch system.
squeue -j JobID	List nodes allocated to a running job in addition to basic information..
scontrol show job JobID	List detailed information on a particular job.
sinfo -a	List summary information on all the partition.

See the manual (man) pages for other available options.

Job Status

NODELIST(REASON)

MaxGRESPerAccount - a user has exceeded the number of cores or gpus allotted per user or project for a given partition.

Useful Batch Job Environment Variables

DESCRIPTION	SLURM ENVIRONMENT VARIABLE	DETAIL DESCRIPTION
JobID	$SLURM_JOB_ID	Job identifier assigned to the job
Job Submission Directory	$SLURM_SUBMIT_DIR	By default, jobs start in the directory that the job was submitted from. So the "cd $SLURM_SUBMIT_DIR" command is not needed.
Machine(node) list	$SLURM_NODELIST	variable name that contains the list of nodes assigned to the batch job
Array JobID	$SLURM_ARRAY_JOB_ID $SLURM_ARRAY_TASK_ID	each member of a job array is assigned a unique identifier

See the sbatch man page for additional environment variables available.

srun

The srun command initiates an interactive job on compute nodes.

For example, the following command:

srun

```
srun -A account_name --time=00:30:00 --nodes=1 --ntasks-per-node=16 \
--partition=gpuA100x4 --gpus=1 --mem=16g --pty /bin/bash
```

will run an interactive job in the gpuA100x4 partition with a wall clock limit of 30 minutes, using one node and 16 cores per node and 1 gpu. You can also use other sbatch options such as those documented above.

After you enter the command, you will have to wait for SLURM to start the job. As with any job, your interactive job will wait in the queue until the specified number of nodes is available. If you specify a small number of nodes for smaller amounts of time, the wait should be shorter because your job will backfill among larger jobs. You will see something like this:

```
srun: job 123456 queued and waiting for resources
```

Once the job starts, you will see:

```
srun: job 123456 has been allocated resources
```

and will be presented with an interactive shell prompt on the launch node. At this point, you can use the appropriate command to start your program.

When you are done with your work, you can use the exit command to end the job.

scancel

The scancel command deletes a queued job or terminates a running job.

- scancel JobID deletes/terminates a job.

Refunds

Refunds are considered, when appropriate, for jobs that failed due to circumstances beyond user control.

Projects wishing to request a refund should email help@ncsa.illinois.edu. Please include the batch job ids and the standard error and output files produced by the job(s).

Visualization

Delta A40 nodes support NVIDIA raytracing hardware.

- describe visualization capabilities & software.
- how to establish VNC/DVC/remote desktop

Top of Page

Containers

Apptainer (formerly Singularity)

Container support on Delta is provided by Apptainer/Singularity.

Docker images can be converted to Singularity sif format via the `singularity pull` command. Commands can be run from within a container using `singularity run` command (or apptainer run).

If you encounter quota issues with Apptainer/Singularity caching in `~/.singularity`, the environment variable `SINGULARITY_CACHEDIR` can be used to use a different location such as a scratch space.

Your $HOME is automatically available from containers run via Apptainer/Singularity. You can "pip3 install --user" against a container's python, setup virtualenv's or similar while useing a containerized application. Just run the container's /bin/bash to get a Apptainer> prompt (or use *apptainer shell <container>* for a quick look from a login node). Here's an srun example of that with tensorflow:

srun the bash from a container to interact with programs inside it

```
$ srun \
 --mem=32g \
 --nodes=1 \
 --ntasks-per-node=1 \
 --cpus-per-task=16 \
 --partition=gpuA100x4-interactive \
 --account=bbka-delta-gpu \
 --gpus-per-node=1 \
 --gpus-per-task=1 \
 --gpu-bind=verbose,per_task:1 \
 --pty \
 apptainer run --nv --bind /projects/bbXX \
 /sw/external/NGC/tensorflow:22.06-tf2-py3 /bin/bash
# job starts ...
Apptainer> hostname
gpua068.delta.internal.ncsa.edu
Apptainer> which python  # the python in the container
/usr/bin/python
Apptainer> python --version
Python 3.8.10
```

NVIDIA NGC Containers

Delta provides NVIDIA NGC Docker containers that we have pre-built with Singularity/Apptainer. Look for the latest binary containers in **/sw/external/NGC/** . The containers are used as shown in the sample scripts below:

PyTorch example script

```
#!/bin/bash
#SBATCH --mem=64g
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=1
#SBATCH --cpus-per-task=16     # <- match to OMP_NUM_THREADS, 64 requests
whole node
#SBATCH --partition=gpuA100x4 # <- one of: gpuA100x4 gpuA40x4 gpuA100x8
gpuMI100x8
#SBATCH --account=bbka-delta-gpu
#SBATCH --job-name=pytorchNGC
### GPU options ###
#SBATCH --gpus-per-node=1
#SBATCH --gpus-per-task=1
#SBATCH --gpu-bind=verbose,per_task:1

module reset # drop modules and explicitly load the ones needed
             # (good job metadata and reproducibility)
             # $WORK and $SCRATCH are now set
module list  # job documentation and metadata

echo "job is starting on `hostname`"

# run the container binary with arguments: python3 <program.py>
# --bind /projects/bbXX  # add to apptainer arguments to mount directory
inside container
apptainer run --nv \
 /sw/external/NGC/pytorch:22.02-py3 python3 tensor_gpu.py
```

Tensorflow example script

```
#!/bin/bash
#SBATCH --mem=64g
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=1
#SBATCH --cpus-per-task=16     # <- match to OMP_NUM_THREADS
#SBATCH --partition=gpuA100x4 # <- one of: gpuA100x4 gpuA40x4 gpuA100x8
gpuMI100x8
#SBATCH --account=bbka-delta-gpu
#SBATCH --job-name=tfNGC
### GPU options ###
#SBATCH --gpus-per-node=1
#SBATCH --gpus-per-task=1
#SBATCH --gpu-bind=verbose,per_task:1

module reset # drop modules and explicitly load the ones needed
             # (good job metadata and reproducibility)
             # $WORK and $SCRATCH are now set
module list  # job documentation and metadata

echo "job is starting on `hostname`"

# run the container binary with arguments: python3 <program.py>
# --bind /projects/bbXX  # add to apptainer arguments to mount directory
inside container
apptainer run --nv \
 /sw/external/NGC/tensorflow:22.06-tf2-py3 python3 \
 tf_matmul.py
```

Container list (as of March, 2022)

catalog.txt

```
caffe:20.03-py3 caffe2:18.08-py3
catalog.txt
cntk:18.08-py3
cp2k_v9.1.0.sif
cuquantum-appliance_22.03-cirq.sif
digits:21.09-tensorflow-py3
gromacs_2022.1.sif
hpc-benchmarks:21.4-hpl
lammps:patch_4May2022
matlab:r2021b
mxnet:21.09-py3
mxnet_22.08-py3.sif
namd_2.13-multinode.sif
namd_3.0-alpha11.sif
paraview_egl-py3-5.9.0.sif
pytorch:22.02-py3
pytorch_22.07-py3.sif
pytorch_22.08-py3.sif
tensorflow_19.09-py3.sif
tensorflow:22.02-tf1-py3
tensorflow:22.02-tf2-py3
tensorflow_22.05-tf1-py3.sif
tensorflow_22.05-tf2-py3.sif
tensorflow:22.06-tf1-py3
tensorflow:22.06-tf2-py3
tensorflow_22.07-tf2-py3.sif
tensorflow_22.08-tf1-py3.sif
tensorflow_22.08-tf2-py3.sif
tensorrt:22.02-py3
tensorrt_22.08-py3.sif
theano:18.08
torch:18.08-py2
```

see also: https://catalog.ngc.nvidia.com/orgs/nvidia/containers

AMD Infinity Hub containers for MI100

The AMD node in partition gpuMI100x8 (-interactive) will run containers from the AMD Infinity Hub. The Delta team has pre loaded the following containers in **/sw/external/MI100** and will retrieve others upon request.

AMD MI100 containers in /sw/external/MI100

```
cp2k_8.2.sif
gromacs_2021.1.sif
lammps_2021.5.14_121.sif
milc_c30ed15e1-20210420.sif
namd_2.15a2-20211101.sif
namd3_3.0a9.sif
openmm_7.7.0_49.sif
pytorch_rocm5.0_ubuntu18.04_py3.7_pytorch_1.10.0.sif
tensorflow_rocm5.0-tf2.7-dev.sif
```

A sample batch script for pytorch resembles:

MI100 sample pytorch script

```
#!/bin/bash
#SBATCH --mem=64g
#SBATCH --nodes=1
#SBATCH --ntasks-per-node=1
#SBATCH --cpus-per-task=16
#SBATCH --partition=gpuMI100x8
#SBATCH --account=bbka-delta-gpu
#SBATCH --job-name=tfAMD
#SBATCH --reservation=amd
#SBATCH --time=00:15:00
### GPU options ###
#SBATCH --gpus-per-node=1
##SBATCH --gpus-per-task=1
##SBATCH --gpu-bind=none     # <- or closest

module purge # drop modules and explicitly load the ones needed
             # (good job metadata and reproducibility)

module list  # job documentation and metadata

echo "job is starting on `hostname`"

# https://apptainer.org/docs/user/1.0/gpu.html#amd-gpus-rocm
# https://pytorch.org/docs/stable/notes/hip.html
time \
apptainer run --rocm \
 ~arnoldg/delta/AMD/pytorch_rocm5.0_ubuntu18.04_py3.7_pytorch_1.10.0.sif \
 python3 tensor_gpu.py

exit
```

Other Containers

Extreme-scale Scientific Software Stack (E4S)

The E4S container with GPU (cuda and rocm) support is provided for users of specific ECP packages made available by the E4S project (https://e4s-project.github.io/). The singularity image is available as :

```
/sw/external/E4S/e4s-gpu-x86_64.sif
```

To use E4S with NVIDIA GPUs

```
$ srun --account=account_name --partition=gpuA100-interactive \
  --nodes=1 --gpus-per-node=1 --tasks=1 --tasks-per-node=1 \
  --cpus-per-task=16 --mem=28g \
  --pty bash
$ singularity exec --cleanenv /sw/external/E4S/e4s-gpu-x86_64.sif \
  /bin/bash --rcfile /etc/bash.bashrc
```

The spack package inside of the image will interact with a local spack installation. If ~/.spack directory exists, it might need to be renamed.

More information can be found at https://e4s-project.github.io/download.html

Top of Page

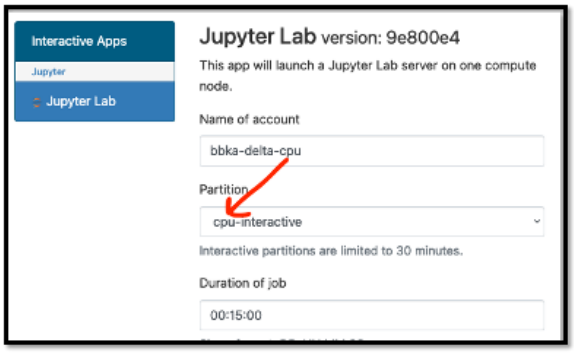
Delta Science Gateway and Open OnDemand

Open OnDemand

The Delta Open OnDemand portal is now available for use. Current supported Interactive apps: Jupyter notebooks.

To connect to the Open OnDemand portal, point a browser to https://openondemand.delta.ncsa.illinois.edu/ and use your NCSA username, password with NCSA Duo with the CILogin page.

Please make sure to match the account to charge with the resource partition as shown below. The account names end in -cpu and -gpu. The matching partition would start with cpu or gpu (as in gpuA100x4 interactive).



To customize your JupyterLab experience for Python or R, see: customizing Delta Open OnDemand

Delta Science Gateway

Protected Data (N/A)

Top of Page

Help

For assistance with the use of Delta

- For ACCESS allocations issues create a ticket via the ACCESS Help page.
- All other issues regardless of allocation type, please send email to help@ncsa.illinois.edu.

Acknowledge

To acknowledge the NCSA Delta system in particular, please include the following

This research is part of the Delta research computing project, which is supported by the National Science Foundation (award OCI 2005572), and the State of Illinois. Delta is a joint effort of the University of Illinois at Urbana-Champaign and its National Center for Supercomputing Applications.

- How to Acknowledge ACCESS

References

Supporting documentation resources:

https://www.rcac.purdue.edu/knowledge/anvil

https://nero-docs.stanford.edu/jupyter-slurm.html