

Introduction on Slurm Job Submission

dicos-support@twgrid.org

Academia Sinica Grid-computing Centre (ASGC)



Outline

- Introduction of Slurm
- User Interfaces (Login Node)
- Basic Usage of Slurm System
- Environment Modules (Lmod)
- Python, Compilation and MPI Enviroment
- Available Software
- Job Submission Example

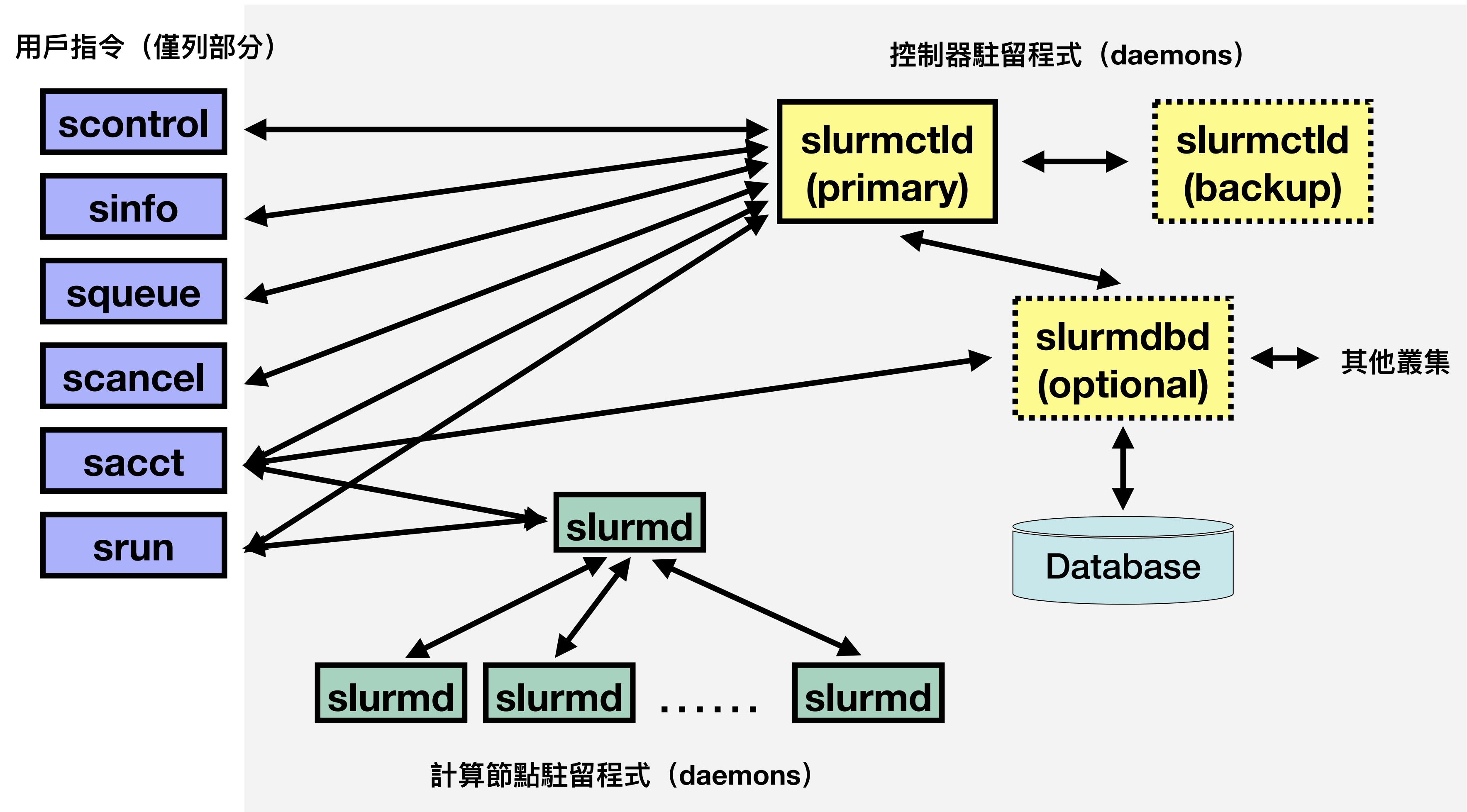
Introduction of Slurm



Introduction of slurm

Overview

- Slurm is an
 - Open source
 - Fault-tolerant
 - Highly scalable
- Cluster management
 - Job scheduling
- system



Introduction of slurm

ASGC resources

- Computing Machine Specifications Computing Nodes :

CPU Cluster	CPU Model	Nodes	RAM-Per-Node	Cores-Per-Node	Total Cores
EDR1	AMD Genoa 9654@2.4GHz	20	1.5 TB	192	3840
Intel-g4	Intel(R) Xeon(R) Gold 6448H	4	1.0 TB	128	512

GPU Cluster	GPU Model	Nodes	GPU-Boards-Per-Node	CPU Model	CPU Cores-Per-Node
GPU-A100	NVIDIA A100	2	8	Intel(R) Xeon(R) Gold 6126 CPU @ 2.60GHz	64
GPU-V100	NVIDIA V100	6	8	AMD EPYC 7302 16-Core Processor	48
GPU-L40S	NVIDIA L40S	1	4	AMD EPYC 9374F 32-Core Processor	64

<https://dicos.grid.sinica.edu.tw/wiki/>

User Interfaces (Login Nodes)

User Interfaces (Login Nodes)

Login into Slurm user interface

- The user interface node for slurm are :

slurm-ui.twgrid.org

- Login in user interface :

`ssh <your account>@slurm-ui.twgrid.org`

Enter your **password** and **2FA verification code**

- You will be prompted with the relative information of your account when login into the slurm user interfaces.
- For Windows users can download and install SSH client software (e.g. **PuTTY**, **MobaXterm**, **VScode**, etc.).
- For macOS users, you can open the built-in **terminal** directly.

```
$ ssh yiruchen0101@slurm-ui.twgrid.org
(yiruchen0101@slurm-ui.twgrid.org) Password:
(yiruchen0101@slurm-ui.twgrid.org) Verification code:

ASGC
slurm-ui

Welcome to slurm-ui01.twgrid.org (Almalinux 9)!

Cluster dashboard: https://grafana01.twgrid.org:3000/dashboards
username: dicos-user
password: Dicos-ASGC00

Notice:
1. Don't remove or edit /dicos_ui_home/<your account>/.google_authenticator (file under your home directory).
2. /dicos_ui_home/ is a temporary storage space. You are fully responsible for the security and integrity of your data in this directory (ASGC does not guarantee the integrity of the data in this directory). Please back up your data to the Ceph directory (/ceph/work/<your group>/) or transfer it to your own storage.
3. If you use /tmp on worker node as an intermediate working space, please remember to include a command in your submission script to remove files from /tmp when your tasks finish. You can include one of the following commands in your submission script:
$ rm -rf /tmp/<your file name>
or
$ ls -al /tmp/ | grep <your account> | awk '{print $9}' | xargs -I {} rm -rf /tmp/{}
4. The /dicos_ui_home/ space migration is scheduled for Jan. 24, 2025. The original /dicos_ui_home/ space has been renamed to /dicos_ui_home_old_20250124. Please copy your data from the old space (/dicos_ui_home_old_20250124) to the new empty /dicos_ui_home/ space by Mar. 15, 2025.
5. Please avoid running computational jobs on login nodes. Use the job scheduler to submit your tasks.

Slurm User Command

$ sinfo          Query partitions and nodes information
$ sinfo -o "%.30P %.5a %.6D %.15A %.16C"  Show status of partitions, nodes and CPUs usage
$ sbatch [your job script]               Submit job with bash script
$ squeue -u [your account]                Query the state of jobs
$ scancel [Job ID]                        Cancel pending or running job
$ scontrol show job [Job ID]              Show the detailed job information
$ scontrol show node [Node name]          Show the detailed node information

Module Command

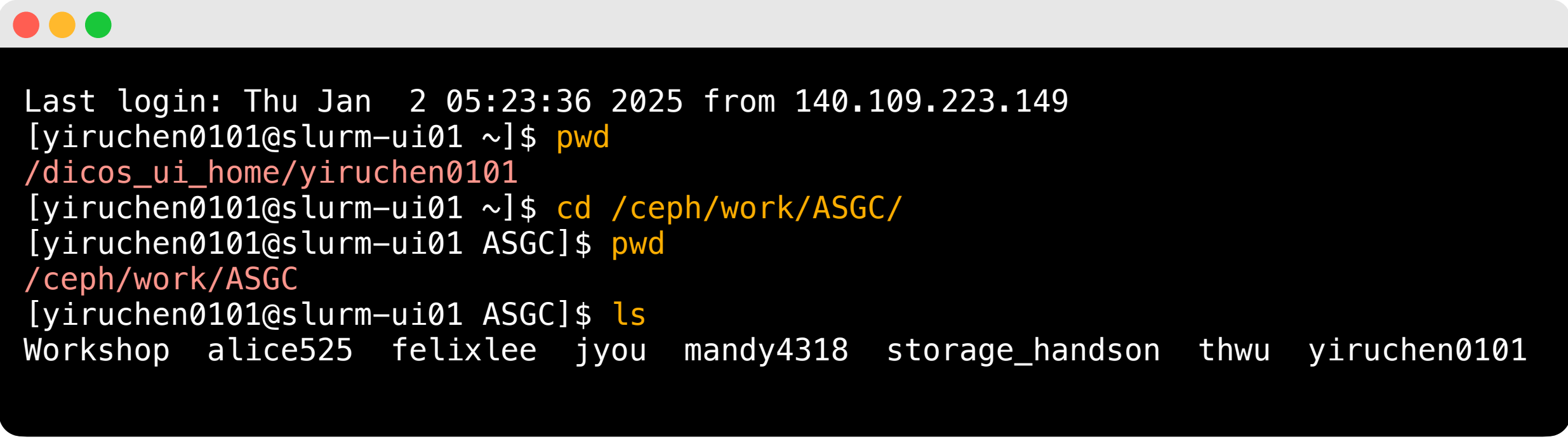
$ module avail   List available packages
$ module list    List currently loaded modules
$ module load [package]  Load package
$ module unload [package]  Unload packages
$ module purge    Remove all modules

[yiruchen0101@slurm-ui01 ~]$
```

User Interfaces (Login Nodes)

Mount Space

- User space (100 GB) : /dicos_ui_home/{user}
- Group Space (3 TB) : /ceph/work/{group}
 - For working and installing software



```
Last login: Thu Jan  2 05:23:36 2025 from 140.109.223.149
[yiruchen0101@slurm-ui01 ~]$ pwd
/dicos_ui_home/yiruchen0101
[yiruchen0101@slurm-ui01 ~]$ cd /ceph/work/ASGC/
[yiruchen0101@slurm-ui01 ASGC]$ pwd
/ceph/work/ASGC
[yiruchen0101@slurm-ui01 ASGC]$ ls
Workshop  alice525  felixlee  jyou  mandy4318  storage_handson  thwu  yiruchen0101
```

Basic Usage of Slurm System

Basic Usage of Slurm System

Partition/ Queues of slurm

- Slurm Partitions (Queues)
- The default queue is “edr1-al9_short”.
- Users could submit to different partitions by assigning partition parameters, e.g.

```
SBATCH -p edr1-al9_large my_script.sh
```

Cluster	Partition	Timelimit	Nodelist
EDR1	edr1-al9_short	03:00:00	hpa-wn[05-24]
	edr1-al9_short_serial	04:00:00	
	edr1-al9_large	14-00:00:00	
	edr1-al9_long_serial	14-00:00:00	
	edr1-al9_moderate_serial	2-00:00:0	
Intel-g4	intel-g4-al9_short	03:00:00	hpi-wn[01-04]
	intel-g4-al9_short_serial	04:00:00	
	intel-g4-al9_large	14-00:00:00	
	intel-g4-al9_long_serial	14-00:00:00	
	intel-g4-al9_moderate_serial	2-00:00:0	
A100	a100-al9	5-00:00:00	hp-teslaa[01,03]
	a100_long-al9	7-00:00:00	
	a100_short-al9	06:00:00	
	a100_devel-al9	20:00	
V100	v100-al9	5-00:00:0	hp-teslav[01-06]
	v100-al9_short	06:00:00	
	v100-al9_long	7-00:00:00	
L40S	l40s-al9	5-00:00:0	sm-gpu21
	l40s-al9_short	06:00:00	
	l40s-al9_long	7-00:00:00	

Basic Usage of Slurm System

User commands : sinfo

- Query partitions and nodes information : `sinfo` or `sinfo -N`

```
[yiruchen0101@slurm-ui01 yiruchen0101]$ sinfo
PARTITION      AVAIL  TIMELIMIT  NODES  STATE NODELIST
intel-g4-a19_short      up    3:00:00     4  alloc hpi-wn[01-04]
intel-g4-a19_short_serial up    4:00:00     4  alloc hpi-wn[01-04]
intel-g4-a19_large      up   14-00:00:0     4  alloc hpi-wn[01-04]
intel-g4-a19_long_serial up   14-00:00:0     4  alloc hpi-wn[01-04]
intel-g4-a19_moderate_serial up  2-00:00:00     4  alloc hpi-wn[01-04]
edr1-a19_short*        up    3:00:00    20  alloc hpa-wn[05-24]
edr1-a19_short_serial  up    4:00:00    20  alloc hpa-wn[05-24]
edr1-a19_large        up   14-00:00:0    20  alloc hpa-wn[05-24]
edr1-a19_long_serial   up   14-00:00:0    20  alloc hpa-wn[05-24]
edr1-a19_moderate_serial up  2-00:00:00    20  alloc hpa-wn[05-24]
v100-a19           up   5-00:00:00     2   mix hp-teslav[01,06]
v100-a19           up   5-00:00:00     4   idle hp-teslav[02-05]
v100-a19_short      up    6:00:00     2   mix hp-teslav[01,06]
v100-a19_short      up    6:00:00     4   idle hp-teslav[02-05]
v100-a19_long       up   7-00:00:00     2   mix hp-teslav[01,06]
v100-a19_long       up   7-00:00:00     4   idle hp-teslav[02-05]
a100-a19           up   5-00:00:00     2   mix hp-teslaa[01,03]
a100_long-a19       up   7-00:00:00     2   mix hp-teslaa[01,03]
a100_short-a19      up    6:00:00     2   mix hp-teslaa[01,03]
a100_devel-a19      up    20:00      2   mix hp-teslaa[01,03]
l40s-a19           up   5-00:00:00     1   mix sm-gpu21
l40s-a19_short      up    6:00:00     1   mix sm-gpu21
l40s-a19_long       up   7-00:00:00     1   mix sm-gpu21
```

```
[yiruchen0101@slurm-ui01 yiruchen0101]$ sinfo -N
NODELIST      NODES      PARTITION STATE
hp-teslaa01      1      a100_long-a19 mix
hp-teslaa01      1      a100_devel-a19 mix
hp-teslaa01      1      a100-a19 mix
hp-teslaa01      1      a100_short-a19 mix
hp-teslaa03      1      a100_long-a19 mix
hp-teslaa03      1      a100_devel-a19 mix
hp-teslaa03      1      a100-a19 mix
hp-teslaa03      1      a100_short-a19 mix
hp-teslav01      1      v100-a19_short mix
hp-teslav01      1      v100-a19 mix
hp-teslav01      1      v100-a19_long mix
hp-teslav02      1      v100-a19_short idle
hp-teslav02      1      v100-a19 idle
hp-teslav02      1      v100-a19_long idle
hp-teslav03      1      v100-a19_short idle
hp-teslav03      1      v100-a19 idle
hp-teslav03      1      v100-a19_long idle
hp-teslav04      1      v100-a19_short idle
hp-teslav04      1      v100-a19 idle
hp-teslav04      1      v100-a19_long idle
hp-teslav05      1      v100-a19_short idle
hp-teslav05      1      v100-a19 idle
:
:
:
```

Basic Usage of Slurm System

User commands : sinfo

- Query partitions and nodes information : `sinfo` or `sinfo -N`

```
[yiruchen0101@slurm-ui01 yiruchen0101]$ sinfo
PARTITION      AVAIL  TIMELIMIT  NODES  STATE NODELIST
intel-g4-a19_short      up    3:00:00     4  alloc hpi-wn[01-04]
intel-g4-a19_short_serial up    4:00:00     4  alloc hpi-wn[01-04]
intel-g4-a19_large      up   14-00:00:00     4  alloc hpi-wn[01-04]
intel-g4-a19_long_serial up   14-00:00:00     4  alloc hpi-wn[01-04]
intel-g4-a19_moderate_serial up  2-00:00:00     4  alloc hpi-wn[01-04]
edr1-a19_short*        up    3:00:00    20  alloc hpa-wn[05-24]
edr1-a19_short_serial  up    4:00:00    20  alloc hpa-wn[05-24]
edr1-a19_large         up   14-00:00:00    20  alloc hpa-wn[05-24]
edr1-a19_long_serial   up   14-00:00:00    20  alloc hpa-wn[05-24]
edr1-a19_moderate_serial up  2-00:00:00    20  alloc hpa-wn[05-24]
v100-a19             up   5-00:00:00     2  mix  hp-teslav[01,06]
v100-a19             up   5-00:00:00     4  idle hp-teslav[02-05]
v100-a19_short        up    6:00:00     2  mix  hp-teslav[01,06]
v100-a19_short        up    6:00:00     4  idle hp-teslav[02-05]
v100-a19_long         up   7-00:00:00     2  mix  hp-teslav[01,06]
v100-a19_long         up   7-00:00:00     4  idle hp-teslav[02-05]
a100-a19             up   5-00:00:00     2  mix  hp-teslaa[01,03]
a100_long-a19         up   7-00:00:00     2  mix  hp-teslaa[01,03]
a100_short-a19        up    6:00:00     2  mix  hp-teslaa[01,03]
a100_devel-a19        up    20:00      2  mix  hp-teslaa[01,03]
l40s-a19             up   5-00:00:00     1  mix  sm-gpu21
l40s-a19_short        up    6:00:00     1  mix  sm-gpu21
l40s-a19_long         up   7-00:00:00     1  mix  sm-gpu21
```

STATE

- idle** : The node is not allocated to any jobs and is available for use.
- alloc** : The node has been allocated to one or more jobs.
- mix** : The node has some of its CPUs **ALLOCATED** while others are **IDLE**.
- down** : The node is unavailable for use.
- drain** : The node is unavailable for use per system administrator request.
- drang** : The node is currently allocated a job, but will not be allocated additional jobs.

Basic Usage of Slurm System

User commands : sbatch

- Submit your job with bash script (recommended) : `sbatch your_script.sh`

```
your_script.sh

#!/bin/bash
#SBATCH --job-name=helloworld          # Job name
#SBATCH --partition=intel-g4-a19_short  # Partiotion name
#SBATCH --nodes=1                      # Numbers of nodes
#SBATCH --ntasks-per-node=1            # Number of tasks per node
#SBATCH --cpus-per-task=1              # Number of CPUs per task
#SBATCH --output=%j.out                # Standard output file (%j: Job ID)
#SBATCH --error=%j.err                 # Standard error file (%j: Job ID)
#SBATCH --time=00-01:00:00             # Time limit
#SBATCH --mail-type=ALL                 # Email notifications = BEGIN, END, FAIL, ALL
#SBATCH --mail-user=jennifer.chen@twgrid.org # Email address to send notifications

srun /bin/echo "Hello World!"
```

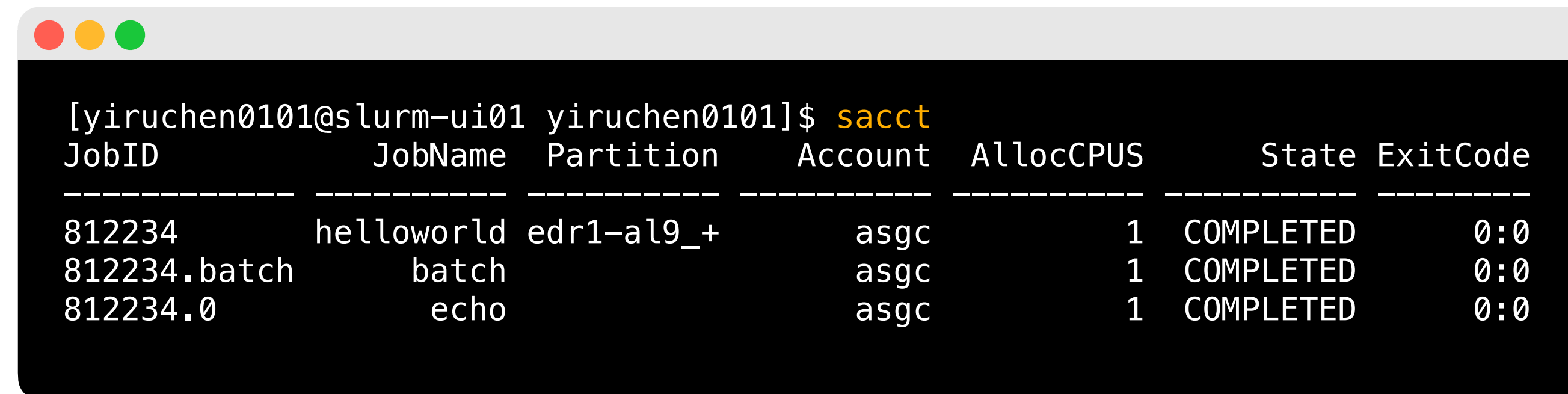
```
[yiruchen0101@slurm-ui01 yiruchen0101]$ sbatch your_script.sh
Submitted batch job 812234
[yiruchen0101@slurm-ui01 yiruchen0101]$
```

Job ID

Basic Usage of Slurm System

User commands : sacct

- Query the jobs submitted by you : `sacct` or `sacct -u <your account>`



```
[yiruchen0101@slurm-ui01 yiruchen0101]$ sacct
```

JobID	JobName	Partition	Account	AllocCPUS	State	ExitCode
812234	helloworld	edr1-al9_+	asgc	1	COMPLETED	0:0
812234.batch	batch		asgc	1	COMPLETED	0:0
812234.0	echo		asgc	1	COMPLETED	0:0

Basic Usage of Slurm System

User commands : `squeue`

- Show queue information : `squeue`
- Show your job in the queue : `squeue -u <your account>`

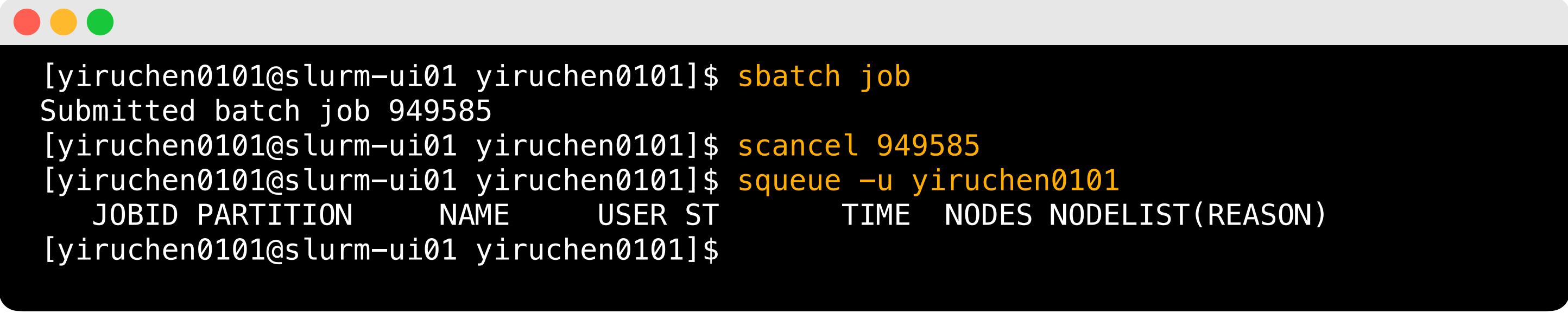
```
[yiruchen0101@slurm-ui01 yiruchen0101]$ squeue
  JOBID PARTITION    NAME     USER ST       TIME  NODES NODELIST(REASON)
  869316 a100-a19 symbreak  gtelo PD        0:00      1 (Priority)
  869315 a100-a19 symbreak  gtelo PD        0:00      1 (Nodes required for
job are DOWN, DRAINED or reserved for jobs in higher priority partitions)
  851811 a100-a19   AIREC  hsinyich  R 2-18:02:00      1 hp-teslaa03
  829335 a100-a19   AIREC  hsinyich  R 4-08:28:54      1 hp-teslaa03
  736972 a100_deve  test0  yungilin PD        0:00      1 (Resources)
  .
  .
  .
```

```
[yiruchen0101@slurm-ui01 yiruchen0101]$ squeue -u yiruchen0101
  JOBID PARTITION    NAME     USER ST       TIME  NODES NODELIST(REASON)
  949585 intel-g4- hellowor yiruchen PD        0:00      1 (None)
```

Basic Usage of Slurm System

User commands : scancel

- Cancel your job : `scancel <your JobID>`



```
[yiruchen0101@slurm-ui01 yiruchen0101]$ sbatch job
Submitted batch job 949585
[yiruchen0101@slurm-ui01 yiruchen0101]$ scancel 949585
[yiruchen0101@slurm-ui01 yiruchen0101]$ squeue -u yiruchen0101
  JOBID PARTITION    NAME     USER ST       TIME  NODES NODELIST(REASON)
[yiruchen0101@slurm-ui01 yiruchen0101]$
```

Basic Usage of Slurm System

User commands : scontrol

- Show the detailed job information : `scontrol show job <your JobID>`
- Show the detailed node information : `scontrol show node <node name>`

```
[yiruchen0101@slurm-ui01 yiruchen0101]$ scontrol show job 949681
JobId=949681 JobName=helloworld
  UserId=yiruchen0101(5019) GroupId=ASGC(525) MCS_label=N/A
  Priority=25084 Nice=0 Account=asgc QOS=normal
  JobState=PENDING Reason=None Dependency=(null)
  Requeue=0 Restarts=0 BatchFlag=1 Reboot=0 ExitCode=0:0
  RunTime=00:00:00 TimeLimit=01:00:00 TimeMin=N/A
  SubmitTime=2025-01-12T18:22:54 EligibleTime=2025-01-12T18:22:54
  AccrueTime=2025-01-12T18:22:54
  StartTime=Unknown EndTime=Unknown Deadline=N/A
  SuspendTime=None SecsPreSuspend=0 LastSchedEval=2025-01-12T18:22:54 Scheduler=Main
  Partition=intel-g4-al9_short AllocNode:Sid=slurm-ui04:1885932
  ReqNodeList=(null) ExcNodeList=(null)
  NodeList=
  NumNodes=1-1 NumCPUs=1 NumTasks=1 CPUs/Task=1 ReqB:S:C:T=0:0:*:*
  ReqTRES=cpu=1,mem=927000M,node=1,billing=1
  AllocTRES=(null)
  Socks/Node=* NtasksPerN:B:S:C=1:0:*:* CoreSpec=*
  MinCPUsNode=1 MinMemoryNode=0 MinTmpDiskNode=0
  Features=(null) DelayBoot=00:00:00
  OverSubscribe=OK Contiguous=0 Licenses=(null) Network=(null)
  Command=/ceph/work/ASGC/yiruchen0101/job
  WorkDir=/ceph/work/ASGC/yiruchen0101
  StdErr=/ceph/work/ASGC/yiruchen0101/949681.err
  StdIn=/dev/null
  StdOut=/ceph/work/ASGC/yiruchen0101/949681.out
  TresPerTask=cpu=1
  MailUser=jennifer.chen@twgrid.org MailType=INVALID_DEPEND,BEGIN,END,FAIL,REQUEUE,STAGE_OUT
```

```
[yiruchen0101@slurm-ui01 yiruchen0101]$ scontrol show node hpa-wn05
NodeName=hp-wn05 Arch=x86_64 CoresPerSocket=96
CPUAlloc=121 CPUEfctv=192 CPUTot=192 CPULoad=108.93
AvailableFeatures=(null)
ActiveFeatures=(null)
Gres=(null)
NodeAddr=hp-wn05 NodeHostName=hp-wn05 Version=24.05.1
OS=Linux 5.14.0-503.16.1.el9_5.x86_64 #1 SMP PREEMPT_DYNAMIC Fri Dec 13 01:47:05 EST
2024
RealMemory=1386000 AllocMem=682880 FreeMem=1163994 Sockets=2 Boards=1
MemSpecLimit=10240
State=MIXED ThreadsPerCore=1 TmpDisk=0 Weight=1 Owner=N/A MCS_label=N/A
Partitions=edr1-al9_short,edr1-al9_short_serial,edr1-al9_large,edr1
al9_long_serial,edr1-al9_moderate_serial
BootTime=2025-08-18T02:20:55 SlurmdStartTime=2025-09-06T06:58:33
LastBusyTime=2025-09-04T00:29:57 ResumeAfterTime=None
CfgTRES=cpu=192,mem=1386000M,billing=192
AllocTRES=cpu=121,mem=682880M
CurrentWatts=0 AveWatts=0
```

Environment Modules (Lmod)

Environment Modules (Lmod)

Introduction

- In DiCOS Slurm system, we have environment modules installed in user interfaces and worker nodes.
- Detailed information please refer to the original document :
<https://modules.readthedocs.io/en/latest/>
- Environment-modules help user to setup environment and environment variables properly for specific software environments.
 - User doesn't need to worry about the complex settings of the environments.

Environment Modules (Lmod)

User commands : module avail

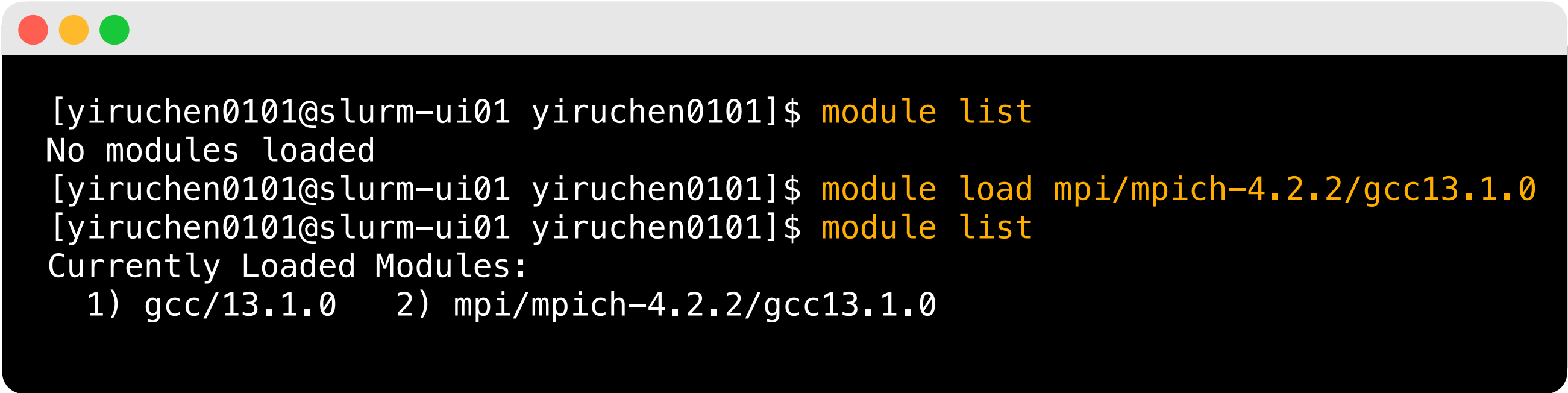
- Show available modules in slurm-ui : `module avail` or `ml av`

```
[yiruchen0101@slurm-ui01 yiruchen0101]$ module avail
----- /ceph/sharedfs/apps/general/almalinux9/modulefiles -----
R/4.2.1          gcc/11.5.0          lapack/v3.12.1          nvhpc/25.1          (D)
R/4.4.0          gcc/13.1.0          mkl/latest              python3/3.9.23
R/4.4.1          (D) gromacs/2022.swaxs-0.1/a100-gpu mkl/2023.2.0          (D) relion/4.0.2
anaconda3/2024.10-1 (D) gromacs/2022.swaxs-0.1/cpu mpi/openmpi-4.1.5/cuda-12.2/gcc-11.5.0 relion/5.0.0 (D)
aocc/5.0.0        (D) gromacs/2022.swaxs-0.1/v100-gpu (D) mpi/openmpi-5.0.5/cuda-12.4/gcc-13.1.0 samtools/1.21
bcftools/1.21     gromacs/2024.0/a100_gpu-al9 mpi/openmpi-5.0.8/gcc-11.5.0 singularity/4.1.2
cmake/3.28        (D) gromacs/2024.0/cpu          nvhpc-byo-compiler/25.1 (D) tbb/latest
cuda/12.2.0       gromacs/2024.0/gpu          nvhpc-hpcx-2.20-cuda12/25.1 tbb/2021.10.0 (D)
cuda/12.4.0       gromacs/2025.2.0/l40s_gpu-al9 nvhpc-hpcx-cuda12/25.1 (D)
cuda/12.6.0       (D) htllib/1.21             nvhpc-hpcx/25.1 (D)
dorado/v0.8.3     julia/1.11.5              (D) nvhpc-nompi/25.1 (D)
----- /ceph/sharedfs/apps/amd/almalinux9/hdr1-al9/modulefiles -----
aocc/4.2.0        gcc/11.5.0          hdf5/1.8.12             mpi/openmpi-5.0.3/aocc420
aocl/4.2.0        gcc/13.1.0          mpi/mpich-4.2.2/gcc13.1.0 mpi/openmpi-5.0.3/gcc13.1.0 (D)
----- /ceph/sharedfs/apps/general/centos7/modulefiles -----
R/4.0.5          gcc/4.8.5          gromacs/2021.swaxs-0.1/gpu mpi/openmpi-2.0.2/gcc485 nvhpc-nompi/20.11
R/4.2.1          gcc/8.2.0          gromacs/2022.swaxs-0.1/gpu mpi/openmpi-3.1.6/cuda/gcc930 nvhpc-nompi/24.3
anaconda3/4.9.2   gcc/8.3.0          gromacs/2024.0/a100_gpu mpi/openmpi-3.1.6/gcc930 nvhpc-openmpi3/24.3
anaconda3/4.10.3  gcc/9.3.0          gromacs/2024.0/cpu      mpi/openmpi-4.1.0/gcc485 nvhpc/20.11
anaconda3/4.12.0  gcc/10.3.0         gromacs/2024.0/gpu      mumax3/cuda-11.3/10_linux nvhpc/24.3
binutils/2.35.2   gcc/11.1.0         hdf5/1.10.5-parallel    nvhpc-byo-compiler/20.11 paraview/5.8.0
cmake/3.20.3      gcc/12.1.0         hdf5/1.10.5             (D) nvhpc-byo-compiler/24.3 python/3.9.5
cuda/11.3.0       git/2.37.1         julia/1.8.0             nvhpc-hpcx-cuda12/24.3 python/3.9.18 (D)
cuda/11.8.0       go/1.21.7          make/4.3                nvhpc-hpcx/24.3 root/v6.30
----- /ceph/sharedfs/apps/intel/centos7/modulefiles -----
clck/2021.6.0     compiler/2022.1.0 (D) dpl/2021.7.0          inspector/2022.1.0 mkl/2022.1.0
compiler-rt/2022.1.0 debugger/2021.6.0 icc/2022.1.0          intel_mpi/2021.6.0 tbb/2021.6.0
compiler/2022.0.2 dev-utilities/2021.6.0 init_opencl/2022.1.0 itac/2021.6.0
```

Environment Modules (Lmod)

User commands : module list & module load

- Show currently loaded modules : `module list` or `ml`
- Load module : `module load <module name>` or `ml <module name>`



```
[yiruchen0101@slurm-ui01 yiruchen0101]$ module list
No modules loaded
[yiruchen0101@slurm-ui01 yiruchen0101]$ module load mpi/mpich-4.2.2/gcc13.1.0
[yiruchen0101@slurm-ui01 yiruchen0101]$ module list
Currently Loaded Modules:
  1) gcc/13.1.0    2) mpi/mpich-4.2.2/gcc13.1.0
```

Environment Modules (Lmod)

User commands : module unload & module purge

- Unload module : `module unload <module name>` or `ml -<module name>`
- Unload all loaded module : `module purge` or `ml purge`

```
[yiruchen0101@slurm-ui01 yiruchen0101]$ module list
Currently Loaded Modules:
  1) gcc/13.1.0    2) mpi/mpich-4.2.2/gcc13.1.0
[yiruchen0101@slurm-ui01 yiruchen0101]$ module unload gcc/13.1.0
[yiruchen0101@slurm-ui01 yiruchen0101]$ module list
Currently Loaded Modules:
  1) mpi/mpich-4.2.2/gcc13.1.0
[yiruchen0101@slurm-ui01 yiruchen0101]$ module load mpi/mpich-4.2.2/gcc13.1.0
[yiruchen0101@slurm-ui01 yiruchen0101]$ module list
Currently Loaded Modules:
  1) gcc/13.1.0    2) mpi/mpich-4.2.2/gcc13.1.0
[yiruchen0101@slurm-ui01 yiruchen0101]$ module purge
[yiruchen0101@slurm-ui01 yiruchen0101]$ module list
No modules loaded
```

Python, Compilation and MPI Environment

Python, Compilation and MPI Environment

Python

- The default system python version is 3.9.18.
- Use python , please consider using anaconda with python first :

`module load anaconda3`

- Install additional applications : `/ceph/work/<groupname>/`

Python, Compilation and MPI Environment

Python

- Before installing a special python package, use the virtual environment :

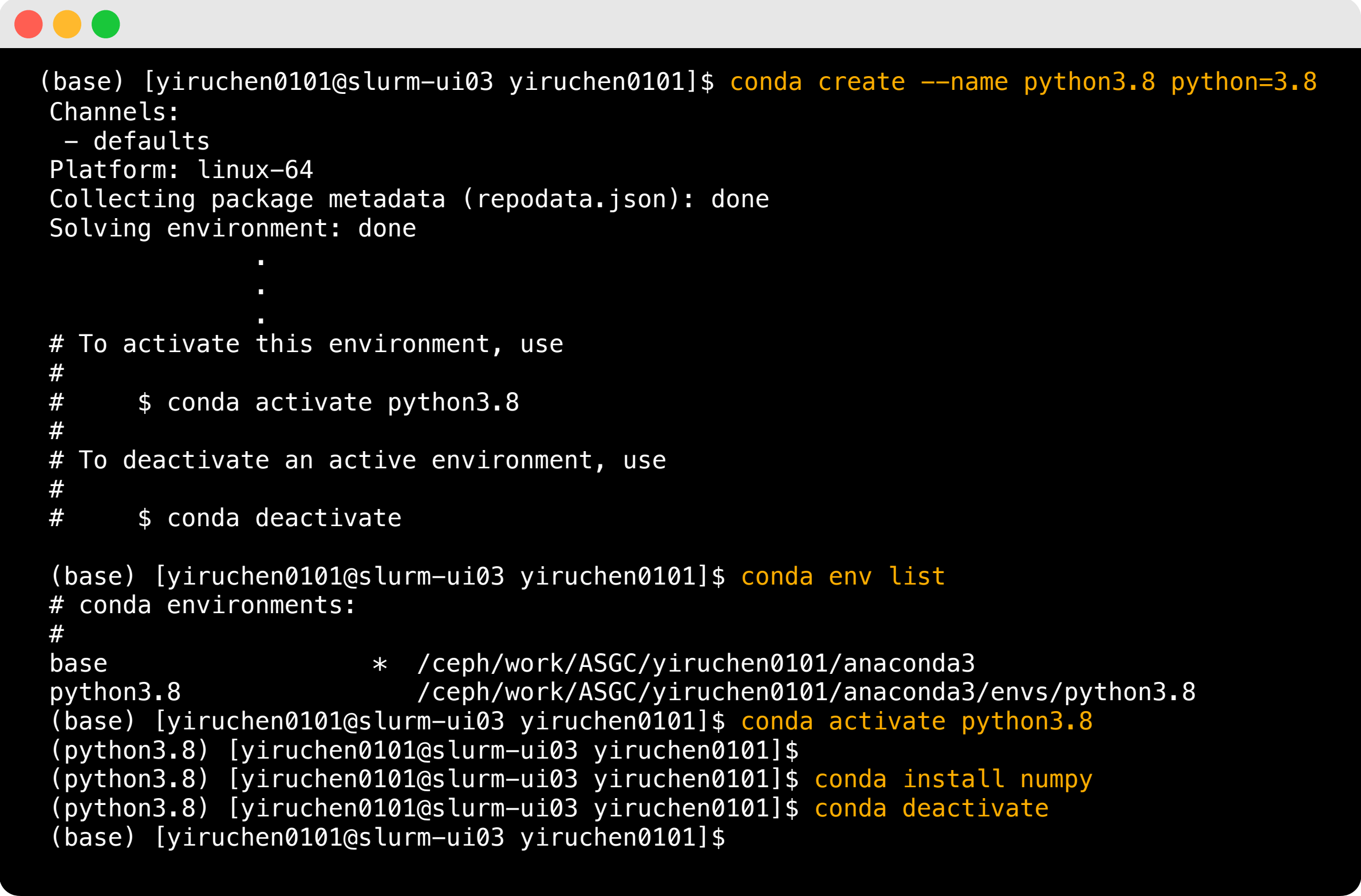
`conda create --name <myenv>`

`conda env list`

`conda activate <myenv>`

`conda install <your_package>`

`conda deactivate`



```
(base) [yiruchen0101@slurm-ui03 yiruchen0101]$ conda create --name python3.8 python=3.8
Channels:
 - defaults
Platform: linux-64
Collecting package metadata (repodata.json): done
Solving environment: done

#
# To activate this environment, use
#
#     $ conda activate python3.8
#
# To deactivate an active environment, use
#
#     $ conda deactivate

(base) [yiruchen0101@slurm-ui03 yiruchen0101]$ conda env list
# conda environments:
#
base                  * /ceph/work/ASGC/yiruchen0101/anaconda3
python3.8             /ceph/work/ASGC/yiruchen0101/anaconda3/envs/python3.8
(base) [yiruchen0101@slurm-ui03 yiruchen0101]$ conda activate python3.8
(python3.8) [yiruchen0101@slurm-ui03 yiruchen0101]$
(python3.8) [yiruchen0101@slurm-ui03 yiruchen0101]$ conda install numpy
(python3.8) [yiruchen0101@slurm-ui03 yiruchen0101]$ conda deactivate
(base) [yiruchen0101@slurm-ui03 yiruchen0101]$
```

Python, Compilation and MPI Environment

Compilation

- Before compiling, enter an interactive session on the desired CPU type (Intel or AMD) using Slurm :
`salloc --partition=(edr1-al9_short / intel-g4-al9_short) ---ntasks=1 --tasks-per-node=1`
- Intel compiler
`module load icc/2022.1.0`
- AMD compiler
`module load aocc/4.2.0`
- GCC
`module load gcc/12.1.0`
- nvidia development kit (nvcc, for GPU program development)
`module load nvhpc/24.3`

```
[yiruchen0101@slurm-ui01 yiruchen0101]$ salloc --partition=edr1-al9_short --ntasks=1 --tasks-per-node=1
salloc: Pending job allocation 1583407
salloc: job 1583407 queued and waiting for resources
salloc: job 1583407 has been allocated resources
salloc: Granted job allocation 1583407
[yiruchen0101@slurm-ui01 yiruchen0101]$ module load aocc/4.2.0
[yiruchen0101@slurm-ui01 yiruchen0101]$ srun hostname
hpa-wn05.twgrid.org
[yiruchen0101@slurm-ui01 yiruchen0101]$ exit
exit
salloc: Relinquishing job allocation 1583407
salloc: Job allocation 1583407 has been revoked.
```

Python, Compilation and MPI Enviroment

MPI enviroment

- Load different MPI implementation

- mpich

- ```
module load mpi/mpich-4.2.2/gcc13.1.0
```

- openmpi

- ```
module load mpi/openmpi-4.1.0/gcc485
```

- ```
module load mpi/openmpi-5.0.3/aocc420
```

# Available Software

# Available Software software

- Anaconda Python packages :  
TensorFlow, PyTorch, PyRoot .....
- CUDA version on GPU cluster : 12.6
- Some Customized Requirements needs to deploy by **Singularity**.  
AlphaFold. (\* Build fee)



# Job Submission Examples

# Job Submission Examples

## Linux commands

- Show current path : `pwd`
- List current folder's file : `ls`
- Change directory : `cd <path>`
- Create directory : `mkdir <dir>`
- Edit text file : `vim <file>`
- Copy : `cp <file> <new file>`
- Move or change file name : `mv <file> <path or new file name>`
- Remove file : `rm <file>`
- Show manual : `man <command>`

# Job Submission Examples

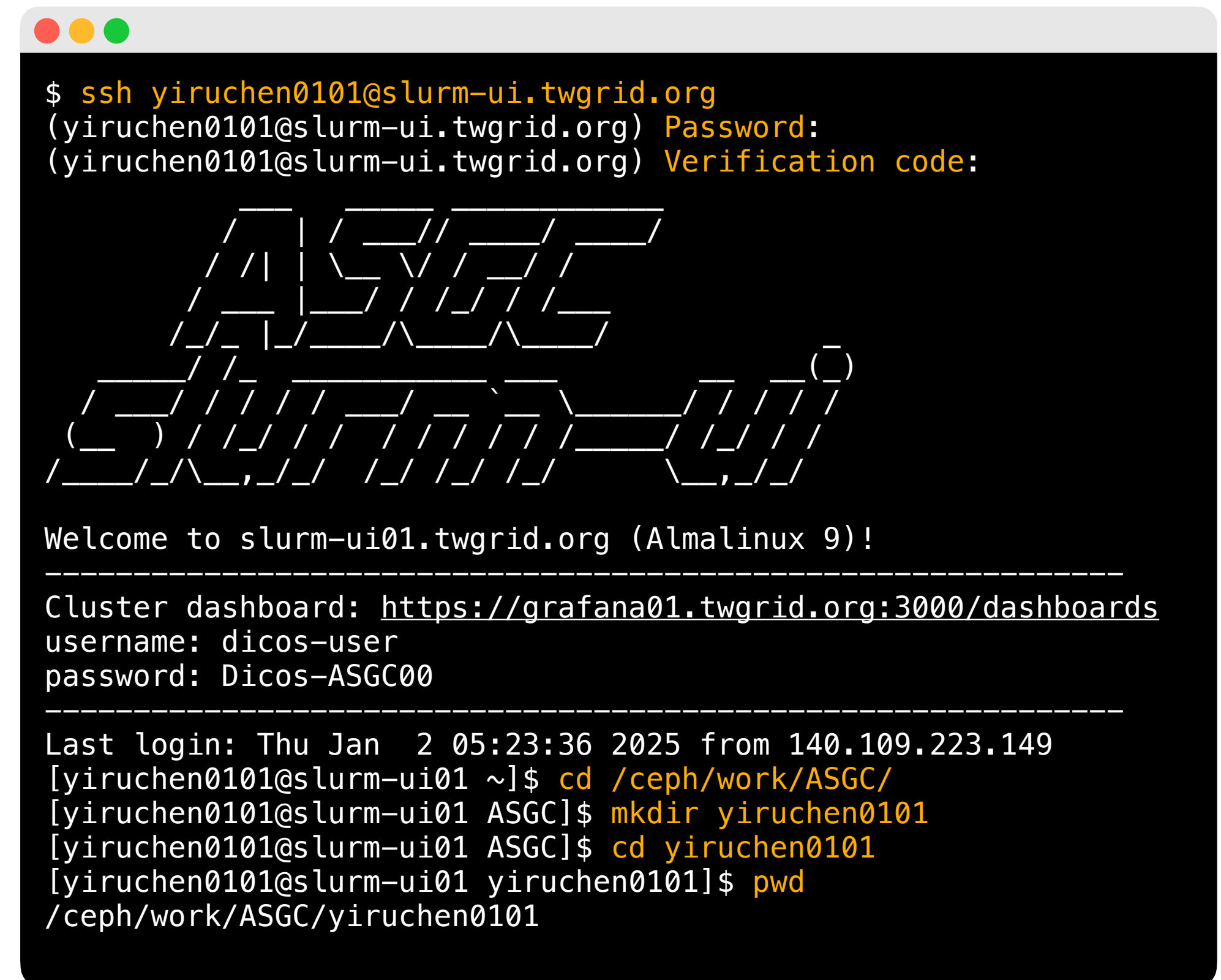
## Preparation

- Open your terminal
- Login : `ssh <your account>@slurm-ui.twgrid.org`
- Go to the working folder : `cd /ceph/work/{group}`
- Build your folder : `mkdir <your account>`
- Go to your folder : `cd <your account>`

PuTTY : <https://www.chiark.greenend.org.uk/~sgtatham/putty/latest.html>

Mobaxterm : <https://mobaxterm.mobatek.net/download-home-edition.html>

VScode : <https://code.visualstudio.com/download>



```
$ ssh yiruchen0101@slurm-ui.twgrid.org
(yiruchen0101@slurm-ui.twgrid.org) Password:
(yiruchen0101@slurm-ui.twgrid.org) Verification code:

 _ _ _ _ _
 / / / / /
/_/_/_/_/_
(_)_/_/_/_/_
/_/_/_/_/_

Welcome to slurm-ui01.twgrid.org (Almalinux 9)!

Cluster dashboard: https://grafana01.twgrid.org:3000/dashboards
username: dicos-user
password: Dicos-ASGC00

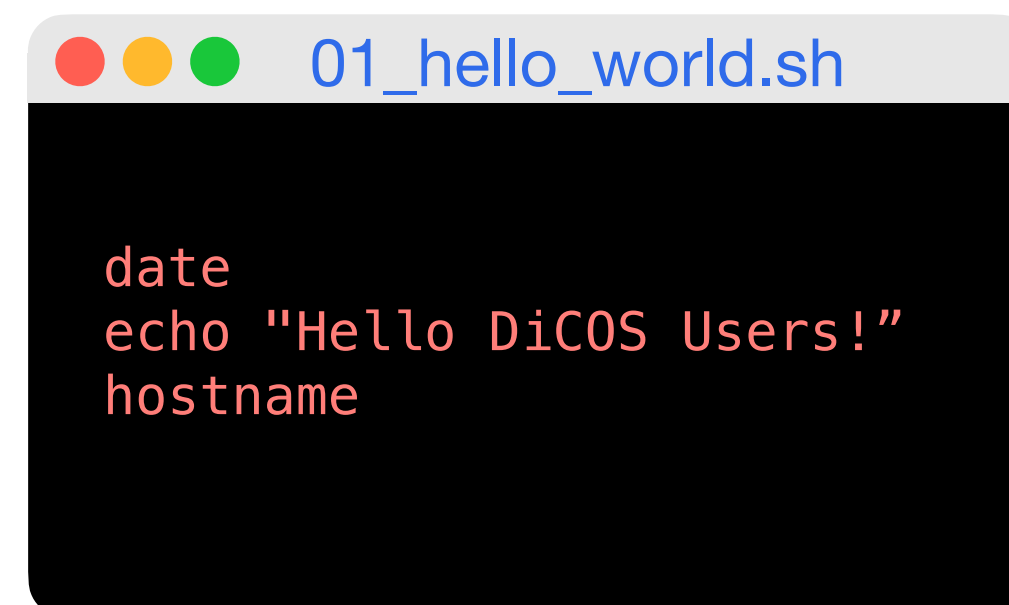
Last login: Thu Jan 2 05:23:36 2025 from 140.109.223.149
[yiruchen0101@slurm-ui01 ~]$ cd /ceph/work/ASGC/
[yiruchen0101@slurm-ui01 ASGC]$ mkdir yiruchen0101
[yiruchen0101@slurm-ui01 ASGC]$ cd yiruchen0101
[yiruchen0101@slurm-ui01 yiruchen0101]$ pwd
/ceph/work/ASGC/yiruchen0101
```

# Job Submission Examples

## Example 1 - Simple Job Submission (Hello World)

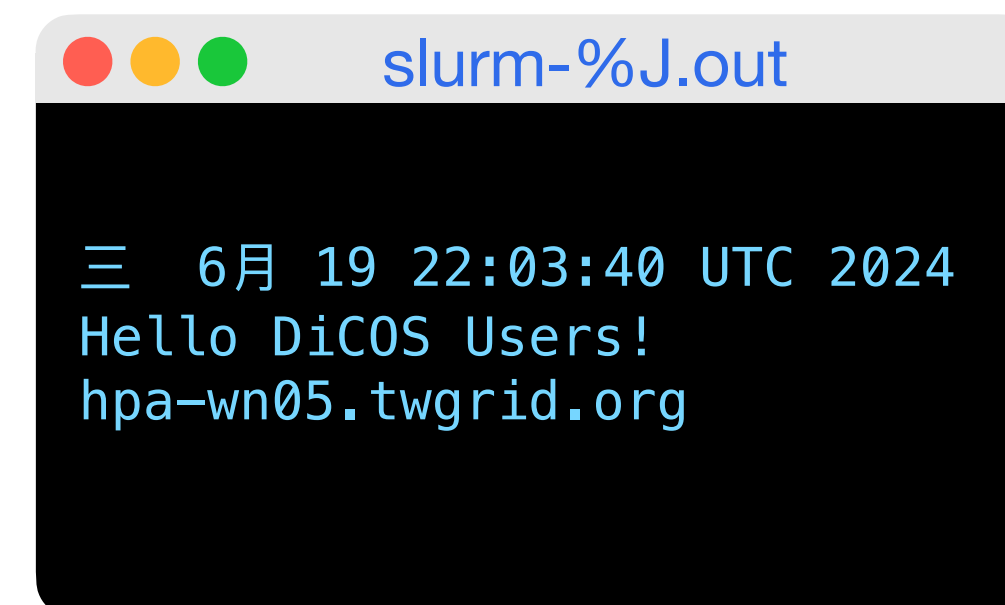
- Prepare a user defined shell script : 01\_hello\_world.sh
- Submit the job with sbatch

`sbatch 01_hello_world.sh`

A terminal window with a title bar containing three colored circles (red, yellow, green) and the text "01\_hello\_world.sh". The window has a black background with red text. The text inside the window is:

```
date
echo "Hello DiCOS Users!"
hostname
```

```
01_hello_world.sh
date
echo "Hello DiCOS Users!"
hostname
```

A terminal window with a title bar containing three colored circles (red, yellow, green) and the text "slurm-%J.out". The window has a black background with cyan text. The text inside the window is:

```
≡ 6月 19 22:03:40 UTC 2024
Hello DiCOS Users!
hpa-wn05.twgrid.org
```

```
slurm-%J.out
≡ 6月 19 22:03:40 UTC 2024
Hello DiCOS Users!
hpa-wn05.twgrid.org
```

# Job Submission Examples

## Example 2 - Submit a MCORE job

- You will need to assign in your preamble of the script for the requesting resources.

E.g. `02_mcore.sh`

- Submit job : `sbatch 02_mcore.sh`
- This example will submit a job which requesting 10 CPU cores

```
02_mcore.sh
#!/bin/bash
#SBATCH --job-name=stress_test # Define the name of your job
#SBATCH --partition=intel-g4-al9_short # Partiotion name
#SBATCH --nodes=1 # Numbers of nodes
#SBATCH --ntasks-per-node=1 # Number of tasks per node
#SBATCH --cpus-per-task=10 # Number of CPUs per task
#SBATCH --output=%j.out # Standard output file (%j: Job ID)
#SBATCH --error=%j.err # Standard error file (%j: Job ID)
#SBATCH --time=00-01:00:00 # Time limit
#SBATCH --mail-type=ALL # Email notifications = BEGIN, END, FAIL, ALL
#SBATCH --mail-user=jennifer.chen@twgrid.org # Email address to send notifications

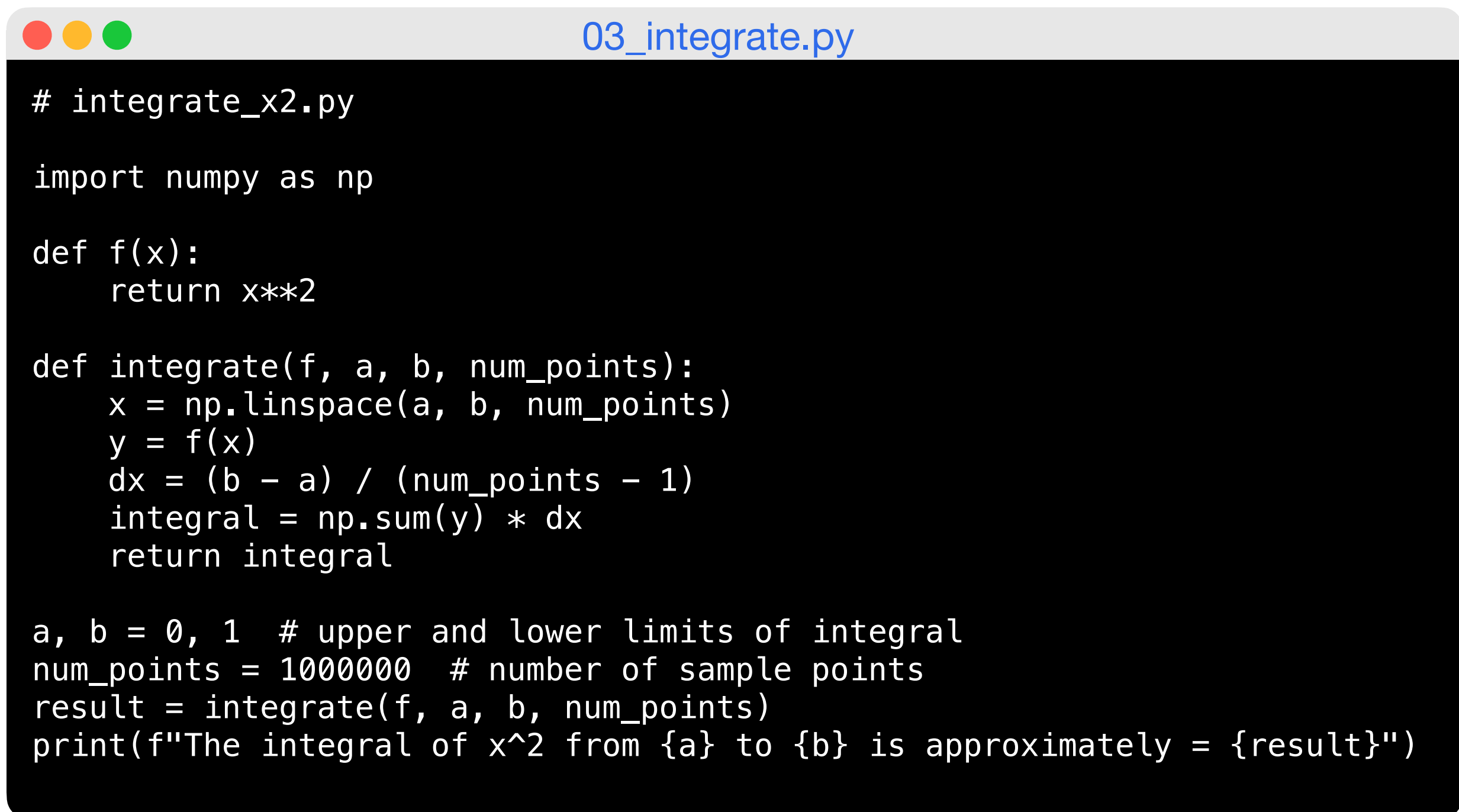
srun stress -c 10 -t 100
```

```
job.%J.out
stress: info: [501543] dispatching hogs: 10 cpu, 0 io, 0 vm, 0 hdd
stress: info: [501543] successful run completed in 100s
```

# Job Submission Examples

## Example 3 - Submit a python job using anaconda3 python3

- Prepare a python script that calculate  $\int_0^1 x^2 dx$  : 03\_integrate.py



```
integrate_x2.py

import numpy as np

def f(x):
 return x**2

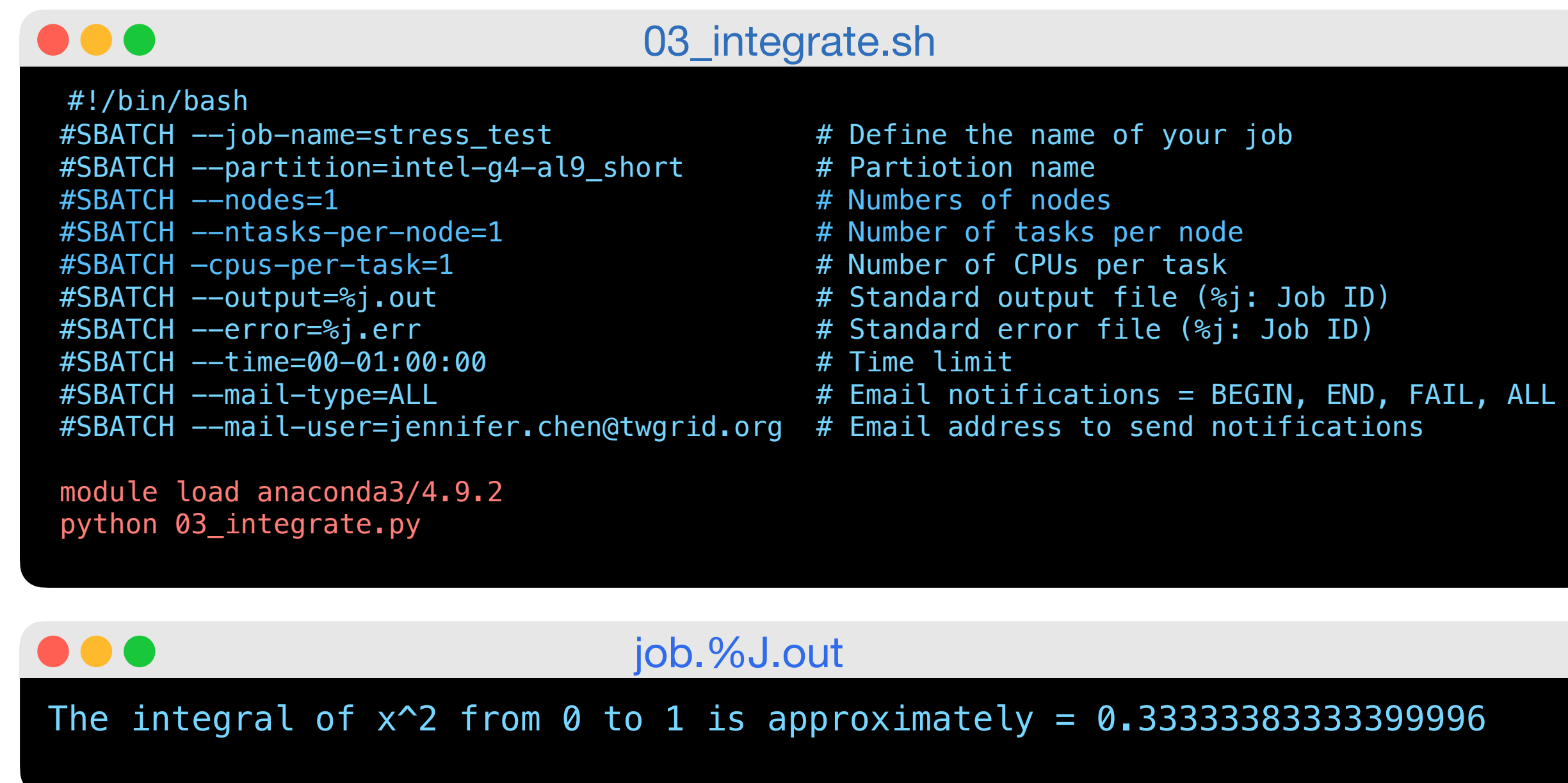
def integrate(f, a, b, num_points):
 x = np.linspace(a, b, num_points)
 y = f(x)
 dx = (b - a) / (num_points - 1)
 integral = np.sum(y) * dx
 return integral

a, b = 0, 1 # upper and lower limits of integral
num_points = 1000000 # number of sample points
result = integrate(f, a, b, num_points)
print(f"The integral of x^2 from {a} to {b} is approximately = {result}")
```

# Job Submission Examples

## Example 3 - Submit a python job using anaconda3 python3

- Prepare a shell script that wrapping the environment modules and run python script: 03\_integrate.sh
- Submit job using sbatch : `sbatch 03_integrate.sh`



```
03_integrate.sh
#!/bin/bash
#SBATCH --job-name=stress_test # Define the name of your job
#SBATCH --partition=intel-g4-al9_short # Partiotion name
#SBATCH --nodes=1 # Numbers of nodes
#SBATCH --ntasks-per-node=1 # Number of tasks per node
#SBATCH -cpus-per-task=1 # Number of CPUs per task
#SBATCH --output=%j.out # Standard output file (%j: Job ID)
#SBATCH --error=%j.err # Standard error file (%j: Job ID)
#SBATCH --time=00-01:00:00 # Time limit
#SBATCH --mail-type=ALL # Email notifications = BEGIN, END, FAIL, ALL
#SBATCH --mail-user=jennifer.chen@twgrid.org # Email address to send notifications

module load anaconda3/4.9.2
python 03_integrate.py

job.%J.out
The integral of x^2 from 0 to 1 is approximately = 0.33333383333399996
```

# Problem Report and FAQ

- Online documents: <https://dicos.grid.sinica.edu.tw/wiki/>
- Email channel to ASGC admins: [DiCOS-Support@twgrid.org](mailto:DiCOS-Support@twgrid.org)
- Regular face-to-face (on-site) video conferences:

ASGC DiCOS user meetings held every Wednesday at 14:30 (UTC+8), please ask our staff for meeting information.