Introduction on Slurm Job Submission

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Outline

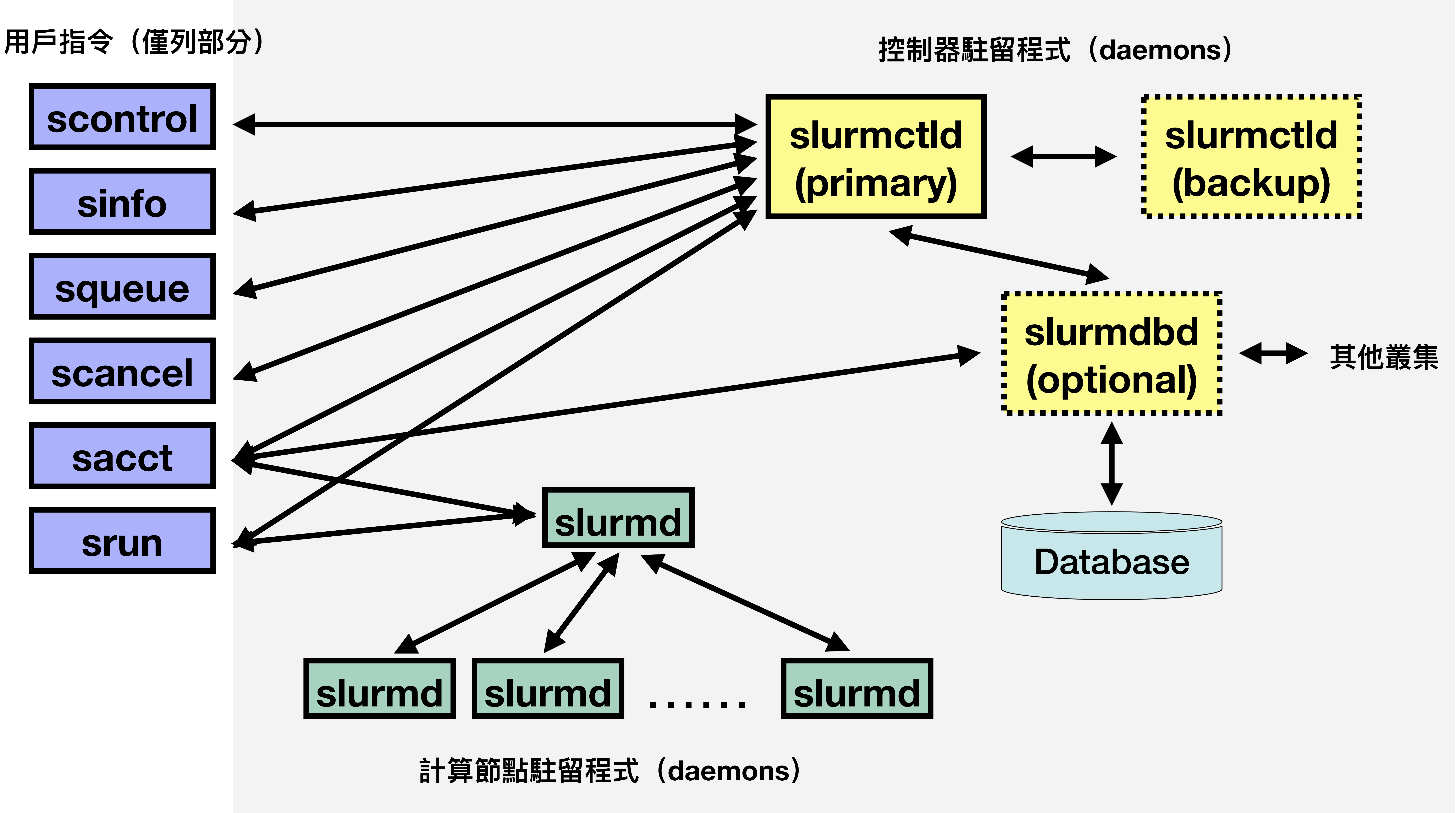
- Introduction of Slurm
- User Interfaces (Login Node)
- Basic Usage of Slurm System
- Environment Modules (Lmod)
- Python, Compilation and MPI Enviroment
- Available Software
- Job Submission Example

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
HDR1	AMD Rome 7662@2.0GHz	6	1.5 TB	128	768
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

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 :

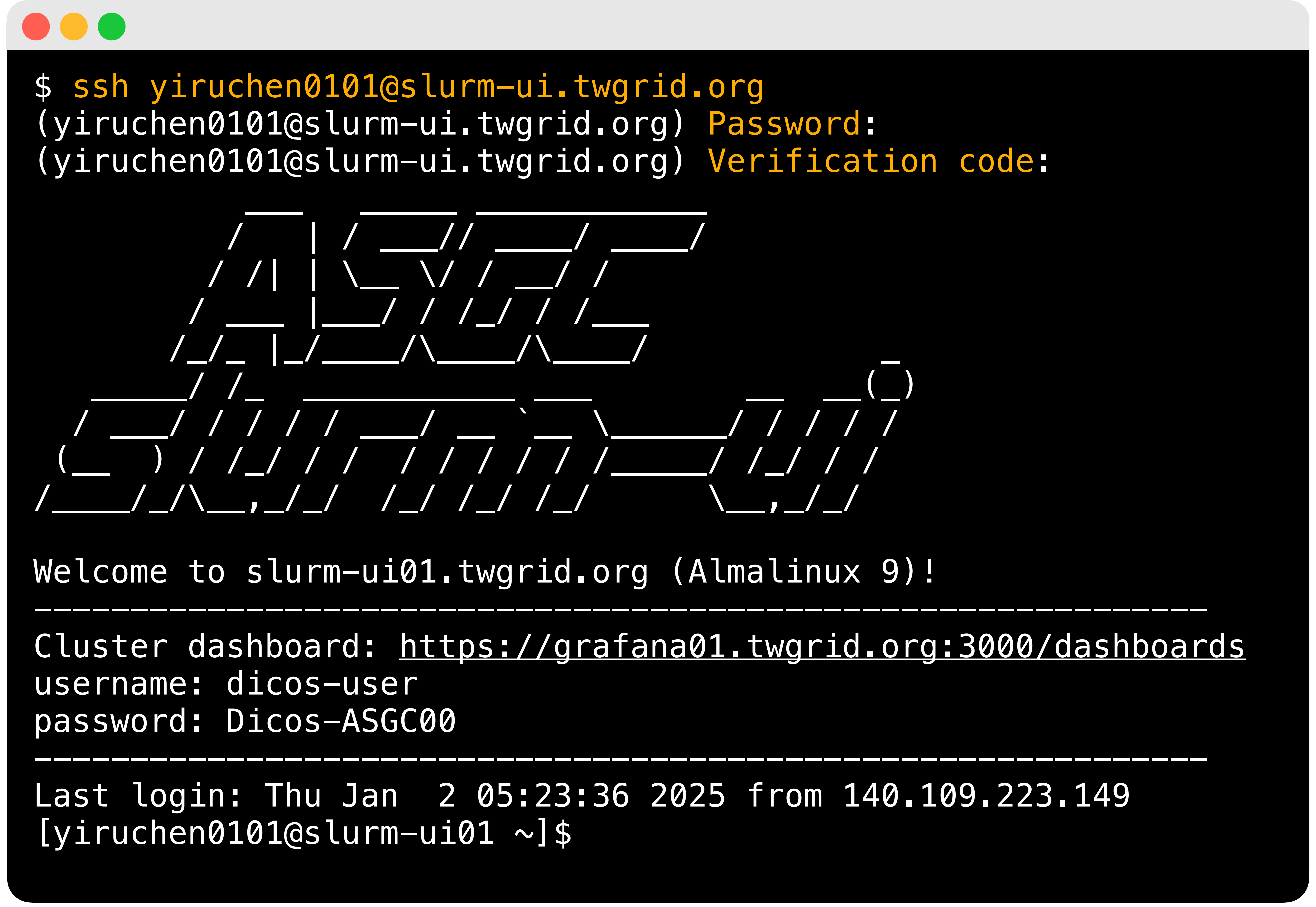
  ssh <your account>@slurm-ui.twgrid.org

  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.

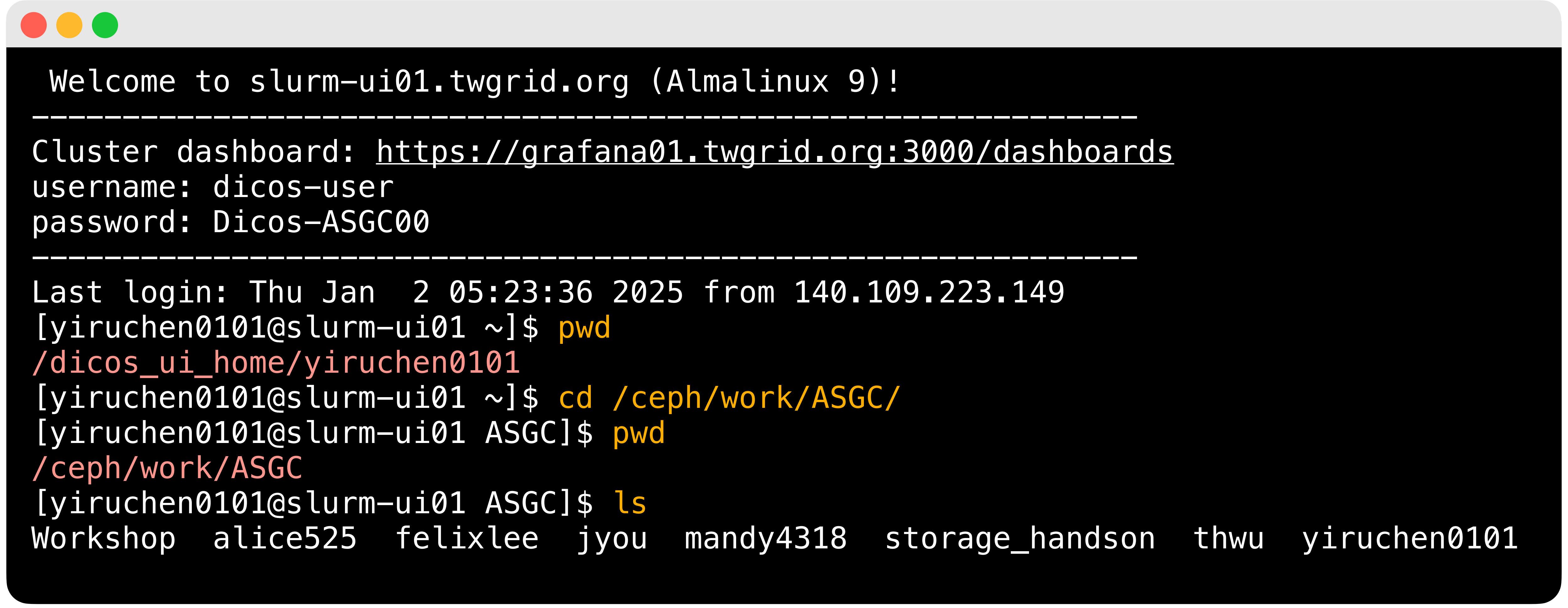


```
$ ssh yiruchen0101@slurm-ui.twgrid.org
(yiruchen0101@slurm-ui.twgrid.org) Password:
(yiruchen0101@slurm-ui.twgrid.org) Verification code:
           ___   _____ ____________
          /   | / ___// ____/ ____/
         / /| | \__ \/ / __/ /
        / ___ |___/ / /_/ / /___
       /_/_ |_/____/\____/\____/            _
   _____/ /_  ___________ ___        __  __(_)
  / ___/ / / / / ___/ __ `__ \______/ / / / /
 (__  ) / /_/ / /  / / / / / /_____/ /_/ / /
/____/_/\__,_/_/  /_/ /_/ /_/      \__,_/_/

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 ~]$
```

User Interfaces (Login Nodes)

Mount Space

- User space : /dicos_ui_home/{user}
- Group Space : /ceph/work/{group}
  - For working and installing software



```
 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 ~]$ 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 hdr1-al9_short my_script.sh
```

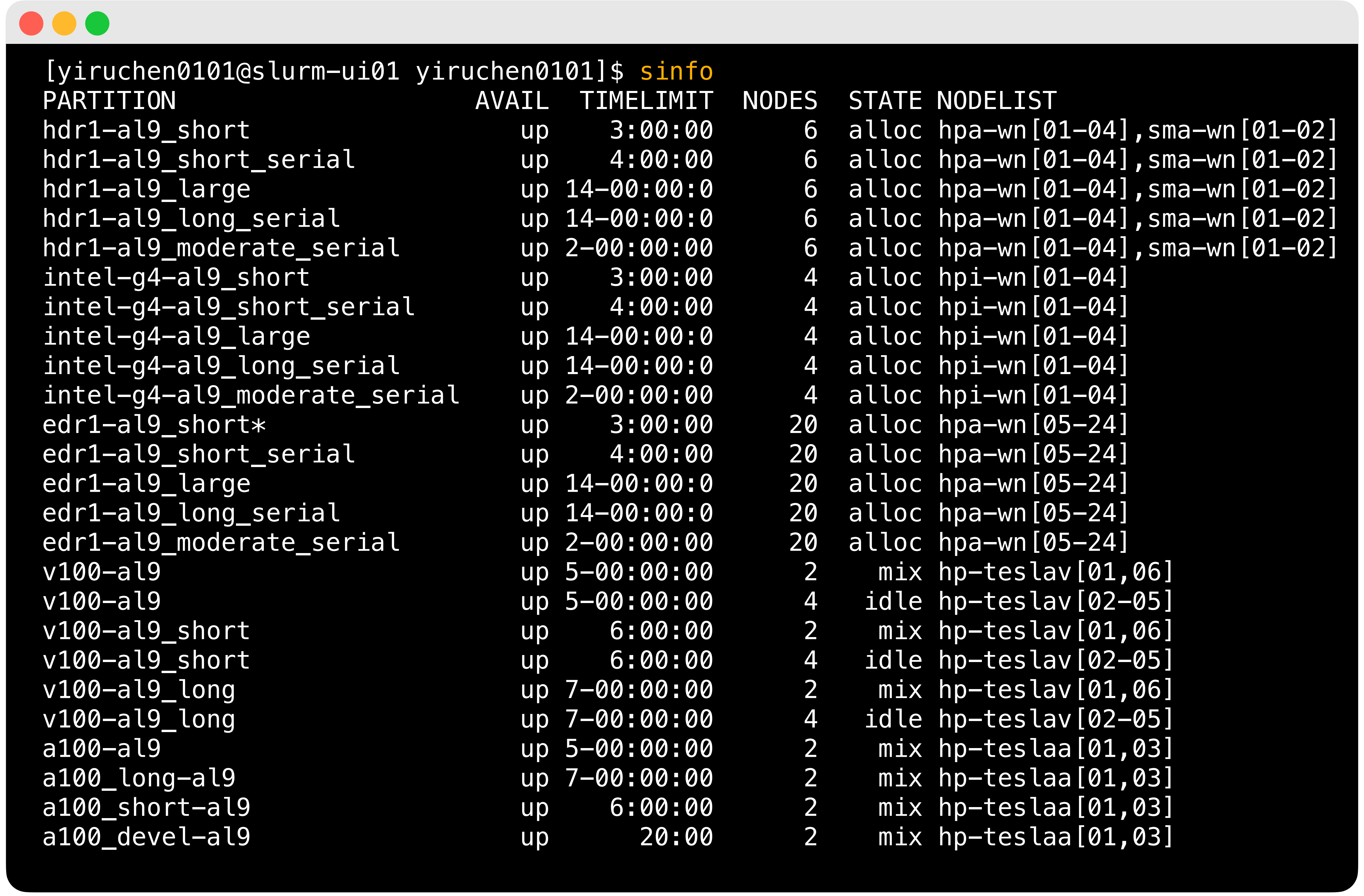
Cluster	Partition	Timelimit	Nodelist
HDR1	**hdr1-al9_short**	3:00:00	sma-wn[01-02] hpa-wn[01-04]
	hdr1-al9_short_serial	4:00:00	
	hdr1-al9_large	14-00:00:00	
	hdr1-al9_long_serial	14-00:00:0	
	hdr1-al9_moderate_serial	2-00:00:0	

Cluster	Partition	Timelimit	Nodelist
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	
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	
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	

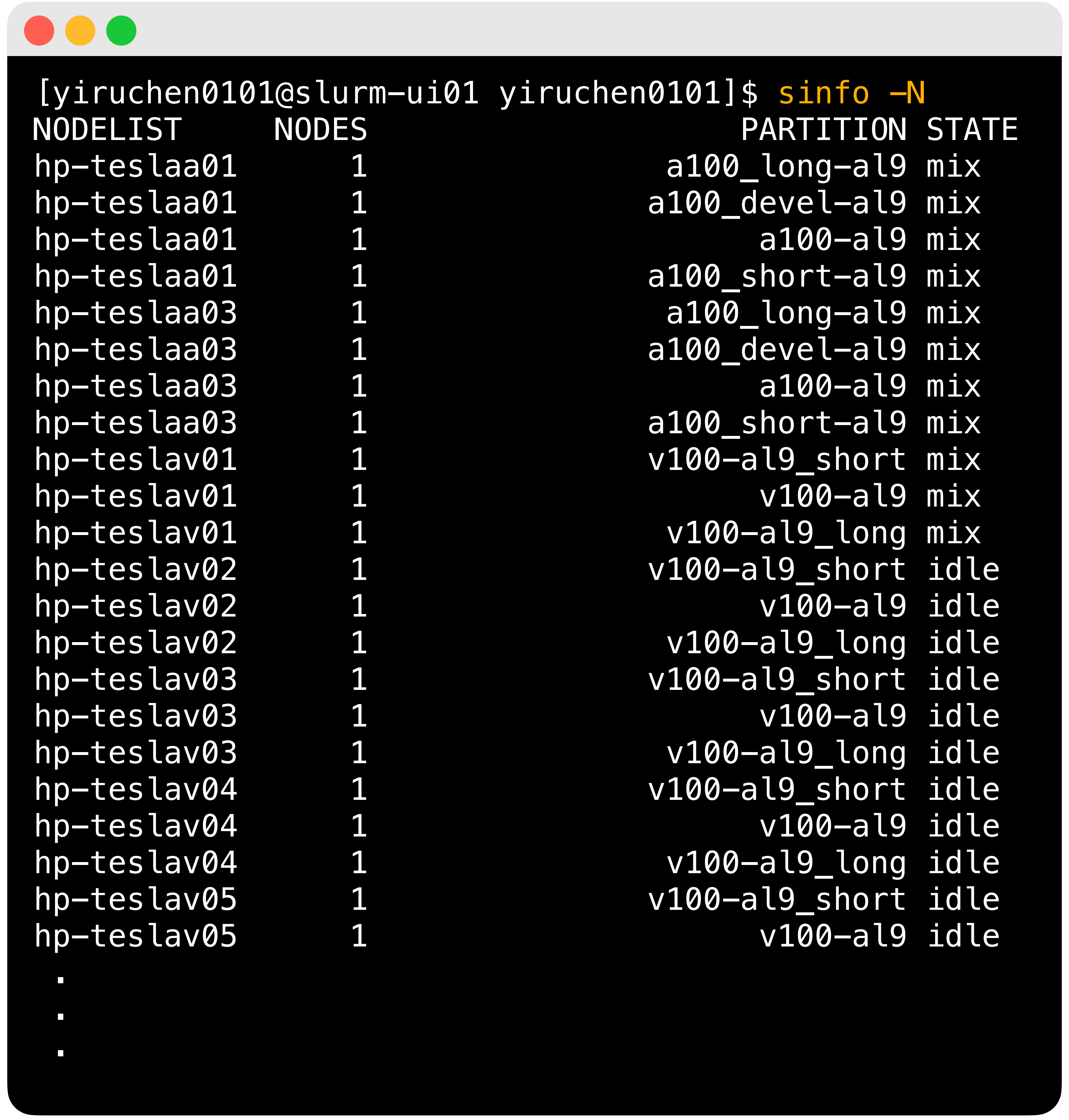
Basic Usage of Slurm System

User commands : sinfo

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



```
[yiruchen0101@slurm-ui01 yiruchen0101]$ sinfo
PARTITION                     AVAIL  TIMELIMIT  NODES  STATE NODELIST
hdr1-al9_short                   up    3:00:00      6  alloc hpa-wn[01-04],sma-wn[01-02]
hdr1-al9_short_serial            up    4:00:00      6  alloc hpa-wn[01-04],sma-wn[01-02]
hdr1-al9_large                   up 14-00:00:0      6  alloc hpa-wn[01-04],sma-wn[01-02]
hdr1-al9_long_serial             up 14-00:00:0      6  alloc hpa-wn[01-04],sma-wn[01-02]
hdr1-al9_moderate_serial         up 2-00:00:00      6  alloc hpa-wn[01-04],sma-wn[01-02]
intel-g4-al9_short               up    3:00:00      4  alloc hpi-wn[01-04]
intel-g4-al9_short_serial        up    4:00:00      4  alloc hpi-wn[01-04]
intel-g4-al9_large               up 14-00:00:0      4  alloc hpi-wn[01-04]
intel-g4-al9_long_serial         up 14-00:00:0      4  alloc hpi-wn[01-04]
intel-g4-al9_moderate_serial     up 2-00:00:00      4  alloc hpi-wn[01-04]
edr1-al9_short*                  up    3:00:00     20  alloc hpa-wn[05-24]
edr1-al9_short_serial            up    4:00:00     20  alloc hpa-wn[05-24]
edr1-al9_large                   up 14-00:00:0     20  alloc hpa-wn[05-24]
edr1-al9_long_serial             up 14-00:00:0     20  alloc hpa-wn[05-24]
edr1-al9_moderate_serial         up 2-00:00:00     20  alloc hpa-wn[05-24]
v100-al9                         up 5-00:00:00      2    mix hp-teslav[01,06]
v100-al9                         up 5-00:00:00      4   idle hp-teslav[02-05]
v100-al9_short                   up    6:00:00      2    mix hp-teslav[01,06]
v100-al9_short                   up    6:00:00      4   idle hp-teslav[02-05]
v100-al9_long                    up 7-00:00:00      2    mix hp-teslav[01,06]
v100-al9_long                    up 7-00:00:00      4   idle hp-teslav[02-05]
a100-al9                         up 5-00:00:00      2    mix hp-teslaa[01,03]
a100_long-al9                    up 7-00:00:00      2    mix hp-teslaa[01,03]
a100_short-al9                   up    6:00:00      2    mix hp-teslaa[01,03]
a100_devel-al9                   up      20:00      2    mix hp-teslaa[01,03]
```

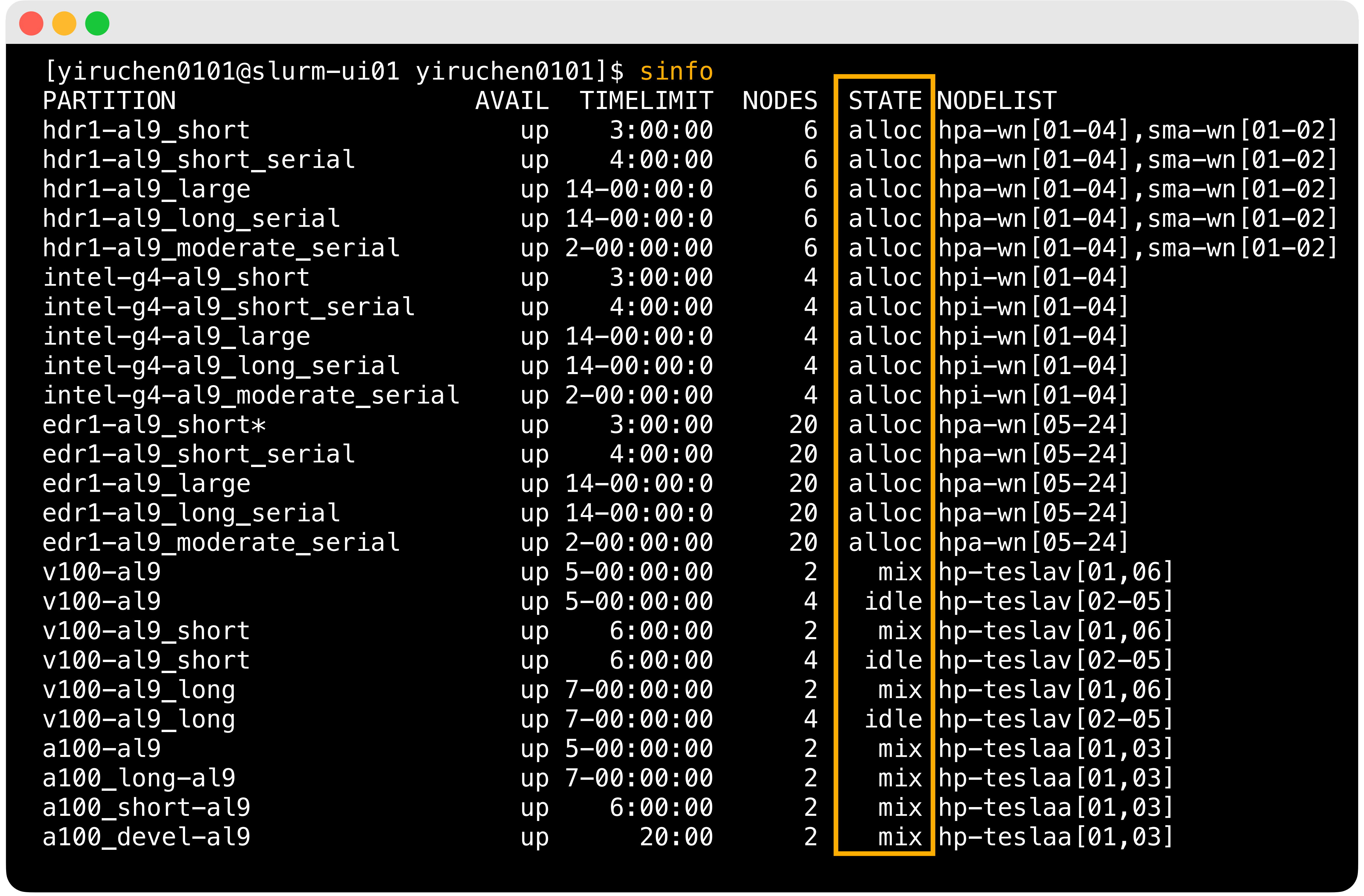


```
[yiruchen0101@slurm-ui01 yiruchen0101]$ sinfo -N
NODELIST      NODES                      PARTITION STATE
hp-teslaa01       1                  a100_long-al9 mix
hp-teslaa01       1                 a100_devel-al9 mix
hp-teslaa01       1                       a100-al9 mix
hp-teslaa01       1                 a100_short-al9 mix
hp-teslaa03       1                  a100_long-al9 mix
hp-teslaa03       1                 a100_devel-al9 mix
hp-teslaa03       1                       a100-al9 mix
hp-teslaa03       1                 a100_short-al9 mix
hp-teslav01       1                 v100-al9_short mix
hp-teslav01       1                       v100-al9 mix
hp-teslav01       1                  v100-al9_long mix
hp-teslav02       1                 v100-al9_short idle
hp-teslav02       1                       v100-al9 idle
hp-teslav02       1                  v100-al9_long idle
hp-teslav03       1                 v100-al9_short idle
hp-teslav03       1                       v100-al9 idle
hp-teslav03       1                  v100-al9_long idle
hp-teslav04       1                 v100-al9_short idle
hp-teslav04       1                       v100-al9 idle
hp-teslav04       1                  v100-al9_long idle
hp-teslav05       1                 v100-al9_short idle
hp-teslav05       1                       v100-al9 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
hdr1-al9_short                  up    3:00:00      6  alloc hpa-wn[01-04],sma-wn[01-02]
hdr1-al9_short_serial           up    4:00:00      6  alloc hpa-wn[01-04],sma-wn[01-02]
hdr1-al9_large                  up 14-00:00:0      6  alloc hpa-wn[01-04],sma-wn[01-02]
hdr1-al9_long_serial            up 14-00:00:0      6  alloc hpa-wn[01-04],sma-wn[01-02]
hdr1-al9_moderate_serial        up 2-00:00:00      6  alloc hpa-wn[01-04],sma-wn[01-02]
intel-g4-al9_short              up    3:00:00      4  alloc hpi-wn[01-04]
intel-g4-al9_short_serial       up    4:00:00      4  alloc hpi-wn[01-04]
intel-g4-al9_large              up 14-00:00:0      4  alloc hpi-wn[01-04]
intel-g4-al9_long_serial        up 14-00:00:0      4  alloc hpi-wn[01-04]
intel-g4-al9_moderate_serial    up 2-00:00:00      4  alloc hpi-wn[01-04]
edr1-al9_short*                 up    3:00:00     20  alloc hpa-wn[05-24]
edr1-al9_short_serial           up    4:00:00     20  alloc hpa-wn[05-24]
edr1-al9_large                  up 14-00:00:0     20  alloc hpa-wn[05-24]
edr1-al9_long_serial            up 14-00:00:0     20  alloc hpa-wn[05-24]
edr1-al9_moderate_serial        up 2-00:00:00     20  alloc hpa-wn[05-24]
v100-al9                        up 5-00:00:00      2    mix hp-teslav[01,06]
v100-al9                        up 5-00:00:00      4   idle hp-teslav[02-05]
v100-al9_short                  up    6:00:00      2    mix hp-teslav[01,06]
v100-al9_short                  up    6:00:00      4   idle hp-teslav[02-05]
v100-al9_long                   up 7-00:00:00      2    mix hp-teslav[01,06]
v100-al9_long                   up 7-00:00:00      4   idle hp-teslav[02-05]
a100-al9                        up 5-00:00:00      2    mix hp-teslaa[01,03]
a100_long-al9                   up 7-00:00:00      2    mix hp-teslaa[01,03]
a100_short-al9                  up    6:00:00      2    mix hp-teslaa[01,03]
a100_devel-al9                  up      20:00      2    mix hp-teslaa[01,03]
```

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.

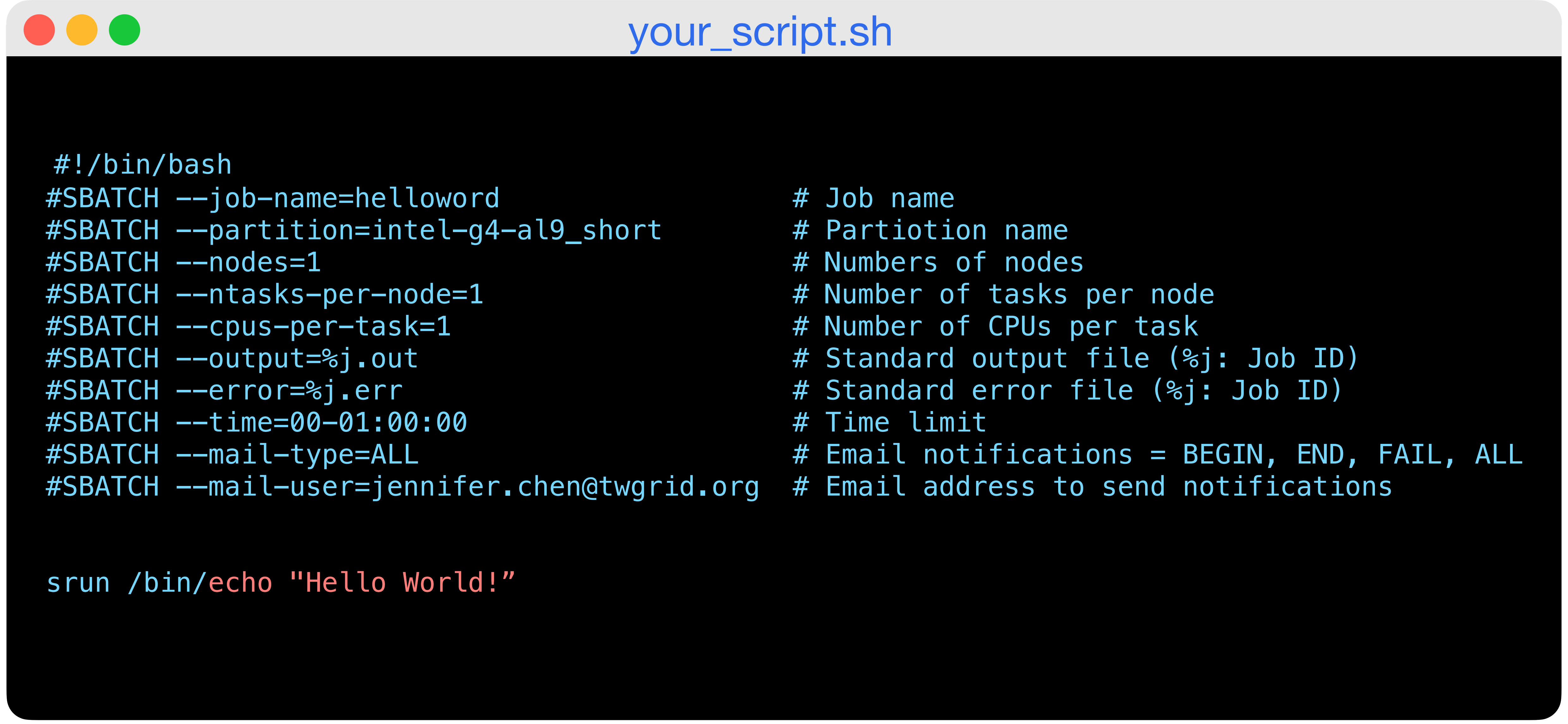
drain : The node is unavailable for use per system administrator request.

drang : The node is currently allocated a job, but will not be allocated additional jobs.

Basic Usage of Slurm System

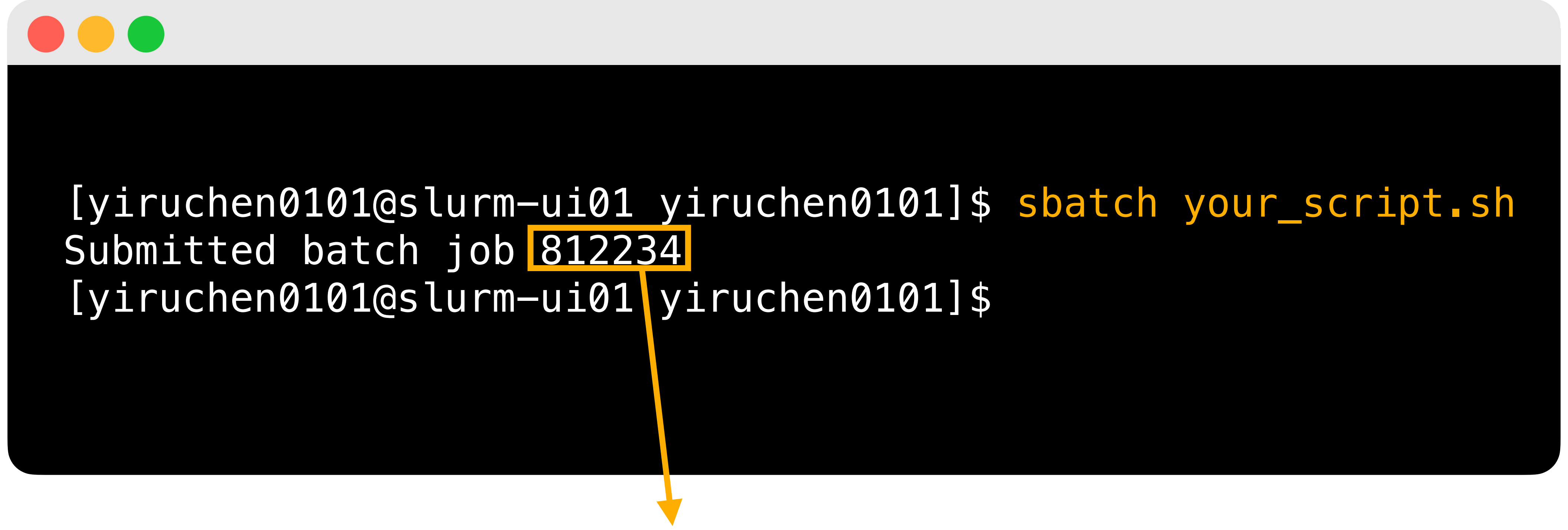
User commands : sbatch

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



your_script.sh

```
 #!/bin/bash
#SBATCH --job-name=helloword                 # Job name
#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


srun /bin/echo "Hello World!”
```



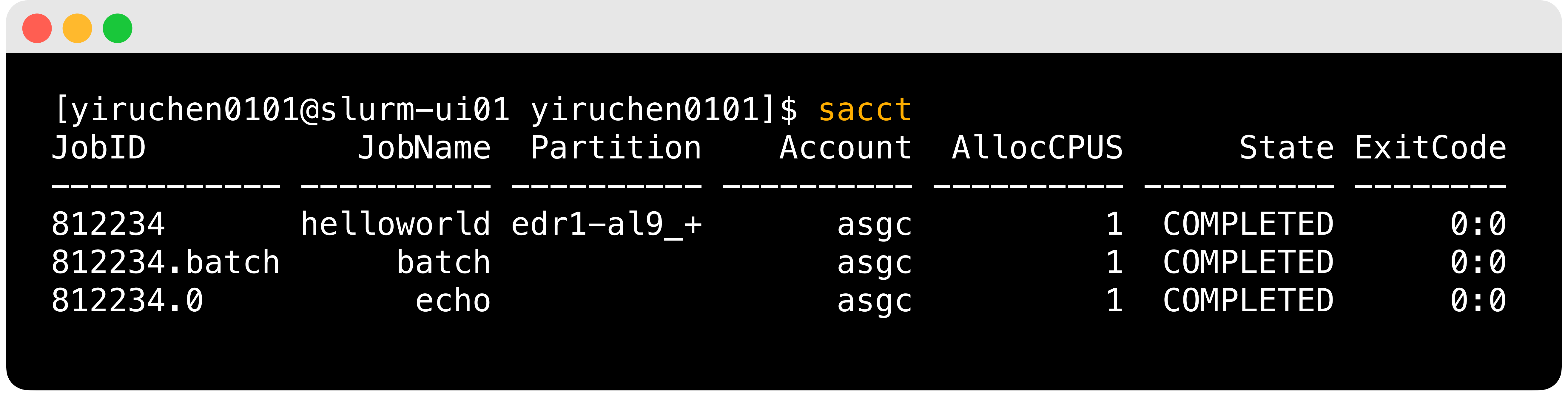
```
[yiruchen0101@slurm-ui01 yiruchen0101]$ sbatch your_script.sh
Submitted batch job 812234
[yiruchen0101@slurm-ui01 yiruchen0101]$
```

Job ID

Basic Usage of Slurm System

User commands : sacct

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

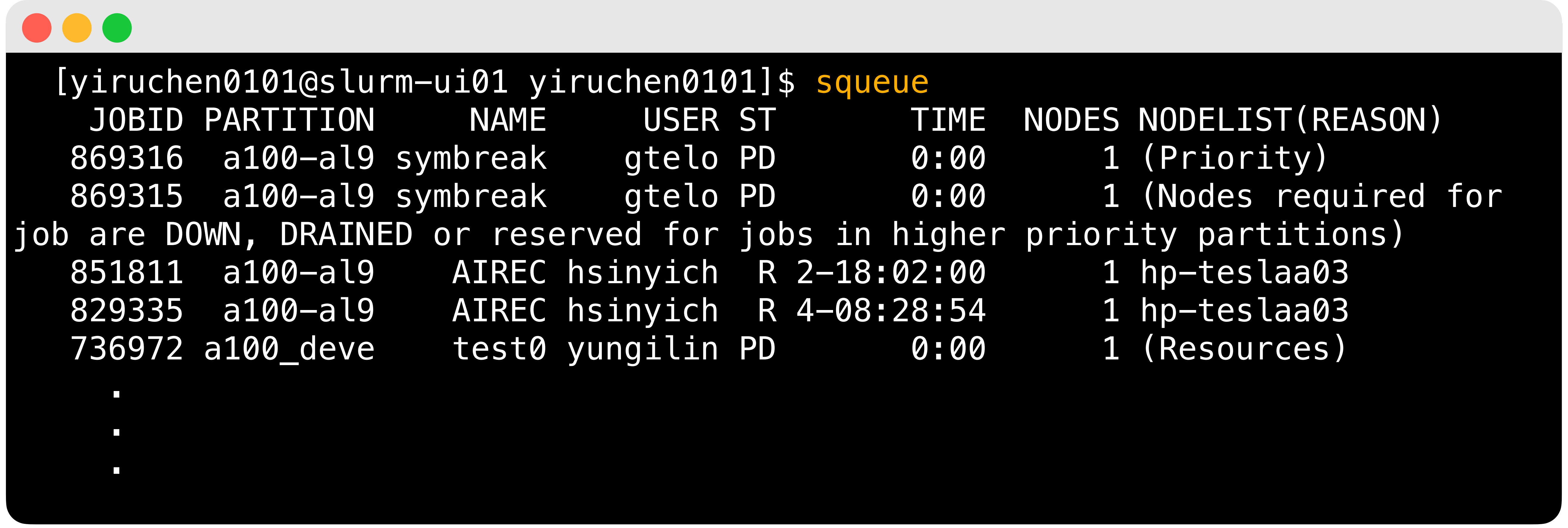


```
[yiruchen0101@slurm-ui01 yiruchen0101]$ sacct
JobID           JobName  Partition    Account  AllocCPUS      State ExitCode
------------ ---------- ---------- ---------- ---------- ---------- --------
812234       helloworld edr1-al9_+       asgc          1  COMPLETED      0:0
812234.batch      batch                  asgc          1  COMPLETED      0:0
812234.0           echo                  asgc          1  COMPLETED      0:0
```

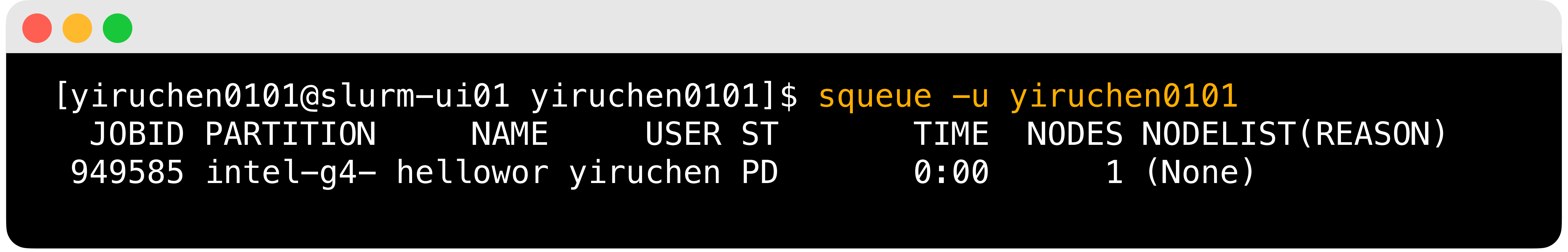
Basic Usage of Slurm System

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-al9 symbreak    gtelo PD       0:00      1 (Priority)
   869315  a100-al9 symbreak    gtelo PD       0:00      1 (Nodes required for
job are DOWN, DRAINED or reserved for jobs in higher priority partitions)
   851811  a100-al9    AIREC hsinyich  R 2-18:02:00      1 hp-teslaa03
   829335  a100-al9    AIREC hsinyich  R 4-08:28:54      1 hp-teslaa03
   736972 a100_deve    test0 yungilin PD       0:00      1 (Resources)
     .
     .
     .
```

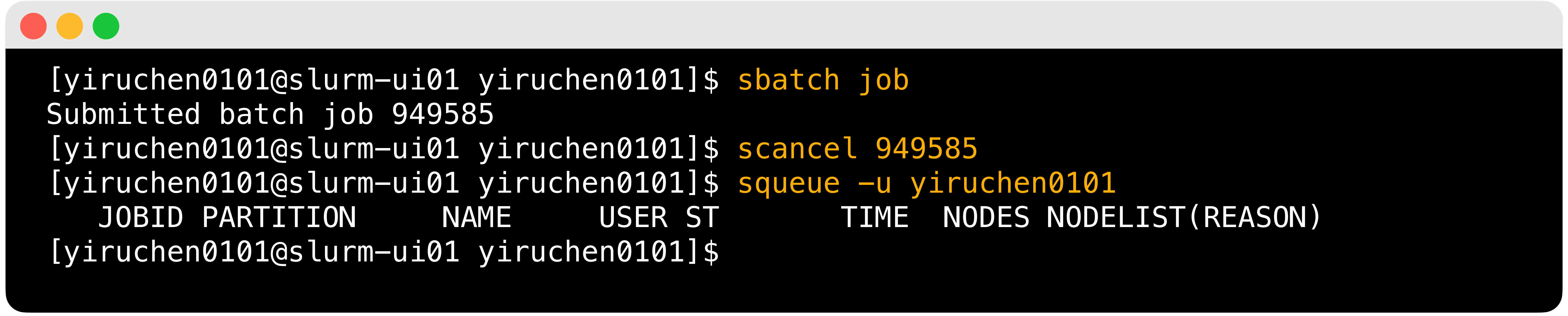


```
  [yiruchen0101@slurm-ui01 yiruchen0101]$ squeue -u yiruchen0101
    JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
   949585 intel-g4- hellowor yiruchen PD       0:00      1 (None)
```

Basic Usage of Slurm System

User commands : scancel

- Cancel your job : scancel <your JobID>

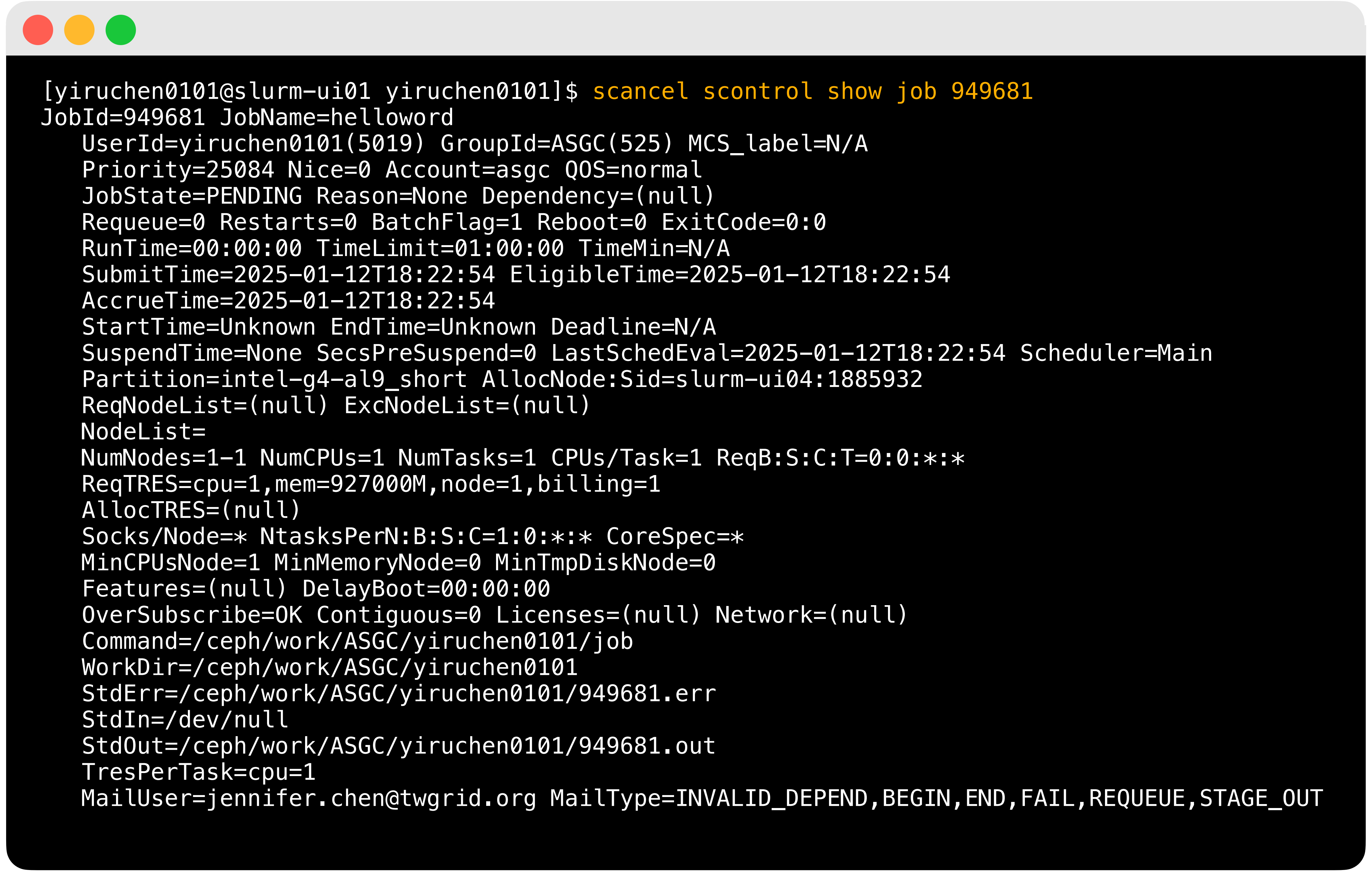


```
[yiruchen0101@slurm-ui01 yiruchen0101]$ sbatch job
Submitted batch job 949585
[yiruchen0101@slurm-ui01 yiruchen0101]$ scancel 949585
[yiruchen0101@slurm-ui01 yiruchen0101]$ squeue -u yiruchen0101
   JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
[yiruchen0101@slurm-ui01 yiruchen0101]$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

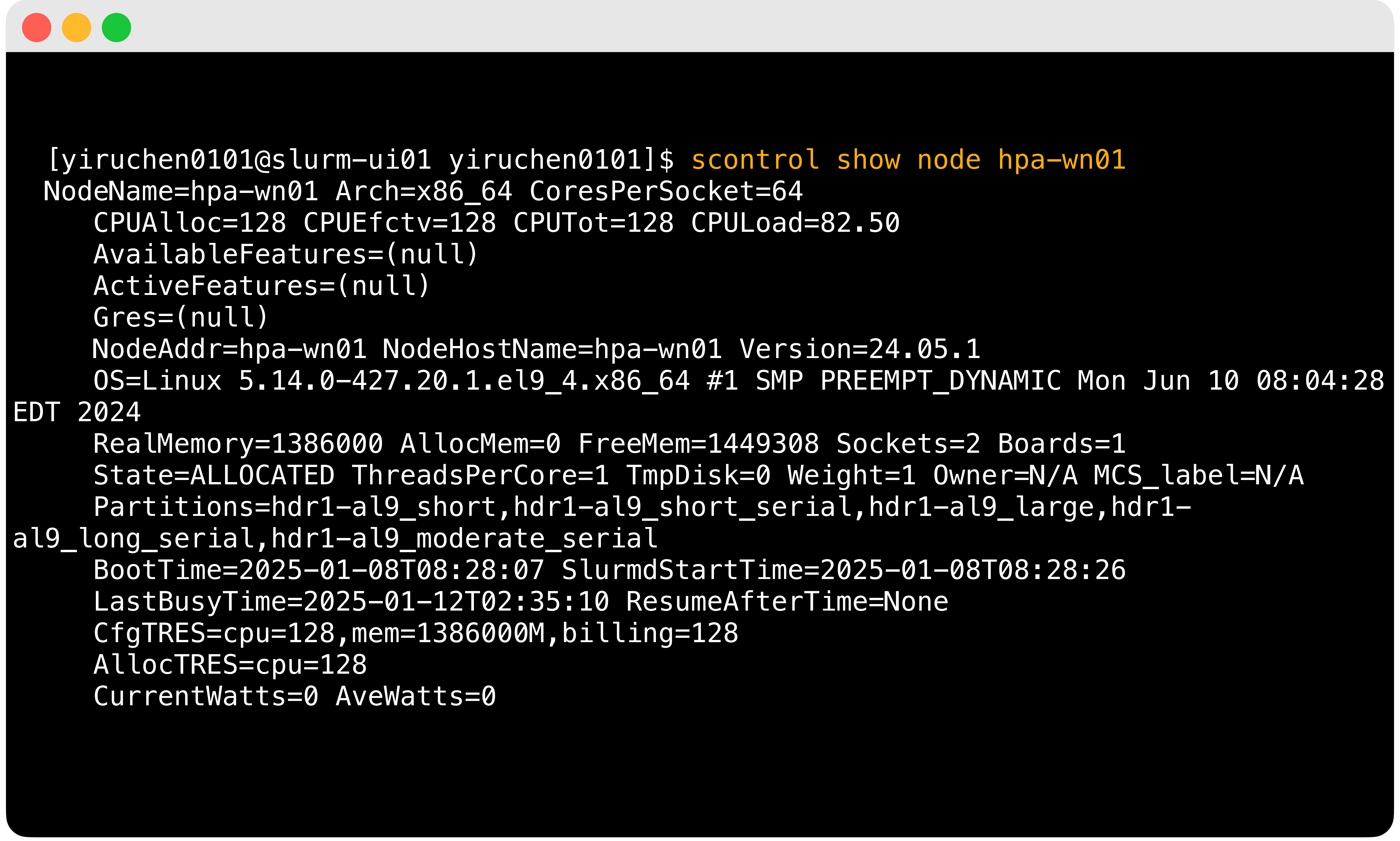
Basic Usage of Slurm System

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]$ scancel scontrol show job 949681
JobId=949681 JobName=helloword
   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-wn01
 NodeName=hpa-wn01 Arch=x86_64 CoresPerSocket=64
    CPUAlloc=128 CPUEfctv=128 CPUTot=128 CPULoad=82.50
    AvailableFeatures=(null)
    ActiveFeatures=(null)
    Gres=(null)
    NodeAddr=hpa-wn01 NodeHostName=hpa-wn01 Version=24.05.1
    OS=Linux 5.14.0-427.20.1.el9_4.x86_64 #1 SMP PREEMPT_DYNAMIC Mon Jun 10 08:04:28
EDT 2024
    RealMemory=1386000 AllocMem=0 FreeMem=1449308 Sockets=2 Boards=1
    State=ALLOCATED ThreadsPerCore=1 TmpDisk=0 Weight=1 Owner=N/A MCS_label=N/A
    Partitions=hdr1-al9_short,hdr1-al9_short_serial,hdr1-al9_large,hdr1-
al9_long_serial,hdr1-al9_moderate_serial
    BootTime=2025-01-08T08:28:07 SlurmdStartTime=2025-01-08T08:28:26
    LastBusyTime=2025-01-12T02:35:10 ResumeAfterTime=None
    CfgTRES=cpu=128,mem=1386000M,billing=128
    AllocTRES=cpu=128
    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 :

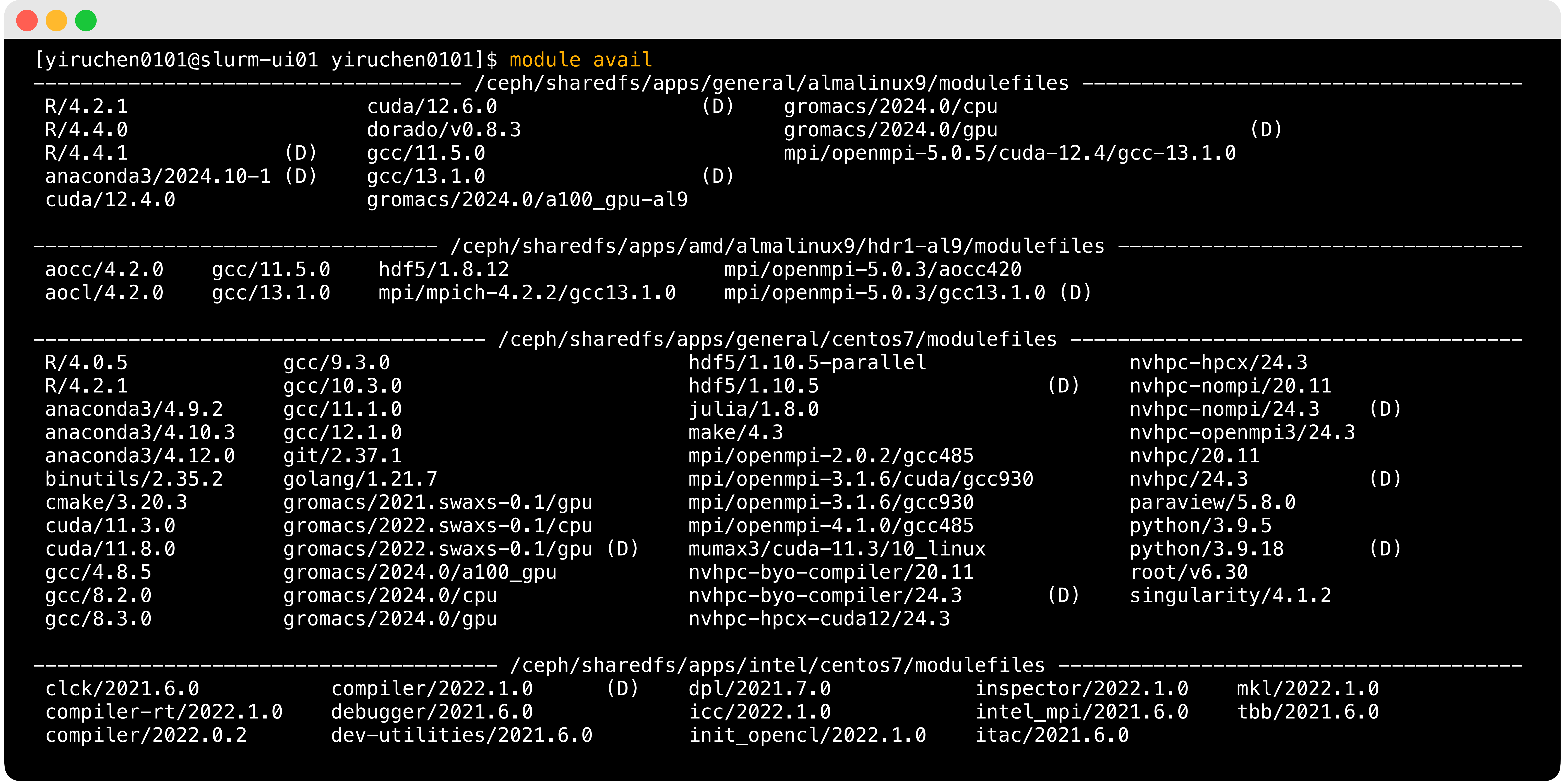
  https://modules.readthedocs.io/en/latest/

- 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

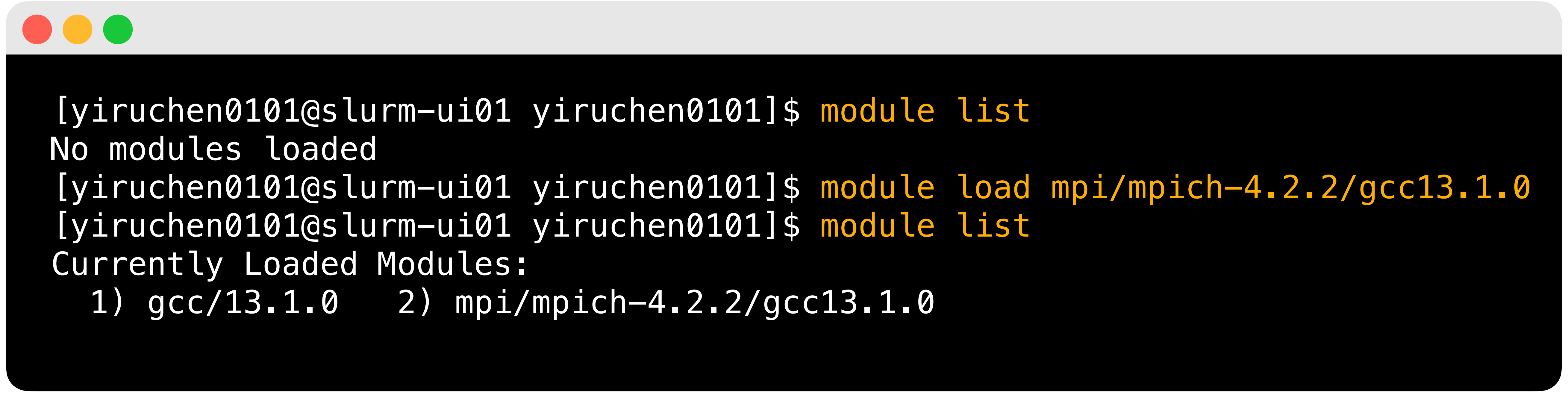


```
[yiruchen0101@slurm-ui01 yiruchen0101]$ module avail
------------------------------------ /ceph/sharedfs/apps/general/almalinux9/modulefiles -------------------------------------
 R/4.2.1                    cuda/12.6.0                 (D)    gromacs/2024.0/cpu
 R/4.4.0                    dorado/v0.8.3                      gromacs/2024.0/gpu                     (D)
 R/4.4.1             (D)    gcc/11.5.0                         mpi/openmpi-5.0.5/cuda-12.4/gcc-13.1.0
 anaconda3/2024.10-1 (D)    gcc/13.1.0                  (D)
 cuda/12.4.0                gromacs/2024.0/a100_gpu-al9

---------------------------------- /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/9.3.0                         hdf5/1.10.5-parallel                 nvhpc-hpcx/24.3
 R/4.2.1             gcc/10.3.0                        hdf5/1.10.5                   (D)    nvhpc-nompi/20.11
 anaconda3/4.9.2     gcc/11.1.0                        julia/1.8.0                          nvhpc-nompi/24.3    (D)
 anaconda3/4.10.3    gcc/12.1.0                        make/4.3                             nvhpc-openmpi3/24.3
 anaconda3/4.12.0    git/2.37.1                        mpi/openmpi-2.0.2/gcc485             nvhpc/20.11
 binutils/2.35.2     golang/1.21.7                     mpi/openmpi-3.1.6/cuda/gcc930        nvhpc/24.3          (D)
 cmake/3.20.3        gromacs/2021.swaxs-0.1/gpu        mpi/openmpi-3.1.6/gcc930             paraview/5.8.0
 cuda/11.3.0         gromacs/2022.swaxs-0.1/cpu        mpi/openmpi-4.1.0/gcc485             python/3.9.5
 cuda/11.8.0         gromacs/2022.swaxs-0.1/gpu (D)    mumax3/cuda-11.3/10_linux            python/3.9.18       (D)
 gcc/4.8.5           gromacs/2024.0/a100_gpu           nvhpc-byo-compiler/20.11             root/v6.30
 gcc/8.2.0           gromacs/2024.0/cpu                nvhpc-byo-compiler/24.3       (D)    singularity/4.1.2
 gcc/8.3.0           gromacs/2024.0/gpu                nvhpc-hpcx-cuda12/24.3

--------------------------------------- /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>

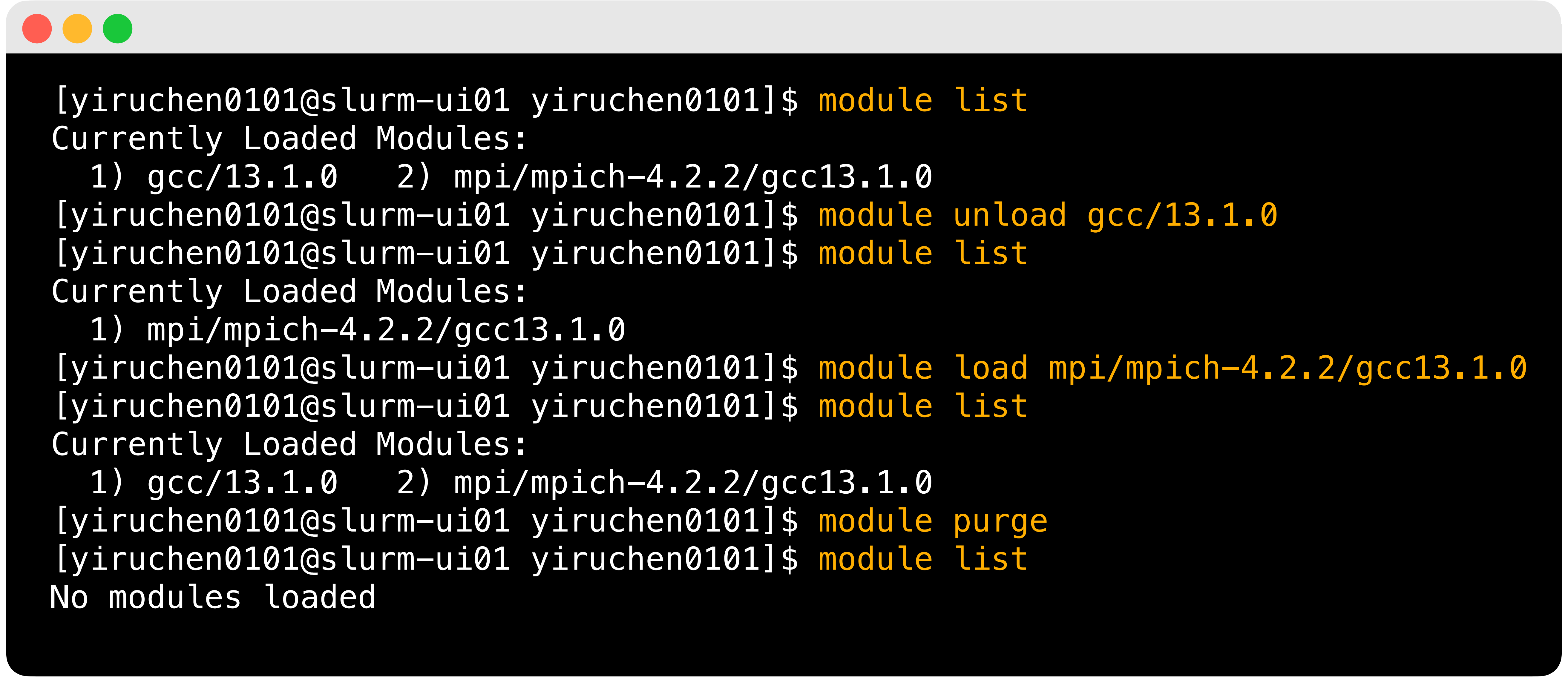


```
[yiruchen0101@slurm-ui01 yiruchen0101]$ module list
No modules loaded
[yiruchen0101@slurm-ui01 yiruchen0101]$ module load mpi/mpich-4.2.2/gcc13.1.0
[yiruchen0101@slurm-ui01 yiruchen0101]$ module list
Currently Loaded Modules:
  1) gcc/13.1.0   2) mpi/mpich-4.2.2/gcc13.1.0
```

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 Enviroment

Python, Compilation and MPI Enviroment

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 Enviroment

Python

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

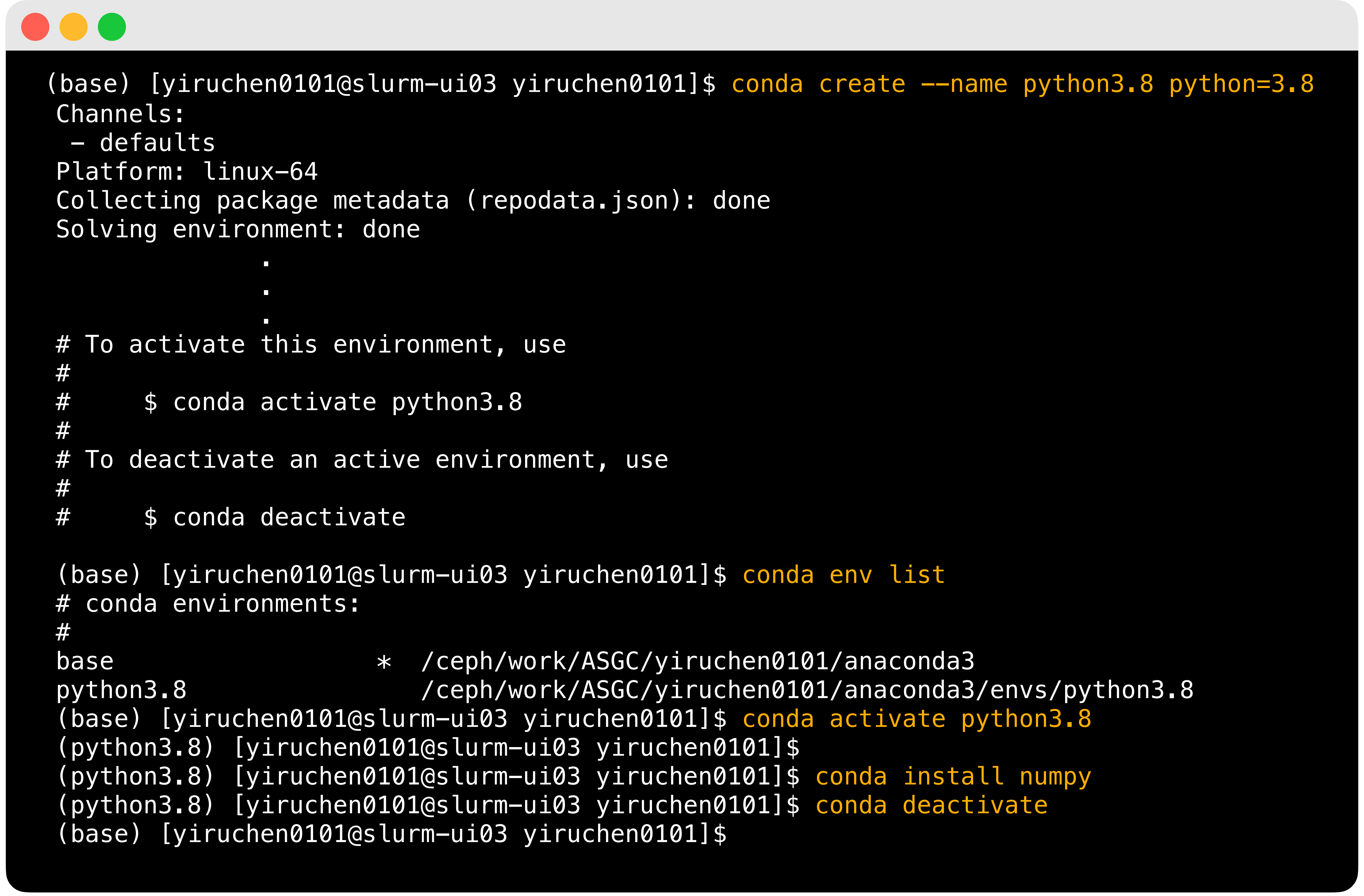
conda create --name <myenv>

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]$
```

https://docs.conda.io/projects/conda/en/latest/commands/index.html#

Python, Compilation and MPI Enviroment

Compilation

- 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

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

/ceph/sharedfs/software/hpc/

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>

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

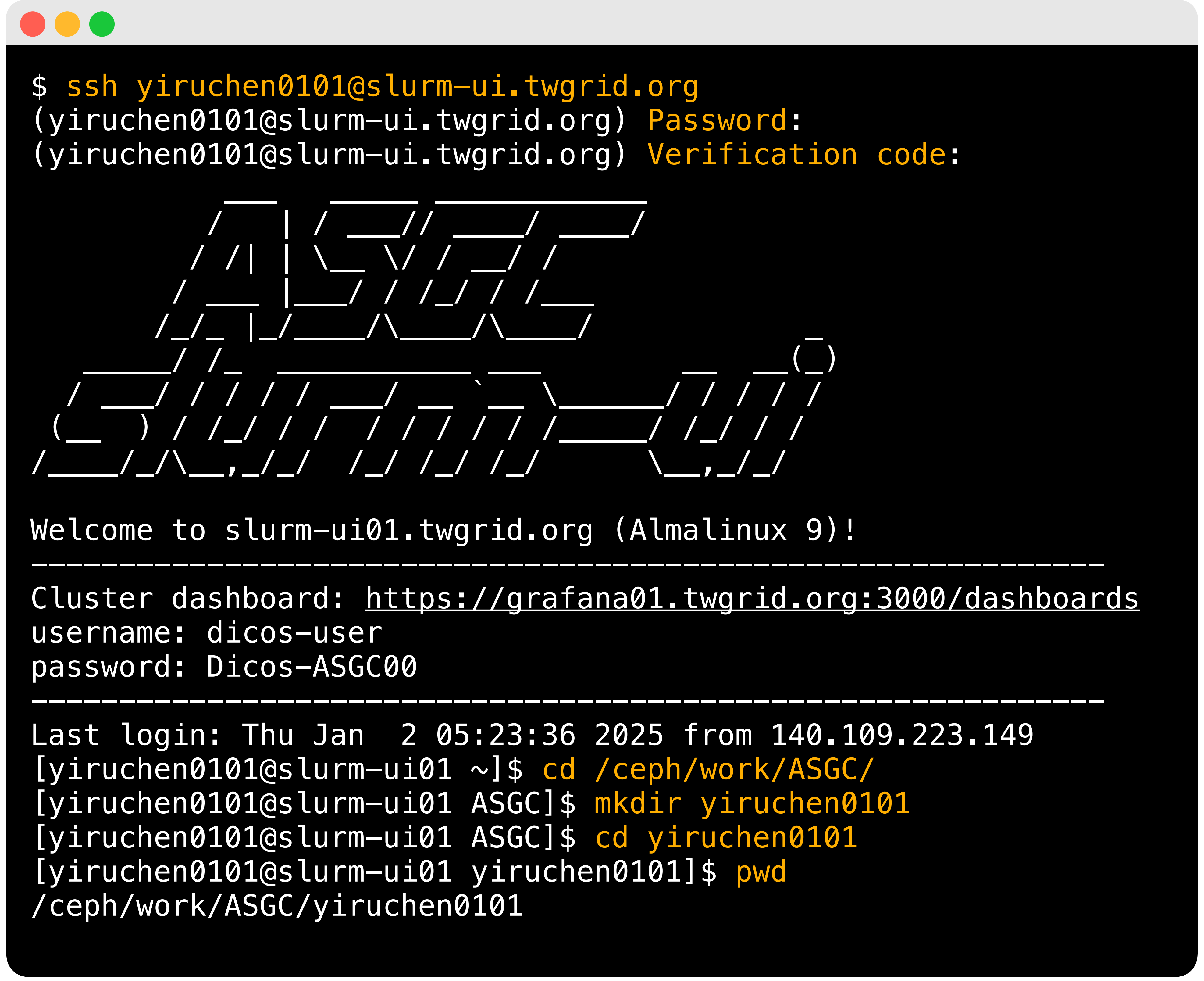
Mobaxterm : https://mobaxterm.mobatek.net/download-home-edition.html

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

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>



```
$ 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
```

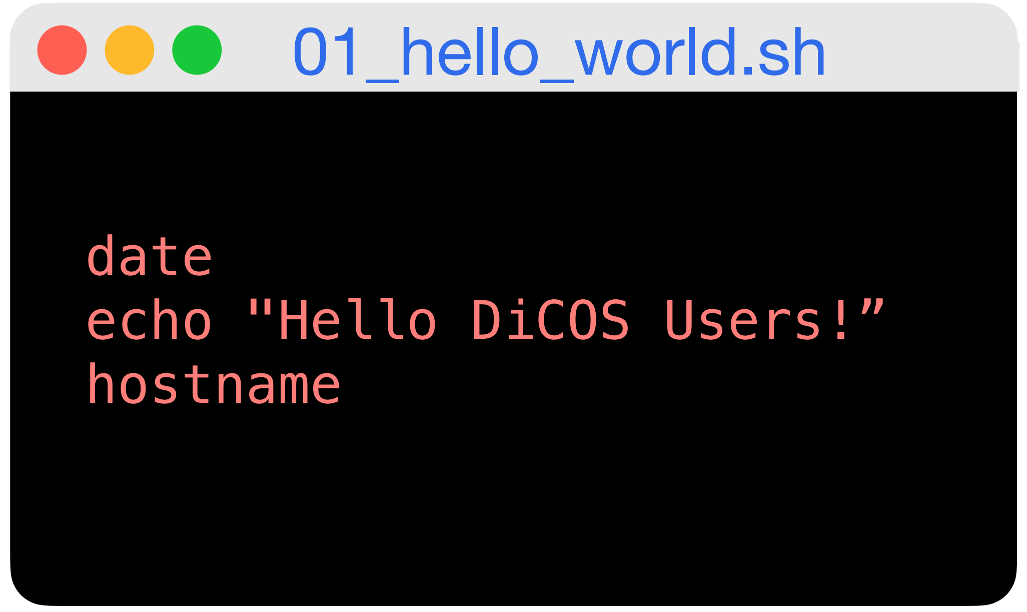
Job Submission Examples

Example 1 - Simple Job Submission (Hello World)

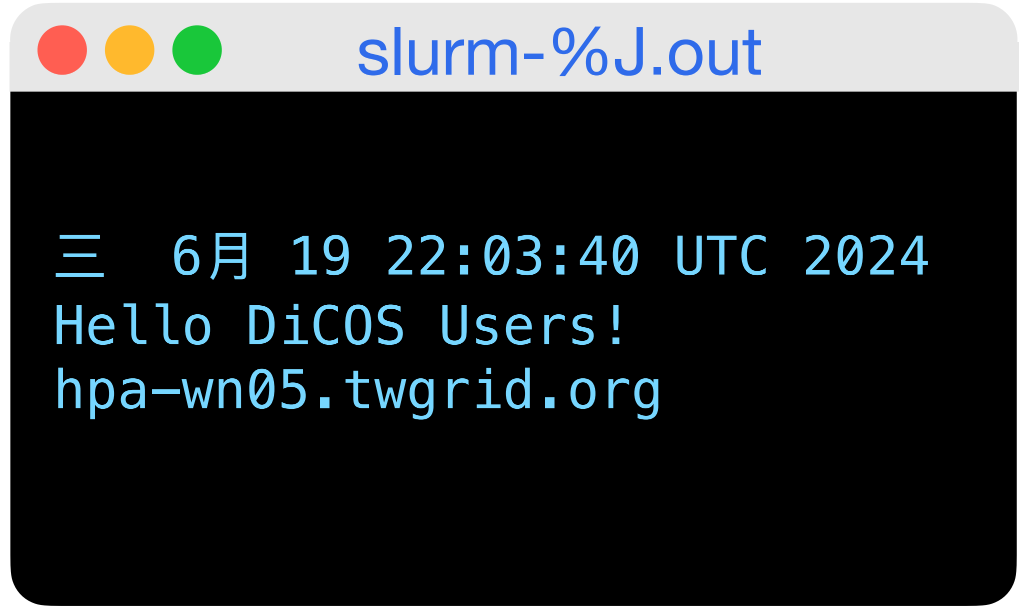
- Prepare a user defined shell script : 01_hello_world.sh

- Submit the job with sbatch

sbatch 01_hello_world.sh



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



```
三  6月 19 22:03:40 UTC 2024
Hello DiCOS Users!
hpa-wn05.twgrid.org
```

Job Submission Examples

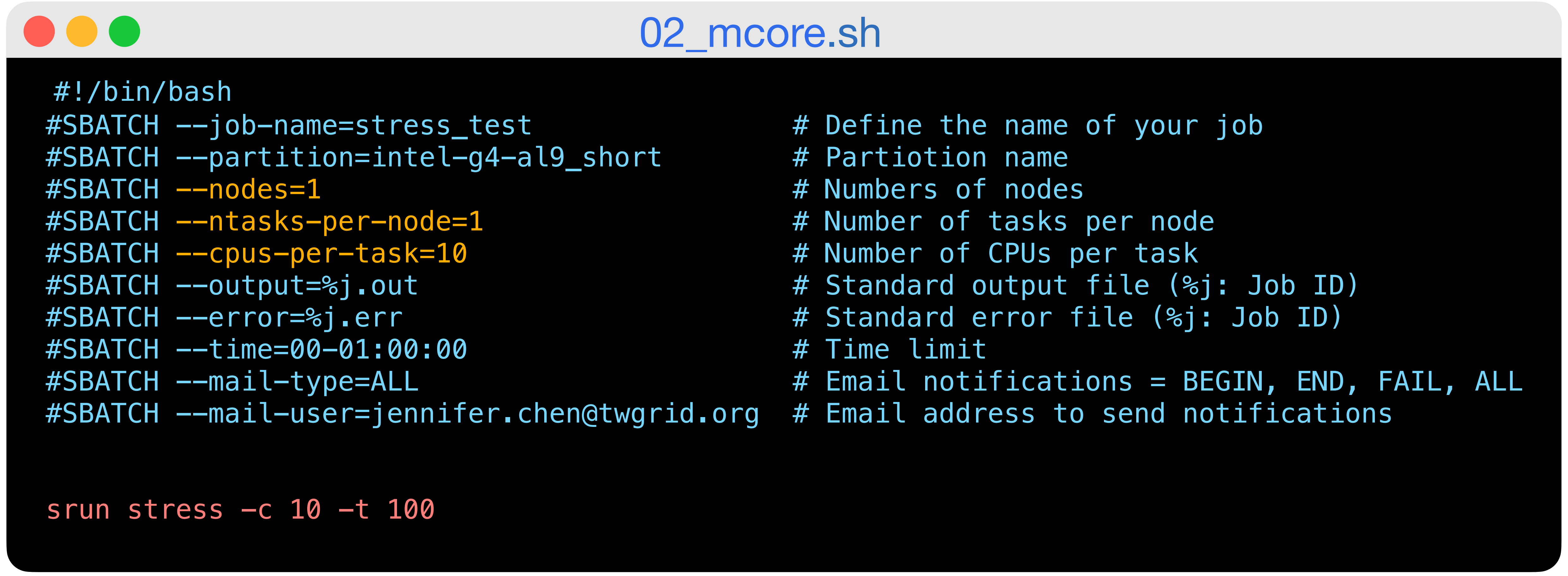
Example 2 - Submit a MCORE job

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

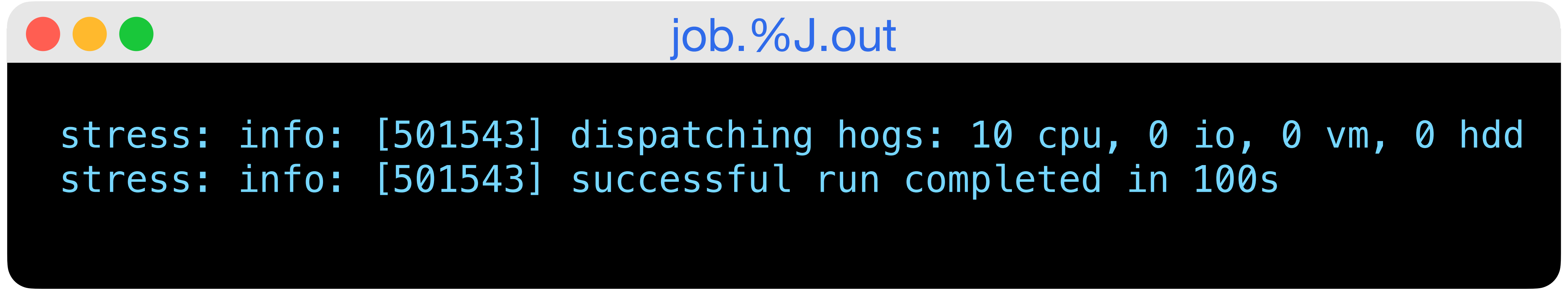
  E.g. 02_mcore.sh

- Submit job : sbatch 02_mcore.sh

- This example will submit a job which requesting 10 CPU cores



```
 #!/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
```

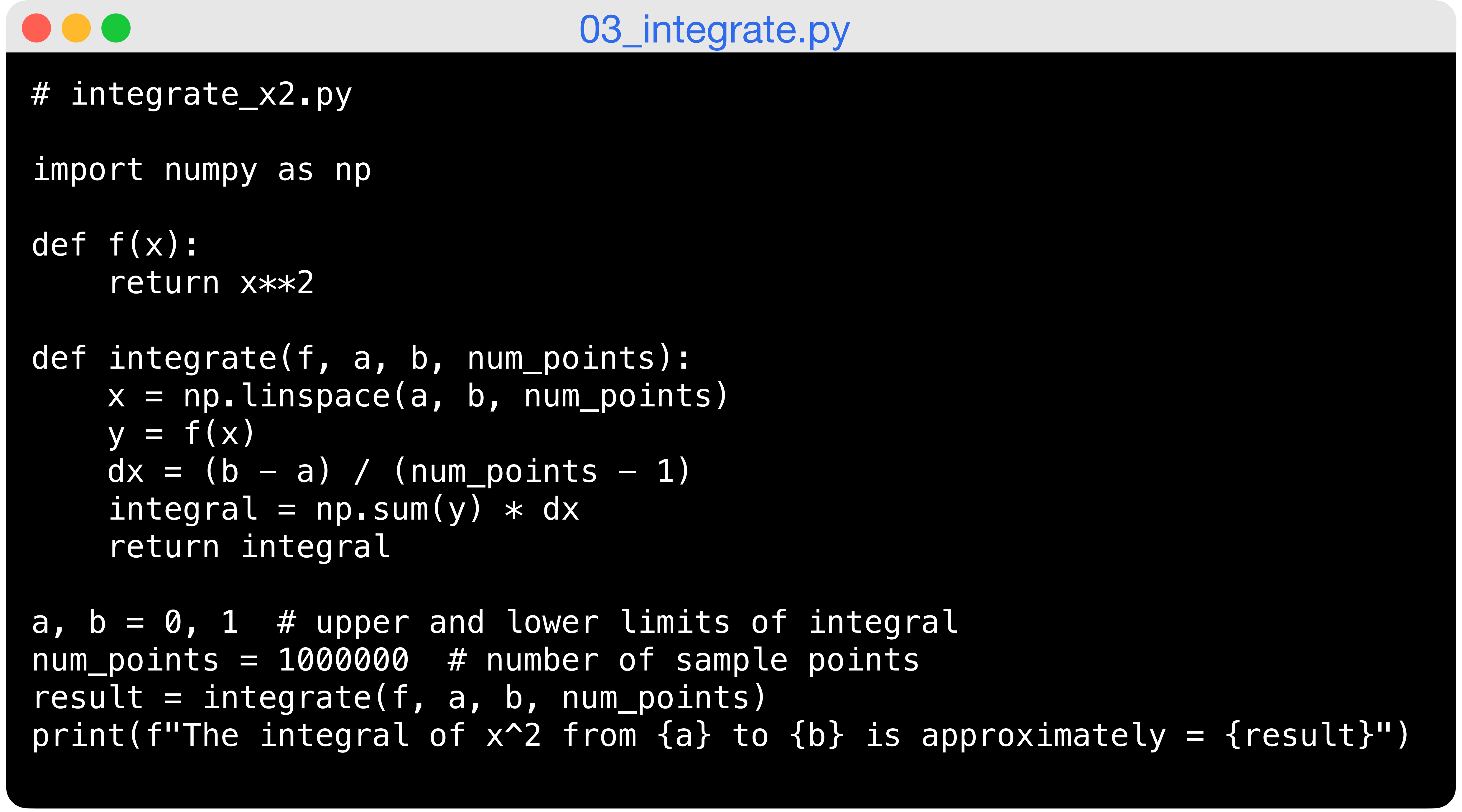


```
stress: info: [501543] dispatching hogs: 10 cpu, 0 io, 0 vm, 0 hdd
stress: info: [501543] successful run completed in 100s
```

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



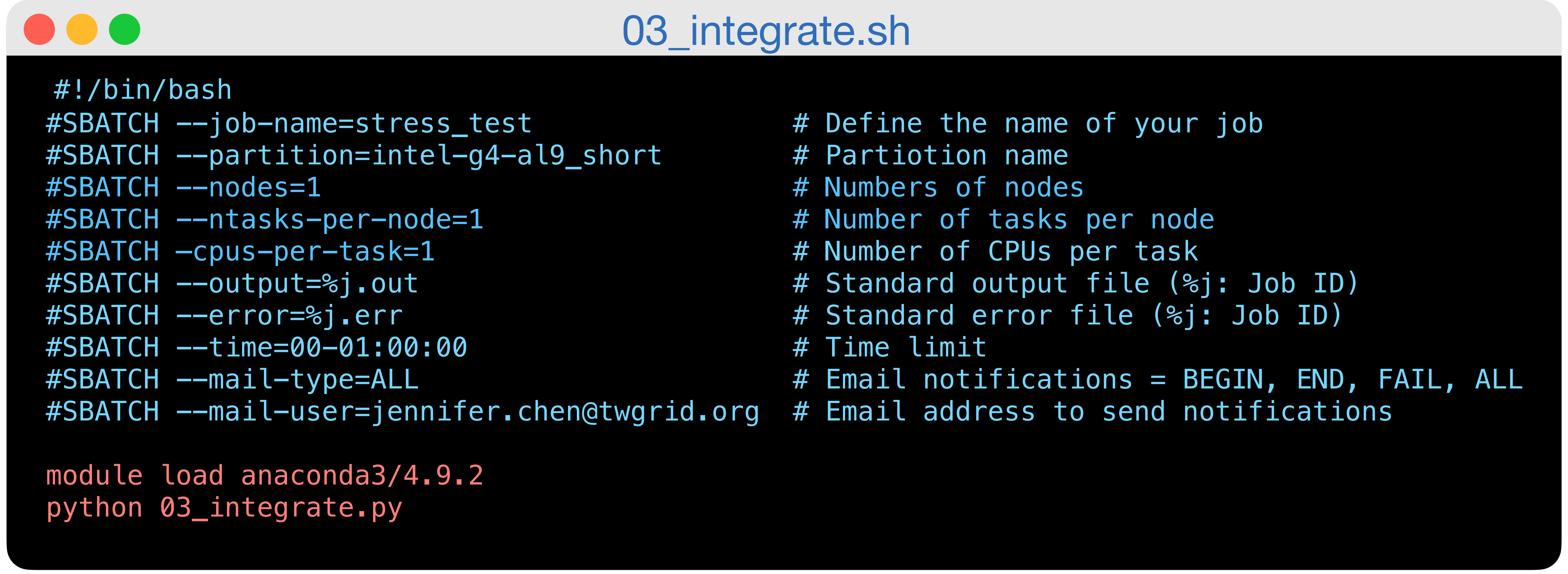
```
# integrate_x2.py

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

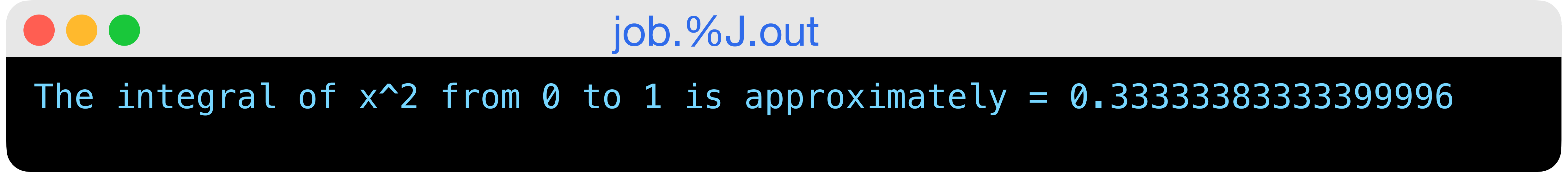
Example 3 - Submit a python job using anaconda3 python3

- Prepare a shell script that wrapping the environment modules and run python script: 03_integrate.sh

- Submit job using sbatch : sbatch 03_integrate.sh



```
#!/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
```



```
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
- 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.