UBAI GUIDE BOOK

hs.hwang

2024-10-16

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1 MAIN

UBAI Cluster .

Chapter .

UBAI Cluster

UBAI Cluster .

Chapter1.

UBAI .

Chapter2.

UBAI .

Chapter3.

, .

Chpater4. Python

Python .

Chpater5.

.

UBAI GUIDE BOOK UBAI .

· AI .

서울시립대학교 | 도시과학빅데이터·AI연구원

2 UBAI Cluster

UBAI

· AI (UBAI) (HPC) .

Slurm AI , , (Job) .

Slurm

Slurm (Job Submit),
(Task Scheduling),
(Resource Management) Linux .

UBAI UBAI Cluster Slurm .

Slurm Slurm .

Visual Studio Code

Visual Studio Code(VScode) Microsoft .
MacOS, Linux, Windows ,
.

UBAI VScode .

VScode . VScode , VScode .

Partition

Slurm Partition .

Partition .

Partition .

Partition	# of Nodes	# of Cores/node	CPU	GPU/node	Memory/node	SSD	Note
gpu1	13	48	Intel Xeon Gold 6240R	RTX3090 (4EA)	768GB	2TB	*
edu1	5	48	Intel Xeon Gold 6240R	A10 (4EA)	768GB	2TB	*
cpu1	30	48	Intel Xeon Gold 6240R	None	768GB	2TB	*
gpu2	10	56	Intel Xeon Gold 6348R	A10 (8EA)	1024GB	2TB	*
gpu3	11	56	Intel Xeon Gold 6348R	A10 (4EA)	1024GB	2TB	*
gpu4	29	56	Intel Xeon Gold 6348R	A6000 (4EA)	1024GB	2TB	*
gpu5	6	64	Intel Xeon Platinum-8358	A6000 (4EA)	1024GB	2TB	*

※ *UBAI 106 , 5,586 CPU , RTX3090 52 , A10 144 , A6000 140 .*

Terminal Partition .

```
sinfo -o "%10P %5D %14F %4c %14G %N"
```

```
PARTITION  NODES  NODES(A/I/O/T)  CPUS  GRES           NODELIST
gpu1       13     10/3/0/13       48    gpu:rtx3090:4  n[001-013]
cpu1       35     16/19/0/35      48    (null)         n[014-048]
hgx        1      0/0/1/1         48    gpu:hgx:8      n050
gpu2       32     26/6/0/32       56    gpu:a10:4      n[051-070,073-080,083-086]
cpu2       14     14/0/0/14       56    (null)         n[087-100]
cpu3       6      4/2/0/6         64    (null)         n[101-106]
test       4      0/4/0/4         56    gpu:a10:4      n[071-072,081-082]
```

MaxJobs( ) 10, MaxSubmit( ) 20, MaxWall( ) 2 .

Partition	MaxJobs	MaxSubmit	MaxWall
*	10	20	2-00:00:00

AI , , .

( ) **AI** .

( ) **The authors acknowledge the Urban Big data and AI Institute of the University of Seoul supercomputing resources (http://ubai.uos.ac.kr) made available for conducting the research reported in this paper.**

3 Chapter1.

UBAI Cluster .

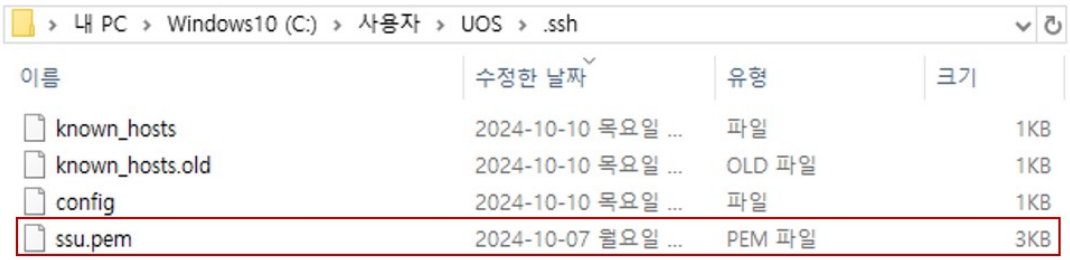
1.

UBAI .

(ubaisysadmin@uos.ac.kr) .

2.

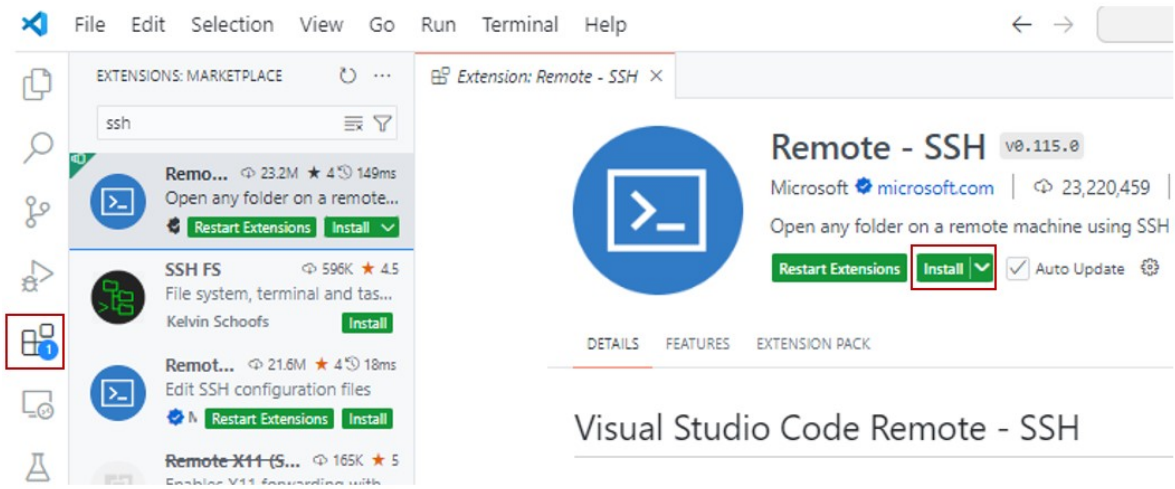
(ID.pem) `C:\User\{ }\.ssh\` .



※ *.ssh* , ***Chapter2.*** *.ssh* .

4 Chapter2.

1. Remote-SSH



VScode Remote-SSH . SSH .

SSH

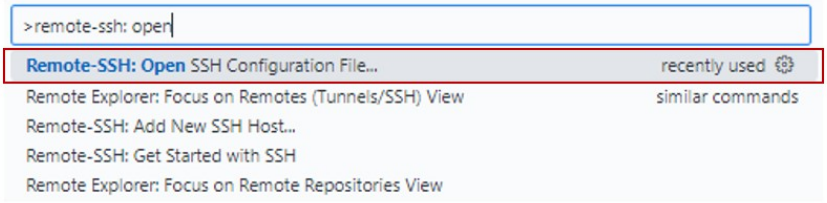
`SSH`
`command` .

SSH , VScode .

VScode Extension Remote-SSH .

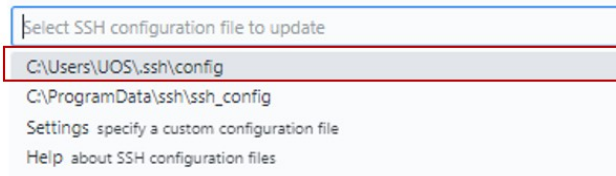
2. Config

1. Remote-SSH , (**CTRL + P**) (search) `>remote-ssh : open ssh`



`configuration` .

※ *`.ssh`* , *`.ssh`* *config* . *`.ssh`* *config* .



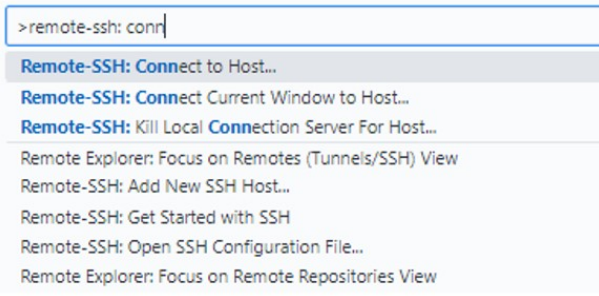
2. , `C:\Users\ \.ssh\config` .
3. `.ssh` config .

config

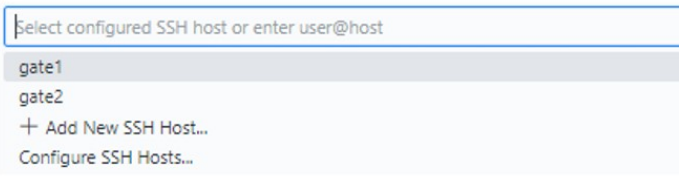
```
Host gate1
    HostName 172.16.10.36
    Port 22
    User   ID
    IdentityFile

Host gate2
    HostName 172.16.10.37
    Port 22
    User   ID
    IdentityFile
```

3. SSH

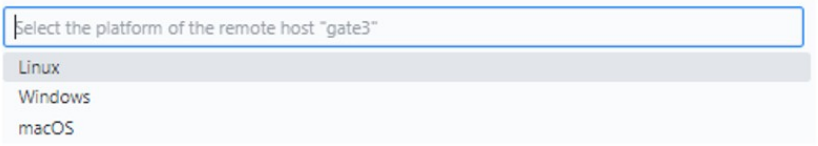
1. VScode (**CRTL+SHIFT+P**) .



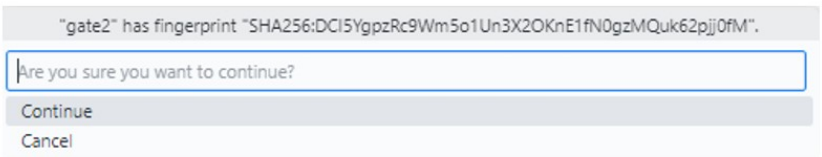
2. `> remote-ssh : connect to host` , .



3. gate1 gate2 . gate1 gate2 .

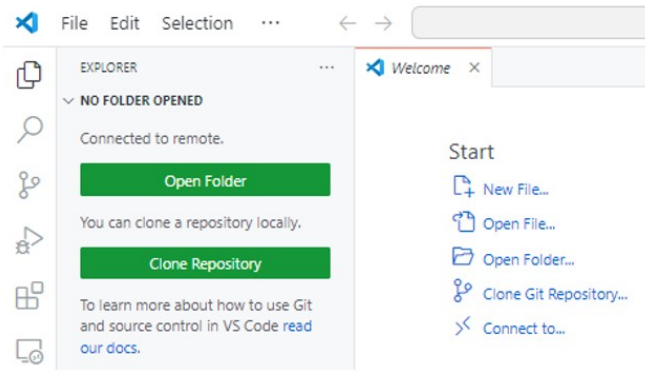


4. Linux .



5. Continue .

6. gate , gate SSH:gate .



7. , (Explorer) , Open Folder .

8. `/home1/{ ID}` , OK . .

9. , SSH !

4.

Mac , .

pem vscode , . pem **LF** .

pem CRLF , LF .

5 Chapter3.

.

(OS), , .

.

OS, , , .

. , .

Linux Conda Enroot . , .

1) Linux Linux .

2) Python Conda Python .

3) Enroot root (sudo) .

. , !

1. Linux

Environment Modules

```
Environment Modules
Unix/Linux                    .
Environment Modules       (PATH  )
                .
```

    (https://modules.sourceforge.net/) .

1.1 Module avail

UBIA Cluster .

```
(ubai) [ssu@gate1 ~]$ module avail

---------------------- /opt/ohpc/pub/modulefiles ----------------------
   CUDA/11.2.2              cmake/3.24.2                  cuda/11.2.2
   EasyBuild/4.9.1          compiler-rt/latest            cuda/11.3.1
   R/4.3.1                  compiler-rt/2023.1.0   (D)    cuda/11.4.4
   advisor/latest           compiler-rt32/latest          cuda/11.5.2
   advisor/2023.1.0 (D)     compiler-rt32/2023.1.0 (D)    cuda/11.6.2
   autotools                compiler/latest               cuda/11.7.1
   ccl/latest               compiler/2023.1.0      (D)    cuda/11.8.0
   ccl/2021.9.0     (D)     compiler32/latest             cuda/12.0.0
   clck/latest              compiler32/2023.1.0    (D)    cuda/12.1.1
   clck/2021.7.3    (D)     cuda/leejihun_cuda            cuda/12.2.1 (D)

  Where:
   D:  Default Module

If the avail list is too long consider trying:

"module --default avail" or "ml -d av" to just list the default modules.
"module overview" or "ml ov" to display the number of modules for each name.

Use "module spider" to find all possible modules and extensions.
Use "module keyword key1 key2 ..." to search for all possible modules matching any of the "k
```

1.2 Module show

.

```
(ubai) [ssu@gate1 ~]$ module show cuda/11.2.2
-------------------------------------------------
   /opt/ohpc/pub/modulefiles/cuda/11.2.2:
-------------------------------------------------
whatis("Name: CUDA Collection")
whatis("Version: 11.2.2")
whatis("Category: cuda")
prepend_path("PATH","/opt/ohpc/pub/cuda/11.2.2/bin")
prepend_path("INCLUDE","/opt/ohpc/pub/cuda/11.2.2/include")
prepend_path("LD_LIBRARY_PATH","/opt/ohpc/pub/cuda/11.2.2/lib64")
family("cuda")
help([[
```

```
This module loads the CUDA

Version 11.2.2

]])
```

1.3 Module load

. .

```
(ubai) [ssu@gate1 ~]$ module load cuda/11.2.2
```

1.4 Module list

.

```
(ubai) [ssu@gate1 ~]$ module list

Currently Loaded Modules:
  1) cuda/11.2.2   2) dal/latest
```

1.5 Module rm

.

```
(ubai) [ssu@gate1 ~]$ module rm dal/latest

Removing dal version 2023.1.0
Use `module list` to view any remaining dependent modules.
```

1.6 Module purge

module rm . module purge module list module
.

```
(ubai) [ssu@gate1 ~]$ module purge

(ubai) [ssu@gate1 ~]$ module list
No modules loaded
```

2. Python

Python

Python , , ,
, .
, .

Anaconda Miniconda . UBAI Miniconda
.

Miniconda

Anaconda
.
.

Miniconda Anaconda .

2.1 Minicoda

Miniconda Miniconda .

1. terminal terminal . Miniconda .

   ```
   wget https://repo.anaconda.com/miniconda/Miniconda3-latest-Linux-x86_64.sh
   ```

2. wget bash .

   ```
   bash Miniconda3-latest-Linux-x86_64.sh
   ```

3. Miniconda . Enter .
   'yes' . Enter .

4. Enter .

5. , conda init . 'yes' enter .

6. .

7. , terminal (base)[ID@ _gate_number] . (Explorer)
   miniconda .

2.2 Minicoda

Miniconda , Python .

Python (Package Dependencies) . Python

.

1. terminal .

```
conda create -n {  _ } python={  _Python_ }
```

ex. `conda create -n ubai python=3.11`

2. .

```
conda activate {  _ }
```

ex. `conda activate ubai`

, `conda activate` .

`conda info --envs` , .

Jupyter notebook , . `pip install ipykernel jupyerlab` or `conda install ipykernel jupyterlab`

※ *Python* ***`pip install`*** .

3. Enroot

enroot evidia , .

, ’ ’ , root .

NVIDIA enroot .

UBAI Rocky Linux 8.8 .

.

, `/home` `/home` root . , sudo .

, Rocky Linux `dnf` , . `dnf search` dnf

, .

, Rocky Linux . , ubuntu centos .

ubuntu OS .

3.1 Enroot

`enroot` . root . 2TB , enroot (/enroot).

enroot , srun ! *(gate1 gate2 .)* , . .

gate .

`srun` . enroot docker . Rocky linux 8.8 , `sudo` `sudo` .

3.2 Image Container

enroot docker image container .

docker , enroot docker , docker image container .

Image

`image` .
 .
 , ubuntu ,
 ,
ubuntu
 .
image dockerhub
 .

Container

`container` .
 .
 ,
 `root` .

3.3 Enroot

(1)

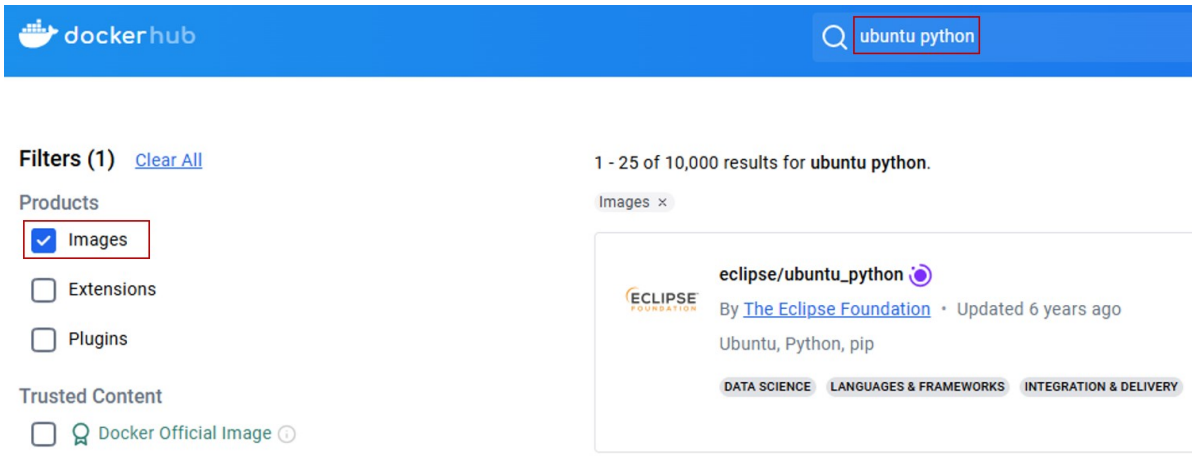
sbatch enroot slurm .
 , Linux .

```
# gpu5
srun --pty -p gpu5 -c 2 /bin/bash
```

```
s(base) [ssu@gate1 ~]$ srun --pty -p gpu5 -c 2 /bin/bash
srun: job 263557 queued and waiting for resources
srun: job 263557 has been allocated resources
```

(2) Enroot

docker hub .



docker hub `docker://` .

```
# dockerhub
enroot import docker://eclipse/ubuntu_python
```

```
(base) [ssu@n101 ~]$ enroot import docker://eclipse/ubuntu_python
[INFO] Querying registry for permission grant
[INFO] Authenticating with user: <anonymous>
[INFO] Authentication succeeded
[INFO] Fetching image manifest list
[INFO] Fetching image manifest
[INFO] Downloading 16 missing layers...
100% 16:0=0s b234f539f7a1d65eabae1617e63c81ac01768abffd48b5cbbf7166
[INFO] Extracting image layers...
100% 15:0=0s b234f539f7a1d65eabae1617e63c81ac01768abffd48b5cbbf7166
[INFO] Converting whiteouts...
100% 15:0=0s b234f539f7a1d65eabae1617e63c81ac01768abffd48b5cbbf7166
```

(3) Enroot

`enroot` .

enroot .

, `ubuntu.sqsh` .

.

```
#       ubuntu.sqsh
enroot create -n mycontainer eclipse_ubuntu_python.sqsh
```

```
(base) [ssu@n101 ~]$ enroot create -n mycontainer eclipse+ubuntu_python.sqsh
[INFO] Extracting squashfs filesystem...

Parallel unsquashfs: Using 2 processors
32434 inodes (38725 blocks) to write

[==========================================================================================

created 27953 files
created 3229 directories
created 4461 symlinks
created 0 devices
created 0 fifos
```

(4) Enroot

```
#         (version.1)
enroot start mycontainer
#         (version.2)
enroot start --root --rw --mount .:/mnt ubuntu-test /bin/bash
```

`--mount .:/mnt` .

mnt home .

(5) Enroot

enroot , .

enroot .

.

, .

```
enroot export mycontainer new_image.sqsh
```

, .

, .

(6) Enroot

```
exit
```

exit Ctrl+D .

6 Chapter4. Python

Python .

Shell **Python** . Shell **Jupyter Notebook** **, Python** .

.

1. BASH

Bash .

(job) , . (ubaisysadmin@uos.ac.kr) . .

1.1

.

(job) , `filename.sh` . Shell `python_project.sh` .

`.sh` .

```
#!/bin/bash
#SBATCH --nodes=1
#SBATCH --partition=gpu2
#SBATCH --cpus-per-task=56
#SBATCH --gres=gpu:4
#SBATCH --job-name=UBAIJOB
#SBATCH -o ./          /jupyter.%N.%j.out  # STDOUT
#SBATCH -e ./          /jupyter.%N.%j.err  # STDERR

echo "start at:" `date`
echo "node: $HOSTNAME"
echo "jobid: $SLURM_JOB_ID"
```

```
module unload CUDA/11.2.2
module load cuda/11.8.0

python cnn.py 12 256 'relu'
```

. .

STDOUT , STDERR . (directory)
.

.

#SBATCH --nodes=1 , . nodes=1 .

#SBATCH --partition=gpu4 Partition . Partition **UBAI Cluster** .

#SBATCH --cpus-per-task=14 . n , 1 CPU/GPU
. #of Cores/node Partition . **UBAI Cluster** .

#SBATCH --gres=gpu:1 GPU . CPU Partition . GPU
, .

#SBATCH --job-name=UBAIJOB .

echo "start at:" 'date' .

echo "node: $HOSTNAME" .

echo "jobid: $SLURM_JOB_ID" jobid .

module ~ Linux . GPU , GPU (CPU Partition) .
Chapter3. module envrionment . .

python cnn.py 12 256 'relu' Python . **.py** . **cnn.py**
. Python sys **sys.argv** . sys .
`python {filename}.py` .

1.2

, Python .

, terminal **sbatch** . (job) .

(job) ID .

```
sbatch filename.sh    # ex) sbatch python_project.sh
```

※ *cnn.py* ***pip install tensorflow && pip install numpy*** .

(job) , STDOUT OUT .

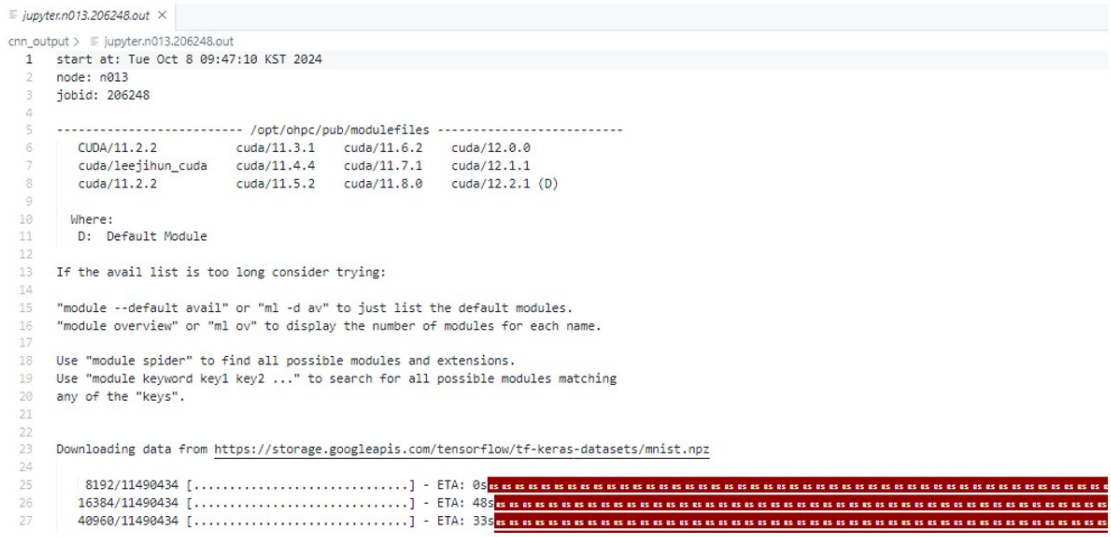
OUT , Partition (job) . terminal `squeue` , ID .

n001, n002 … , (*Resources, Priority*) .

, .

Partition Partition cpus-per-task, gpu Partition (job) .

STDOUT OUT .



2. Jupyter Notebook

Jupyter notebook .

(job) , . (ubaisysadmin@uos.ac.kr)

.

.

2.1

.

(job) , `filename.sh` . Shell `jupyter_notebook.sh` .

`.sh` .

```
#!/bin/bash
#SBATCH --nodes=1
#SBATCH --partition=gpu4
#SBATCH --cpus-per-task=14
#SBATCH --gres=gpu:1
#SBATCH --job-name=UBAIJOB
#SBATCH -o ./          /jupyter.%N.%j.out  # STDOUT
#SBATCH -e ./          /jupyter.%N.%j.err  # STDERR

echo "start at:" `date`
echo "node: $HOSTNAME"
echo "jobid: $SLURM_JOB_ID"

module unload CUDA/11.2.2
module load cuda/11.8.0

python -m jupyter lab $HOME \
        --ip=0.0.0.0 \
        --no-browser
```

. .

STDOUT , STDERR . (directory) .

.

`#SBATCH --nodes=1` , . nodes=1 .

`#SBATCH --partition=gpu4` Partition . Partition UBAI Cluster .

`#SBATCH --cpus-per-task=14` . n , 1 CPU/GPU . #of Cores/node Partition . UBAI Cluster .

`#SBATCH --gres=gpu:1` GPU . CPU Partition . GPU , .

`#SBATCH --job-name=UBAIJOB` .

`echo "start at:" 'date'` .

`echo "node: $HOSTNAME"` .

`echo "jobid: $SLURM_JOB_ID"` jobid .

`module ~` Linux . GPU , GPU (CPU Partition) . Chapter3. module envrionment . .

`python -m jupyter lab $HOME \ --ip=0.0.0.0 \ --no-browse` Jupyter notebook .

2.2

, Python .

, terminal `sbatch` . (job) .

(job) ID .

```
sbatch filename.sh    # ex) sbatch jupyter.sh
```

(job) , STDOUT OUT .

OUT , Partition (job) . terminal `squeue` , ID .

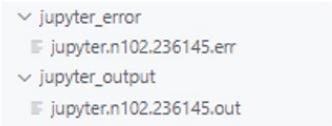
n001, n002 ... , (*Resources, Priority*) .

, .

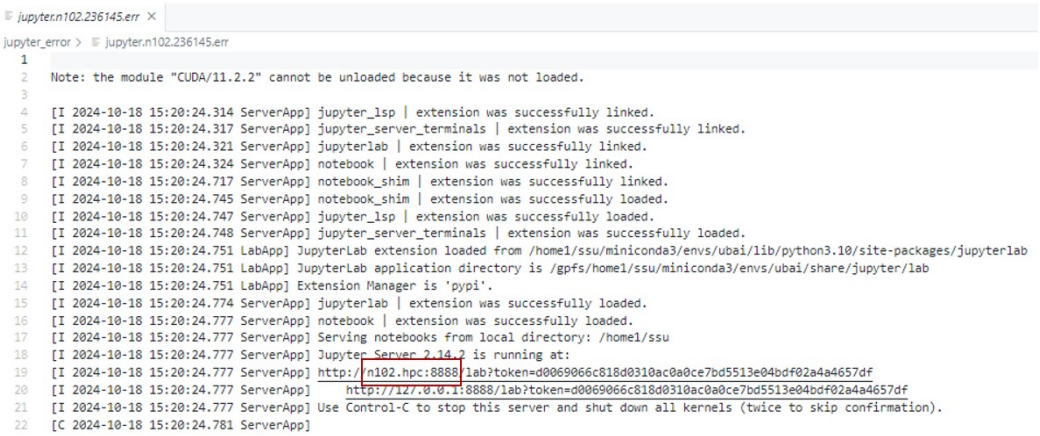
Partition Partition cpus-per-task, gpu Partition (job) .

ERR , Jupyter Notebook .

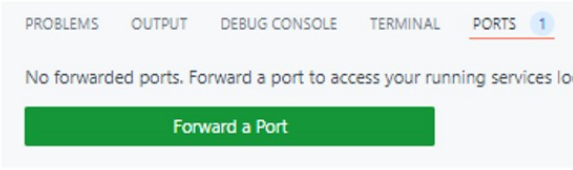
2.3



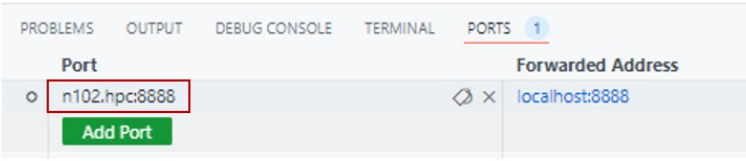
1. STDERR ERR .



2. .



3. VScode PORTS , Forward a Port .



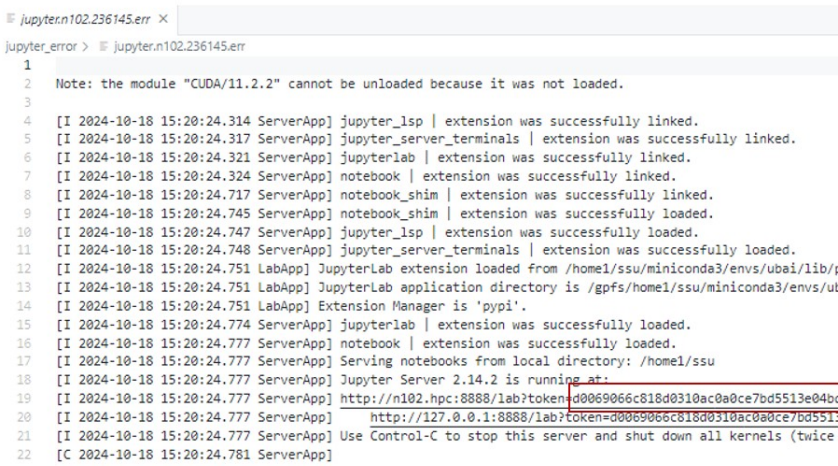
4. 2 Port , Open in Browser .

5. Jupyter .

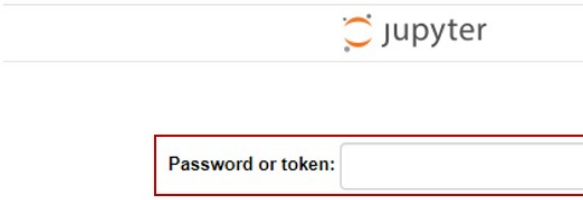
2.4 Jupyter Notebook

Jupyter , . Jupyter Notebook . .

1.



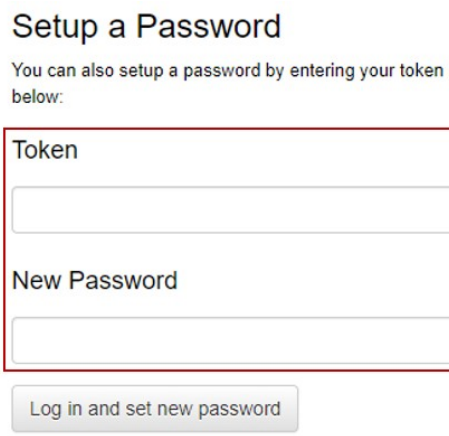
STDERR ERR Token .



Token . Token , Password .

1 , Token .

2.



Token , Token New Password Password .

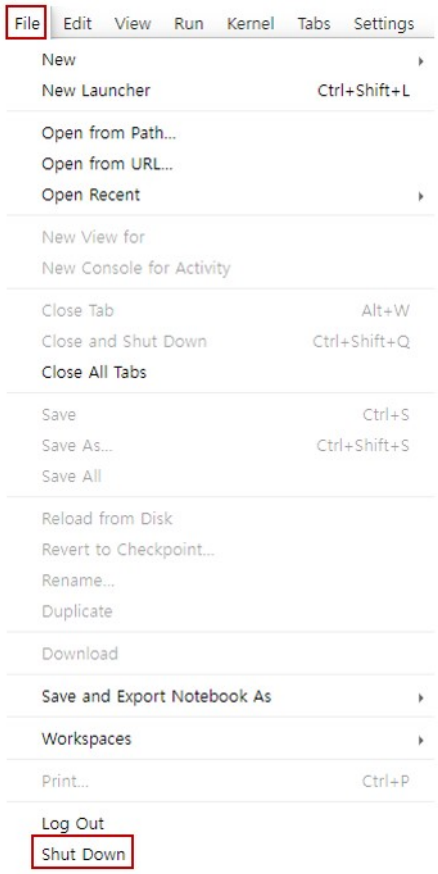
2 , Password .

Jupyter Notebook .

2.5 Jupyter Notebook

Jupyter Nobetook **File → Shut Down** , VScode terminal `scancel {job_ID}` . , job_ID job_ID .

(job) . .



7 Chapter5.

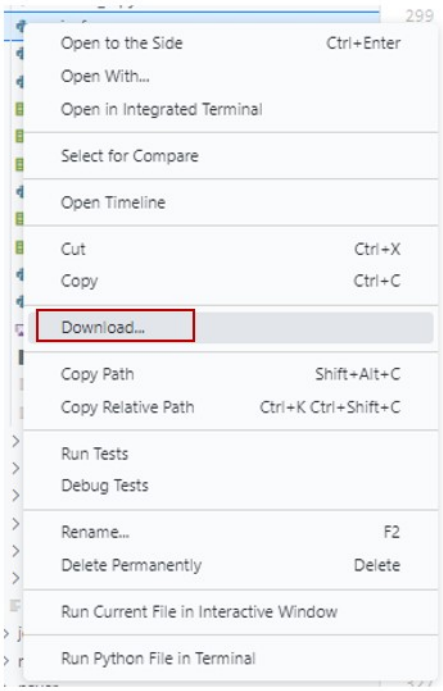
UBAI SSD 100GB . .

※ *(ubaisysadmin@uos.ac.kr)* *1TB* .

1.

VScode .

7.0.1 1.1



Download .

7.0.2 1.2

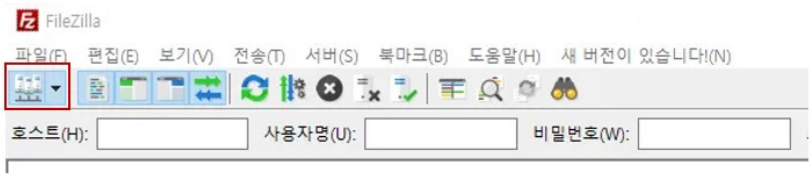
, (Explorer) .

2.

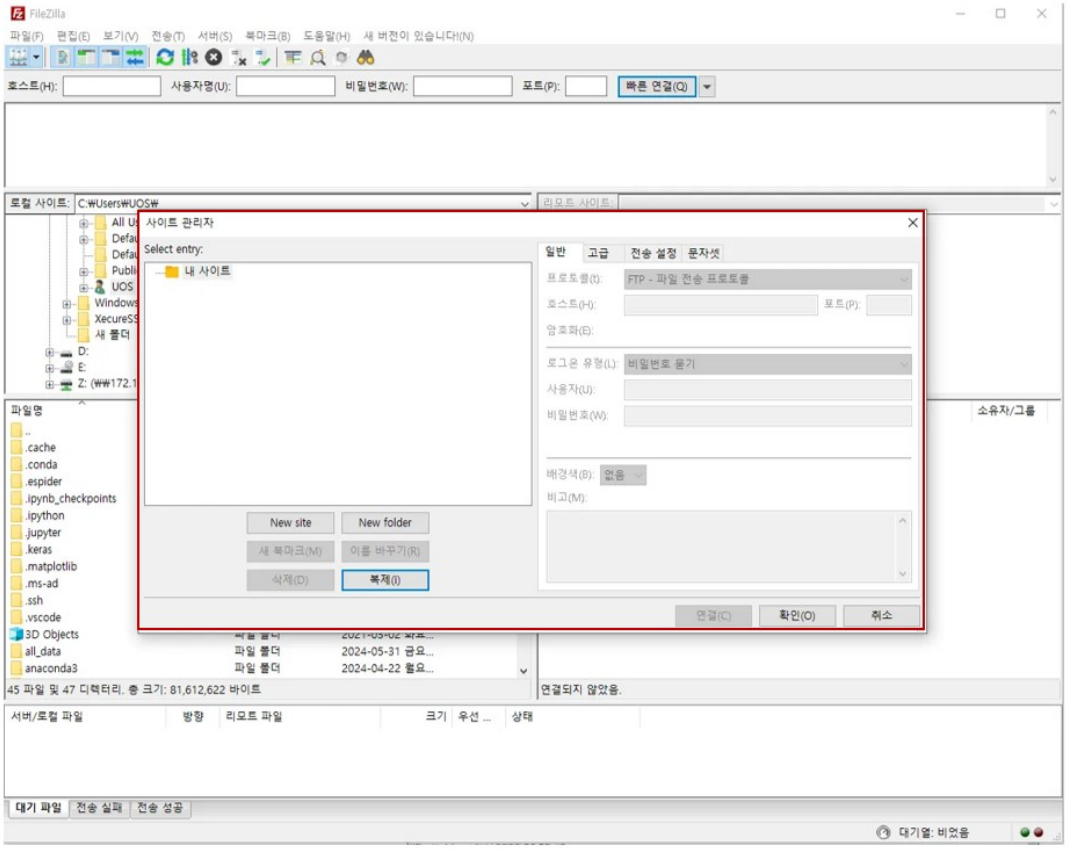
. FileZilla . FileZilla .

FileZilla , .

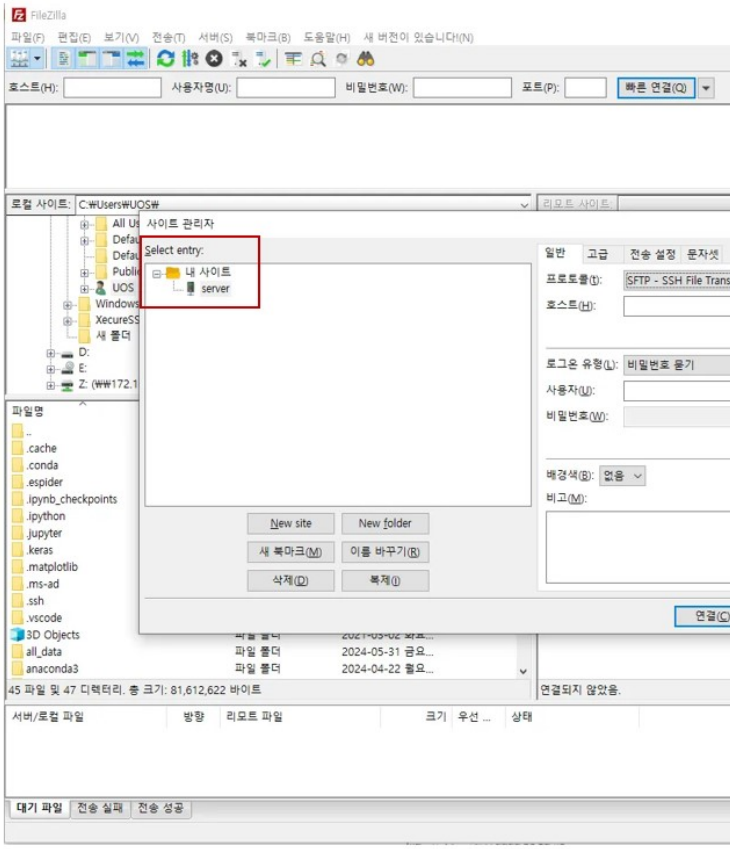
7.0.1 2.1



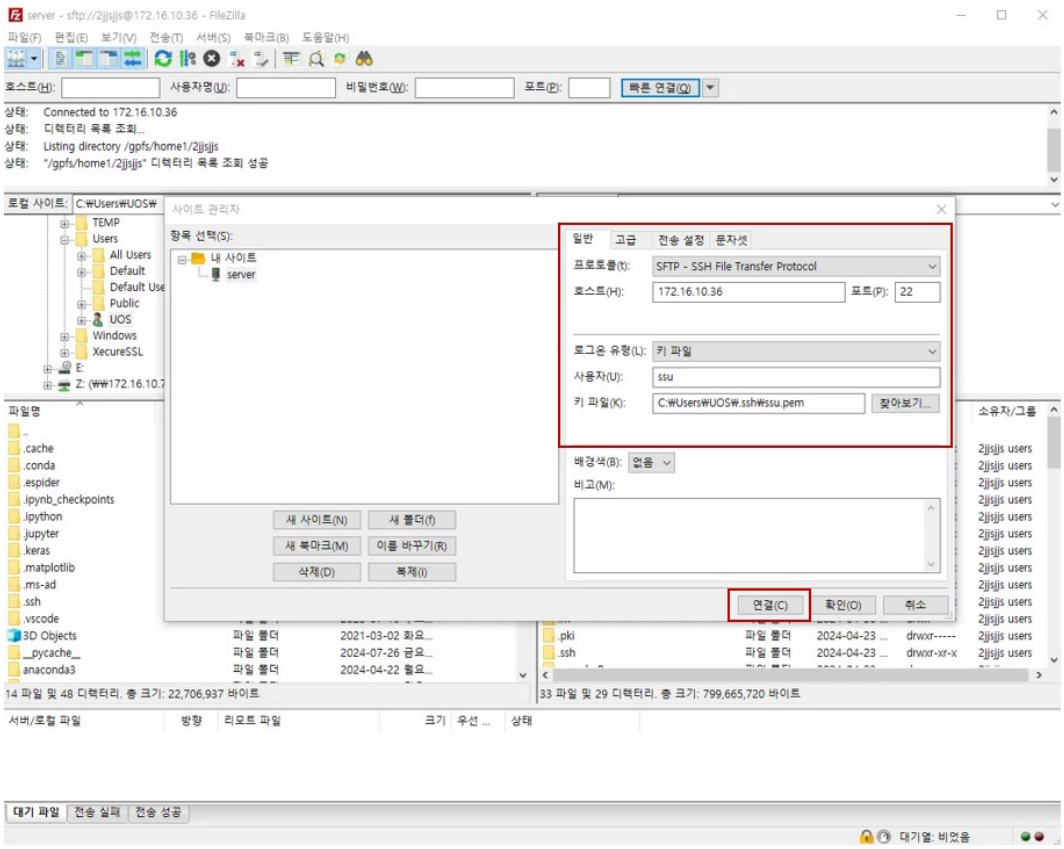
1. .


FileZilla
사이트 관리자
Select entry:
내 사이트
New site
New folder
새 북마크(M)
이름 바꾸기(R)
삭제(D)
복제(I)
일반
고급
전송 설정
문자셋
확인(O)
취소

2. New site .

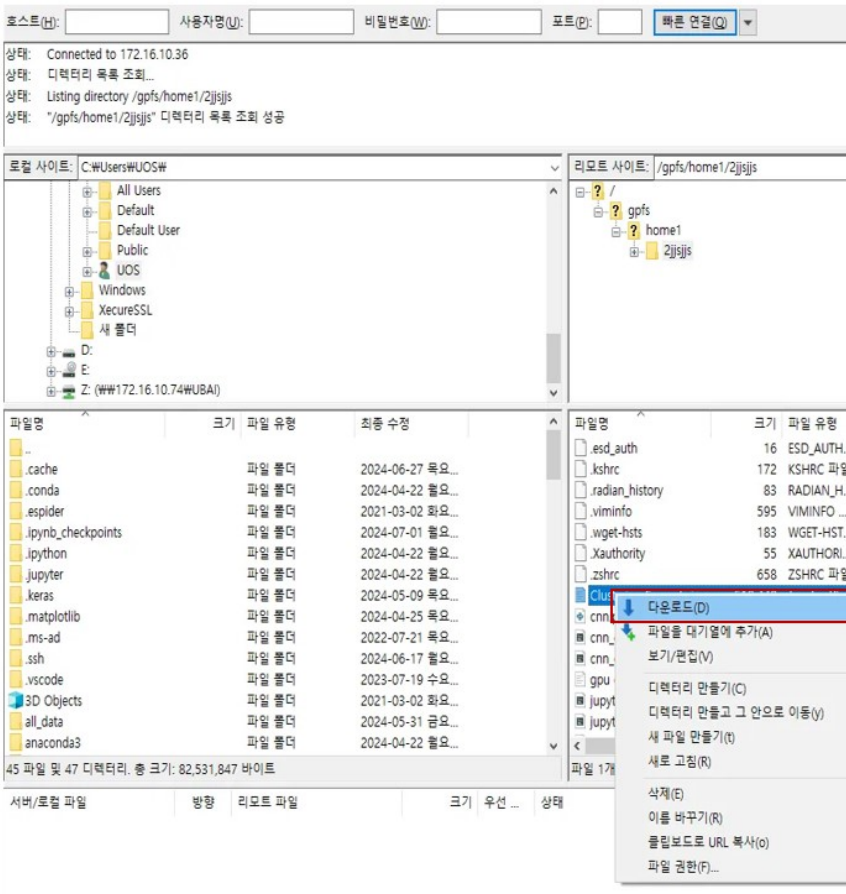


3. “SFTP - SSH File Transfer Protocol” .



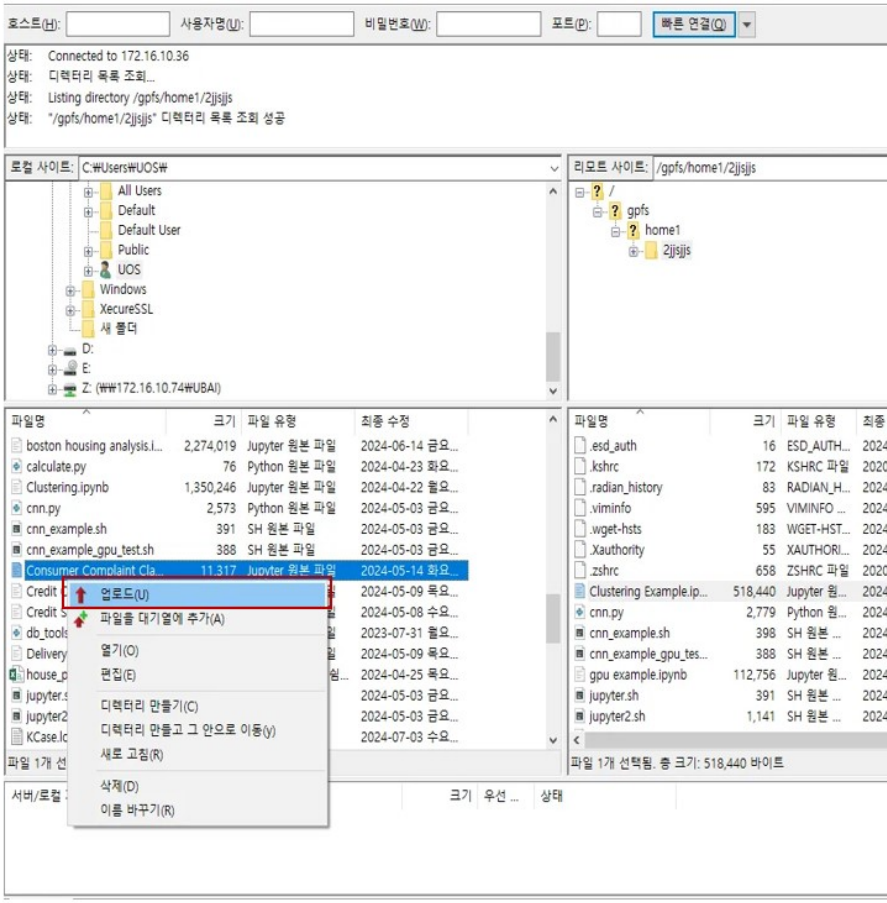
4. .

- : SFTP
- : IPv4
- : 22
- :
- : (ex. ubuntu)
- : (.pem)
-


호스트(H):
사용자명(U):
비밀번호(W):
포트(P):
빠른 연결(Q)
상태: Connected to 172.16.10.36
상태: 디렉터리 목록 조회...
상태: Listing directory /gpfs/home1/2jjsjjs
상태: "/gpfs/home1/2jjsjjs" 디렉터리 목록 조회 성공
로컬 사이트: C:₩Users₩UOS₩
All Users
Default
Default User
Public
UOS
Windows
XecureSSL
새 폴더
D:
E:
Z: (₩₩172.16.10.74₩UBAI)
리모트 사이트: /gpfs/home1/2jjsjjs
/
gpfs
home1
2jjsjjs
파일명 크기 파일 유형 최종 수정
.cache 파일 폴더 2024-06-27 목요...
.conda 파일 폴더 2024-04-22 월요...
.espider 파일 폴더 2021-03-02 화요...
.ipynb_checkpoints 파일 폴더 2024-07-01 월요...
.ipython 파일 폴더 2024-04-22 월요...
.jupyter 파일 폴더 2024-04-22 월요...
.keras 파일 폴더 2024-05-09 목요...
.matplotlib 파일 폴더 2024-04-25 목요...
.ms-ad 파일 폴더 2022-07-21 목요...
.ssh 파일 폴더 2024-06-17 월요...
.vscode 파일 폴더 2023-07-19 수요...
3D Objects 파일 폴더 2021-03-02 화요...
all_data 파일 폴더 2024-05-31 금요...
anaconda3 파일 폴더 2024-04-22 월요...
45 파일 및 47 디렉터리. 총 크기: 82,531,847 바이트
파일명 크기 파일 유형
.esd_auth 16 ESD_AUTH.
.kshrc 172 KSHRC 파일
.radian_history 83 RADIAN_H.
.viminfo 595 VIMINFO ...
.wget-hsts 183 WGET-HST.
.Xauthority 55 XAUTHORI.
.zshrc 658 ZSHRC 파일
다운로드(D)
파일을 대기열에 추가(A)
보기/편집(V)
디렉터리 만들기(C)
디렉터리 만들고 그 안으로 이동(y)
새 파일 만들기(t)
새로 고침(R)
삭제(E)
이름 바꾸기(R)
클립보드로 URL 복사(o)
파일 권한(F)...
서버/로컬 파일 방향 리모트 파일 크기 우선 ... 상태

( ) .

7.0.2 2.2


호스트(H):
사용자명(U):
비밀번호(W):
포트(P):
빠른 연결(Q)
상태: Connected to 172.16.10.36
상태: 디렉터리 목록 조회...
상태: Listing directory /gpfs/home1/2jjsjjs
상태: "/gpfs/home1/2jjsjjs" 디렉터리 목록 조회 성공
로컬 사이트: C:₩Users₩UOS₩
All Users
Default
Default User
Public
UOS
Windows
XecureSSL
새 폴더
D:
E:
Z: (₩₩172.16.10.74₩UBAI)
리모트 사이트: /gpfs/home1/2jjsjjs
/
gpfs
home1
2jjsjjs
파일명 크기 파일 유형 최종 수정
boston housing analysis.i... 2,274,019 Jupyter 원본 파일 2024-06-14 금요...
calculate.py 76 Python 원본 파일 2024-04-23 화요...
Clustering.ipynb 1,350,246 Jupyter 원본 파일 2024-04-22 월요...
cnn.py 2,573 Python 원본 파일 2024-05-03 금요...
cnn_example.sh 391 SH 원본 파일 2024-05-03 금요...
cnn_example_gpu_test.sh 388 SH 원본 파일 2024-05-03 금요...
Consumer Complaint Cla... 11,317 Jupyter 원본 파일 2024-05-14 화요...
업로드(U)
파일을 대기열에 추가(A)
열기(O)
편집(E)
디렉터리 만들기(C)
디렉터리 만들고 그 안으로 이동(y)
새로 고침(R)
삭제(D)
이름 바꾸기(R)
파일명 크기 파일 유형 최종
.esd_auth 16 ESD_AUTH... 2024
.kshrc 172 KSHRC 파일 2020
.radian_history 83 RADIAN_H... 2024
.viminfo 595 VIMINFO ... 2024
.wget-hsts 183 WGET-HST... 2024
.Xauthority 55 XAUTHORI... 2024
.zshrc 658 ZSHRC 파일 2020
Clustering Example.ip... 518,440 Jupyter 원... 2024
cnn.py 2,779 Python 원... 2024
cnn_example.sh 398 SH 원본 ... 2024
cnn_example_gpu_tes... 388 SH 원본 ... 2024
gpu example.ipynb 112,756 Jupyter 원... 2024
jupyter.sh 391 SH 원본 ... 2024
jupyter2.sh 1,141 SH 원본 ... 2024
파일 1개 선택됨. 총 크기: 518,440 바이트
서버/로컬
크기 우선 ... 상태

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