

*AMD Computing & User Training Workshop for
NSTCCore Computing Service 2024*

Introduction of NSTCCore Computing & Storages Services

<https://nstccore.twgrid.org>

Introduction of NSTCCore Computing Service

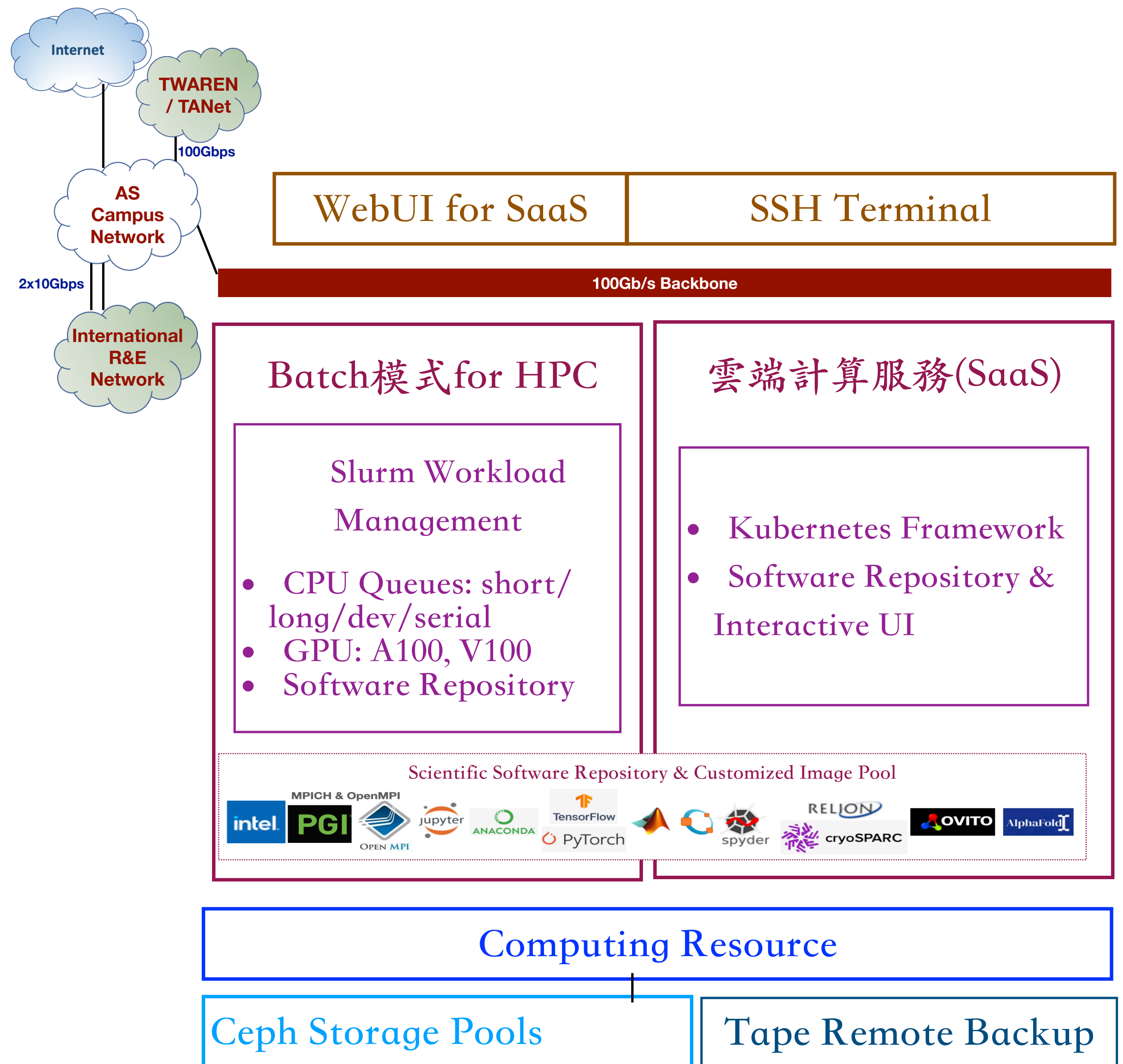
- Computing Service
- Storage Service
- Technical Support
- User Management

	2024.04 ~	2024.09~2025.08	2025.08~2026.06	
CPU	1920 Cores *AMD Genoa + 768 Cores *AMD Rome + 528 Cores *Intel FDR5	1920 Cores *New + 2688 Cores *AMD Rome + Genoa	3840 Cores *New + 2688 Cores *AMD Rome + Genoa	* 後續 計算 能量 依計 畫核 定狀 況決 定
GPU	V100 - 32 boards A100 - 8 boards *Current Resources	V100 - 32 boards A100 - 8 boards *Current Resources	V100 - 32 boards A100 - 8 boards *Current Resources	
Storage (PB)	3 *Buy-in every year	6	9	
Tape (PB)	4 *Buy-in every year	8	12	

表、計算資源購置規劃表 2024.03

Scientific & HPC Computing Service

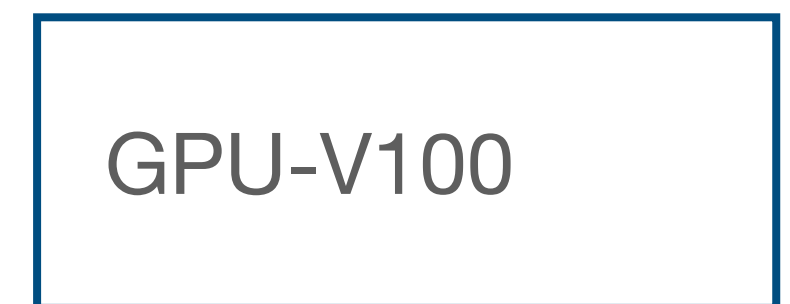
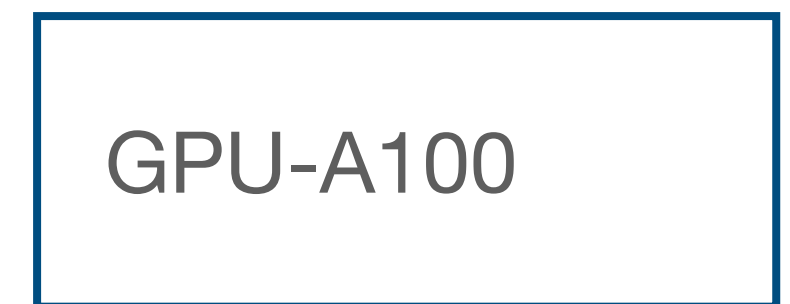
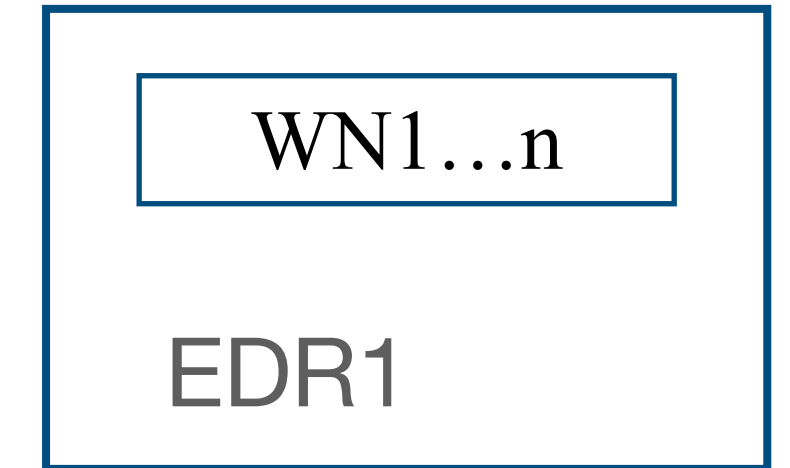
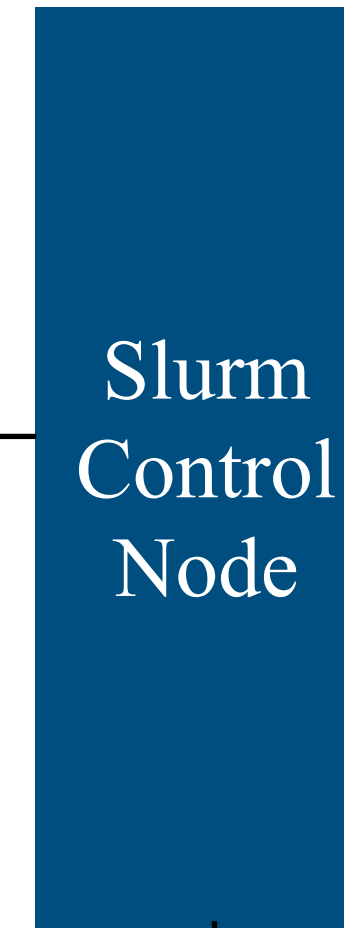
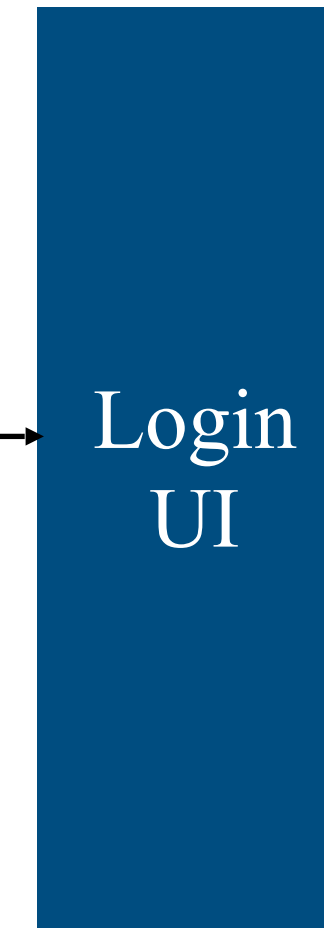
- Batch Jobs Computing Service
 - Slurm Work Management System
- Interactive Jobs Computing Service
 - Scalable & Virtualized Service-as-Service (SaaS) Service Model
 - Software on-demand Web-based UI
 - Customized Application Deployment



System Architecture of NSTCCore Computing Service

Batch Jobs Computing Service

- Slurm System Architecture
 - Scalable Cluster Management and Job Scheduling System
 - GPU - A100 、 V100
 - Jobs Working Space:
 - Ceph Cloud Filesystem
 - Local Disk [HDR1] SSD 1TB & [FDR5] NO SSD
- Computing Nodes
 - CPU



Cluster	CPU	Nodes	Cores-Per-Node	Cores	RAM(GB)	Inter-connection
FDR5	Intel® Xeon® CPU E5-2650 v4@2.20GHz	22	24	528	128	IB:FDR, Eth:10Gbps
HDR1	AMD Rome 7662 @2.0GHz	6	128	768	1536	IB:HDR, Eth:100Gbps
EDR1	AMD Genoa 9654@2.4GHz	10	192	1920	1536	Eth: 100Gbps

Slurm System Architecture

Batch Jobs Computing Service - Slurm

System Spec

- OS : CentOS 7
- Login (SSH) : slurm-ui.twgrid.org
- Mount Space :
 - User Space : /dicos_ui_home/{user}
 - Group Space : /ceph/work/{group}
 - Backup Space : /ceph/project/{group}
(*in the future)
- Compiler : Intel gcc 、 AOCC, openACC and MPI & OpenMP repository
- Software Repository :
 - Scientific Packages : Root 、 MATLAB 、 R 、 Octave
 - Anaconda Python packages : TensorFlow, PyTorch, PyRoot..etc
 - GPU - CUDA v12.1
 - Some Customized Requirements needs to deploy by Singularity, like AlphaFold. (* Build fee)

Interactive Jobs - SaaS Computing Service

- Kubernetes and Openstack
 - High extensible and reliable virtual environment
- Customized Application Deployment
- Images Repository
 - JupyterLab and various scientific applications
 - Built by user's requirements
- Software-on-demand Web UI
 - No installation and easy to adopt
- Working Space
 - Ceph Filesystem

System Spec

- Node Spec : NVIDIA GPU V100 、 A100 、 RTX3090
- Service Web Portal :
 - dicos.grid.sinica.edu.tw
- Mount Space :
 - User Space : /dicos_ui_home/{user}
 - Group Space : /ceph/work/{group}
 - Backup Space : /ceph/project/{group} will be available in the future

SaaS for Virtualized Computing Service

Scientific Software Repository


- Interactive : Ovito(Molecular Dynamics) 、 cisTEM 、 RELION(Medical Image Reconstruction)
- BioMedical : Cryosparc (* License required from users)
- Anaconda Python packages for ML : JupyterLab 、 TensorFlow 、 PyTorch 、 PyRoot 、 DeepMD(Molecular Dynamics)···etc.



When your job needs


- Interactive UI
- Specific OS or Application required
- Dedicate node for rapid development for multi-core or GPU to develop and testing your task

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




CryoSPARC 1080ti
Version: 3.3.2
Resources: 52%

Launch




CryoSPARC RTX3090
Version: 4.0.2
Resources: 44%

Launch




PyRoot
Version: GPU with 1080ti
Resources: 52%

Launch ▾




RELION 4 beta
Version: V4
Resources: 52%

Launch ▾



Triton
Version: 22.01-py3 (GPU P100)
Resources: 50%

Launch ▾



Jupyter Lab GPU A100
Version: GPU with Tensorflow A100
Resources: 62%

Launch ▾

- 2 hours
- 3 days
- 7 days
- 10 days

The path of Disk Space

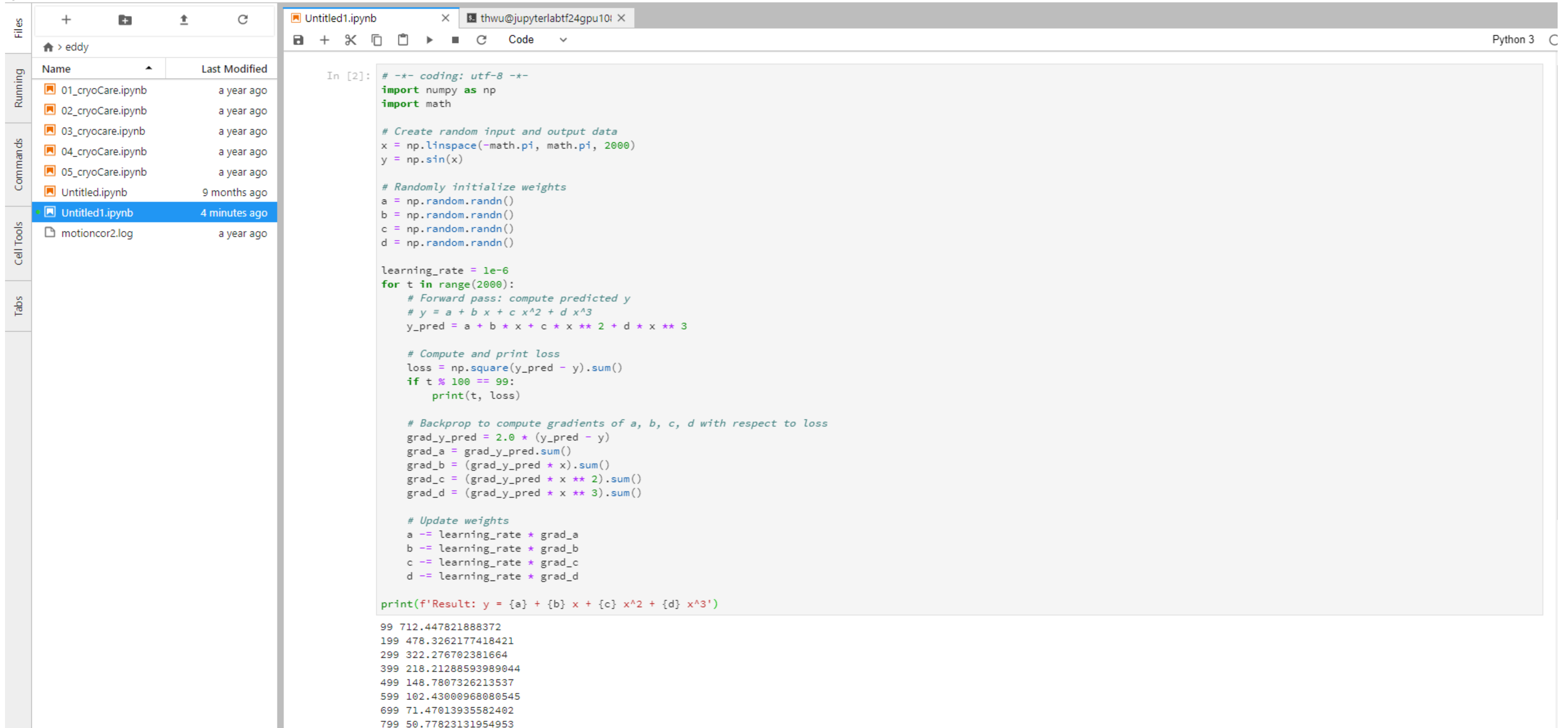
- All user:
 /dicos_ui_home/{user} (UI)
- cryoEM group:
 /activeEM/data/{group}/{user}
- NSTCCore group:
 /ceph/work/{group}/{user}

Example 1.1 (Open a Jupyter RTX 3090)

The screenshot displays the JupyterLab interface. The top menu bar includes File, Edit, View, Run, Kernel, Tabs, Settings, and Help. The left sidebar contains a 'Files' panel with a '+' button and a file browser for the 'eddy' directory. Below this are panels for 'Running' (listing notebooks like 01_cryoCare.ipynb), 'Commands', 'Cell Tools', and 'Tabs'. The main area is the 'Launcher' view, which shows a grid of application icons: Python 2 and Python 3 notebooks, a Console, another Python 2 and Python 3 notebook, and 'Other' options like Terminal and Text File. The Python 3 notebook icon in the top row is highlighted with a blue border.

Name	Last Modified
01_cryoCare.ipynb	a year ago
02_cryoCare.ipynb	a year ago
03_cryocare.ipynb	a year ago
04_cryoCare.ipynb	a year ago
05_cryoCare.ipynb	a year ago
Untitled.ipynb	9 months ago
Untitled1.ipynb	6 minutes ago
motioncor2.log	a year ago

Example 1.2 (Open a Jupyter RTX 3090)



The screenshot displays a JupyterLab environment. On the left, a sidebar shows a file browser with a table of files:

Name	Last Modified
01_cryoCare.ipynb	a year ago
02_cryoCare.ipynb	a year ago
03_cryocare.ipynb	a year ago
04_cryoCare.ipynb	a year ago
05_cryoCare.ipynb	a year ago
Untitled.ipynb	9 months ago
Untitled1.ipynb	4 minutes ago
motioncor2.log	a year ago

The main area shows a code cell for 'Untitled1.ipynb' with the following Python code:

```
In [2]: # -*- coding: utf-8 -*-
import numpy as np
import math

# Create random input and output data
x = np.linspace(-math.pi, math.pi, 2000)
y = np.sin(x)

# Randomly initialize weights
a = np.random.randn()
b = np.random.randn()
c = np.random.randn()
d = np.random.randn()

learning_rate = 1e-6
for t in range(2000):
    # Forward pass: compute predicted y
    # y = a + b x + c x^2 + d x^3
    y_pred = a + b * x + c * x ** 2 + d * x ** 3

    # Compute and print loss
    loss = np.square(y_pred - y).sum()
    if t % 100 == 99:
        print(t, loss)

    # Backprop to compute gradients of a, b, c, d with respect to loss
    grad_y_pred = 2.0 * (y_pred - y)
    grad_a = grad_y_pred.sum()
    grad_b = (grad_y_pred * x).sum()
    grad_c = (grad_y_pred * x ** 2).sum()
    grad_d = (grad_y_pred * x ** 3).sum()

    # Update weights
    a -= learning_rate * grad_a
    b -= learning_rate * grad_b
    c -= learning_rate * grad_c
    d -= learning_rate * grad_d

print(f'Result: y = {a} + {b} x + {c} x^2 + {d} x^3')
```

The output of the code cell shows the loss values at intervals of 100 iterations:

```
99 712.447821888372
199 478.3262177418421
299 322.276702381664
399 218.21288593989044
499 148.7807326213537
599 102.43000968080545
699 71.47013935582402
799 50.77823131954953
```

Example 1.3 (Open a Jupyter RTX 3090 with terminal)

The screenshot displays the JupyterLab interface. On the left, a sidebar shows the file explorer with a list of files and folders. The main area is a terminal window showing the output of the 'nvidia-smi' command.

Files Explorer:

Name	Last Modified
01_cryoCare.ipynb	a year ago
02_cryoCare.ipynb	a year ago
03_cryocare.ipynb	a year ago
04_cryoCare.ipynb	a year ago
05_cryoCare.ipynb	a year ago
Untitled.ipynb	9 months ago
Untitled1.ipynb	2 minutes ago
motioncor2.log	a year ago

Terminal Output:

```
[thwu@jupyterlabtf24gpu1080ti-thwu ~]$ nvidia-smi
Mon Nov 28 07:32:53 2022
+-----+
| NVIDIA-SMI 418.56      Driver Version: 418.56      CUDA Version: 10.1     |
+-----+-----+
| GPU   Name           Persistence-M| Bus-Id        Disp.A | Volatile Uncorr. ECC |
| Fan  Temp  Perf    Pwr:Usage/Cap|  Memory-Usage | GPU-Util  Compute M. |
+-----+-----+
| 0   GeForce GTX 108...  On          | 00000000:0F:00.0 Off  |          N/A         |
| 29%   34C   P8      8W / 250W | 1MiB / 11178MiB |    0%      Default   |
+-----+-----+
+-----+
| Processes:                                                       GPU Memory |
|  GPU       PID    Type   Process name                               Usage      |
+-----+-----+
| No running processes found                                     |
+-----+
[thwu@jupyterlabtf24gpu1080ti-thwu ~]$
```

Storage Service

- Ceph Filesystem
 - An open source distributed filesystem
 - High-Throughput

User Home Space

- /dicos_ui_home/{user_account}
- 100GB Free space

Working Space

- /ceph/work/{group_account}
- Every Group has 3TB free space, PI has full permissions for data in this space. Buy more space according to your computing needs, 1TB/days as a purchase unit.

Backup Space *will be available in 2024

Tape as Backup and Preservation Service in the future

- /ceph/project/{group_account}
- Backup and long-term preserved space. Buy as needed. 1TB/years as a purchase unit.

Data Transfer

- Transfer by SFTP via dicos-sftp.twgrid.org

Technical Support

- Help Desk & Service Notification



- Rocketchat online chat - <https://rocketchat.twgrid.org/channel/general>
- Email - dicos-support@twgrid.org
- Portal - <https://nstccore.twgrid.org>
 - Release up-to-date services status, group usage, pricing and technical relevant information
- Service Portal - <https://dicos.grid.sinica.edu.tw>
 - SaaS Computing Service
 - PI & User Management
- Training & Workshop
 - Regular workshops every 3 months
 - Technical support & consulting services

User Management - User Account



- Apply your account
 - Group Account: <https://canew.twgrid.org/ApplyAccount/groupcreate.php>
 - User Account: <https://canew.twgrid.org/ApplyAccount/ApplyAccount.php>
 - PI approval for Member's application
 - Password & Account Expiration (ISO security)
 - 1 year validation, password & account expiry notification will be sent on 7, 15 and 30 days to expiration.
 - Account Deletion: Your account & user space(UI home directory, work directory and DiCOSBox) will be removed after 6 months of expiration.

User Management - Group

- Members management
 - Members list
 - Abnormal member usage report
 - Member's usage review
- Resource usage Management & Budget Control
 - Monthly Bill will be delivered
 - <https://dicos.grid.sinica.edu.tw/accounting/bill/>
 - Resource Usage
 - Payment Management

使用者 (username)	姓名(name)	Email	Expired Date	Active	Joined Date	Last Login	Storage Usage (UI Home)
chiong	CHAN-HIN IONG	chiong@me.com	Jun. 13, 2024, 00:00 AM	True	Aug. 22, 2018, 00:00 AM	Jul. 31, 2023, 03:41 AM	33.4G/100G <small>Latest Update: 2023-07-31 00:50:03</small>
dickie	Dickie Chang	dickie.chang@twgrid.org	Oct. 12, 2023, 00:00 AM	True	Dec. 15, 2022, 07:16 AM		
eric	嚴漢偉 嚴漢偉	Eric.Yen@twgrid.org	Oct. 18, 2023, 00:00 AM	True	Mar. 11, 2019, 09:13 AM	Jul. 06, 2023, 04:37 AM	0.0G/100G <small>Latest Update: 2023-07-31 00:50:03</small>
ericyen	Eric YEN	Eric.Yen@twgrid.org					
etomo	etomo etomo	etomo@twgrid.org					
felixlee	Felix Lee	felix@twgrid.org					

使用統計摘要(TOTAL SUMMARY TABLE)
使用明細(DETAILED USAGE ACCOUNTING)

• 計算資源使用統計(COMPUTING USAGE OF GROUP) – 預估使用費(INITIAL COST): NT \$15,878

使用者(username)	姓名(name)	CPU (SRU)	GPU (SRU)	預估費用 (Initial Cost Estimation)
chiong	CHAN-HIN IONG	175	7,601	15,552
jyou	Jingya You	1	54	110
rudy	陳侑廷	3	0	6
thwu	Tsung-Hsun Wu	4	101	210

使用統計摘要(TOTAL SUMMARY TABLE)
使用明細(DETAILED USAGE ACCOUNTING)

使用明細(DETAILED USAGE ACCOUNTING)
使用者(username): chiong (CHAN-HIN IONG)

用量異常回報(submit issue)

Alert	#Instance	A100		FDR5		P100		RTX3090		V100	
		CPU (SRU)	GPU (SRU)	CPU (SRU)	GPU (SRU)	CPU (SRU)	GPU (SRU)	CPU (SRU)	GPU (SRU)	CPU (SRU)	GPU (SRU)
<input type="checkbox"/>	relion311rtx3090	3						151	6,320		
<input type="checkbox"/>	jupyterlabtf24gpu3090	2						11	474		
<input type="checkbox"/>	matlab	2								0	6
<input type="checkbox"/>	jupyterlabgpu26a100	1	1	519							
<input type="checkbox"/>	openaccp100	1				11	282				
<input type="checkbox"/>	FDR5 slurm	2			0	0					
<input type="checkbox"/>	STORAGE USAGE (0.0 TB)										

說明(note)

- Group使用空間
- User使用空間
- User使用空間
- User使用空間
- User使用空間

User Management - User

- User Profile

- Change Group

- Change Password

- <http://canew.twgrid.org/ApplyAccount/nocertModify.php>

- Resource Usage

- Free \$200 Credits for Trial

- Storage Usage

[使用統計摘要\(TOTAL SUMMARY TABLE\)](#)
[使用明細\(DETAILED USAGE ACCOUNTING\)](#)

使用明細(DETAILED USAGE ACCOUNTING)

使用者(username): robert10096901 (Po-Han Tseng) Free Period: 2024-02-27 08:28:09~2024-03-27 08:28:09, Remain: NT \$199 用量異常回報(submit issue)

Alert	#Instance	EDR1	
		CPU	GPU
<input type="checkbox"/>	EDR1 slurm	140	7,220

使用者(username): steven20720 (可奕 郭) Free Period: 2024-03-11 08:44:09~2024-04-11 08:44:09

Alert	#Instance	A100		EDR1		QDR6		RTX3090		V100	
		CPU	GPU	CPU	GPU	CPU	GPU	CPU	GPU	CPU	GPU
<input type="checkbox"/>	jupyterlabcpu	4				14	0				