

# User Training Workshop for NSTC Core Computing Service & NVIDIA GPU Computing

( 26 June, 2024)

# Introduction of NSTCCore Computing & Storages Services

<https://nstccore.twgrid.org>

# Introduction of NSTCCore Computing Service

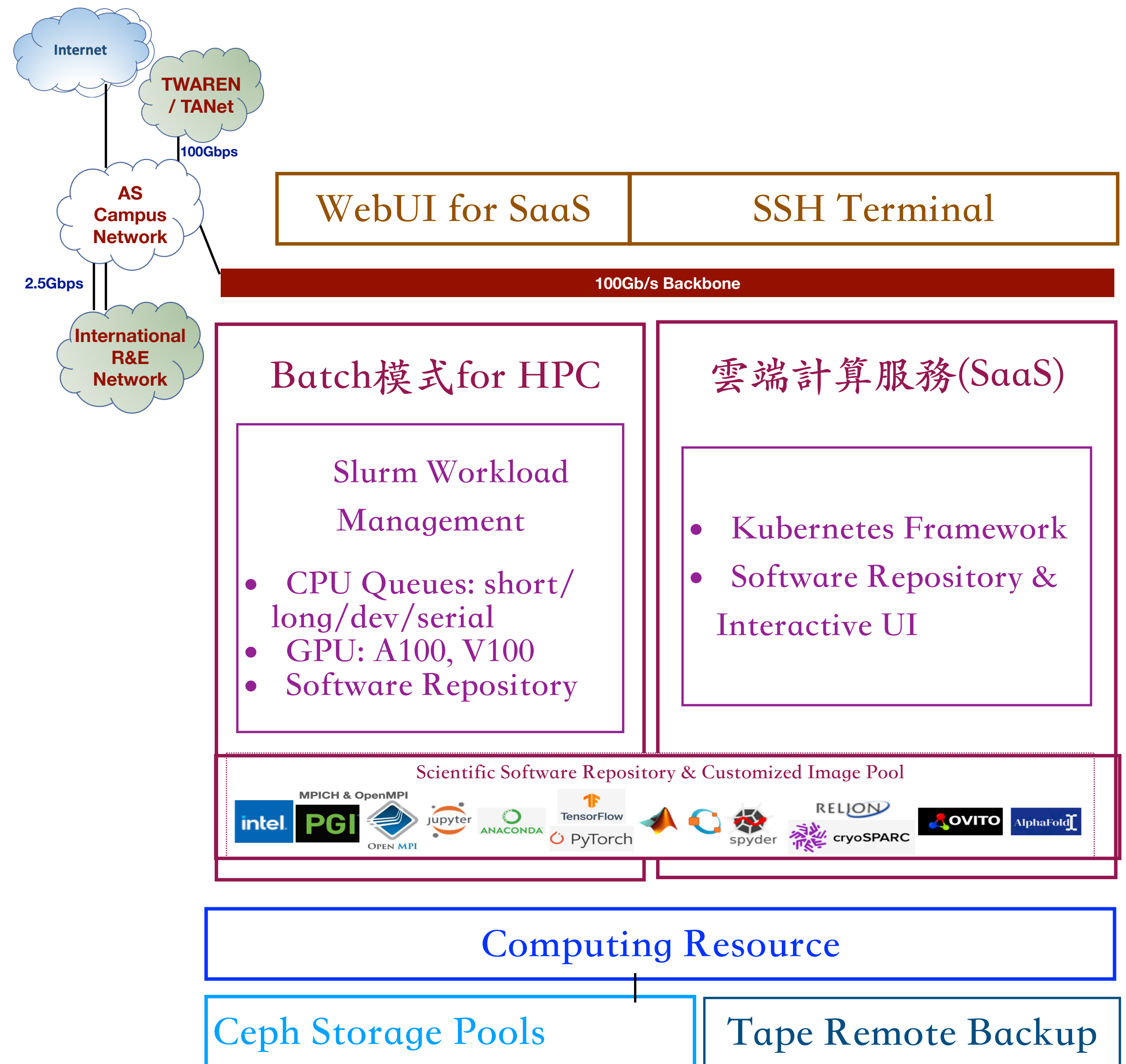
- Computing Service
- Storage Service
- Technical Support
- User Management

	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

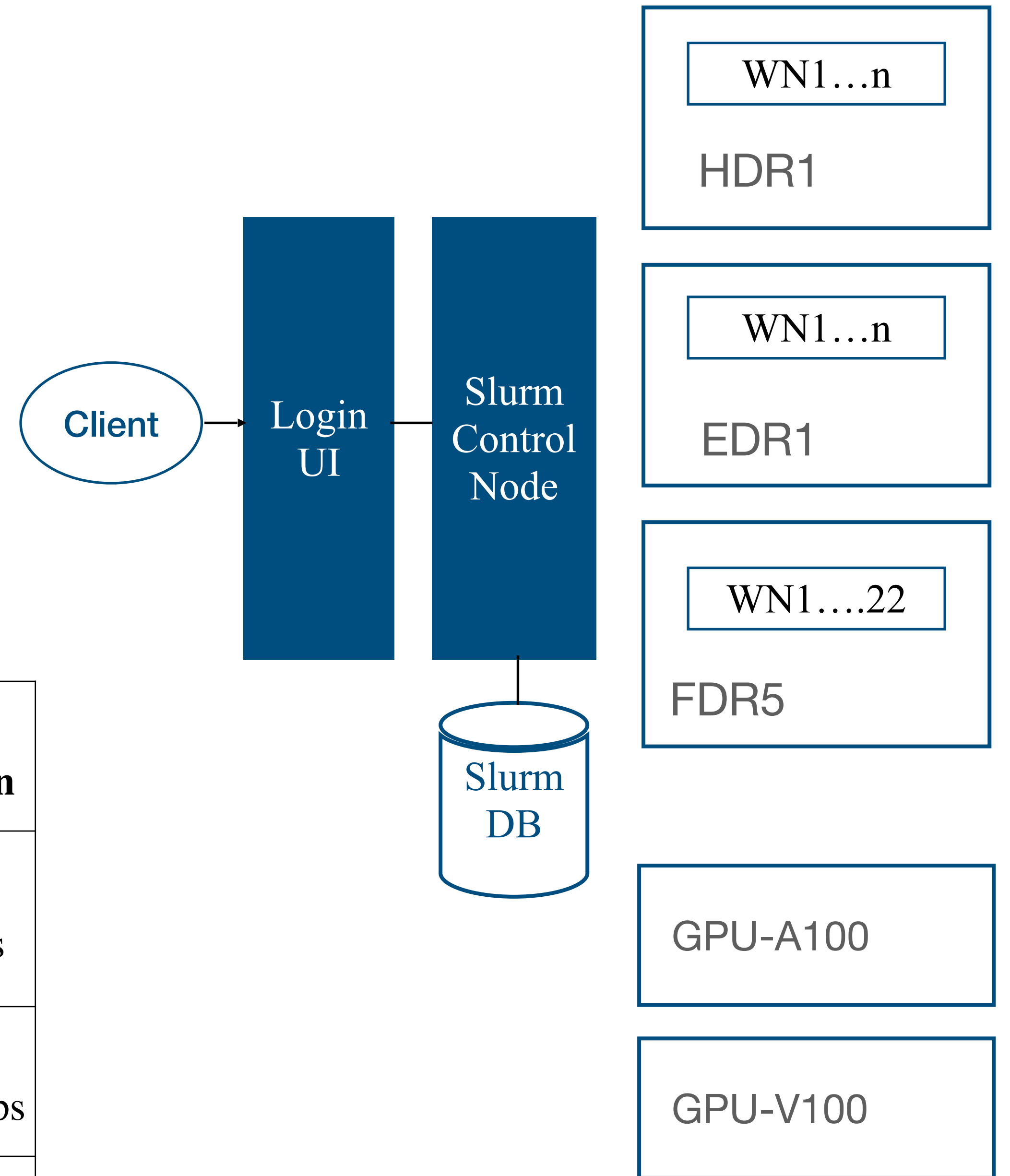
- Batch Jobs Computing Service
  - Slurm Work Management System
- Interactive Jobs Computing Service
  - Scalable & Virtualized Service-as-Service (SaaS) Service Model
  - Software on-demand Web-based UI
  - Customized Application Deployment



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](http://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](https://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}

# 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](https://dicos-sftp.twgrid.org)

# Technical Support

- Help Desk & Service Notification



- Rocketchat online chat - <https://rocketchat.twgrid.org/channel/general>
- Email - [dicos-support@twgrid.org](mailto: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	<b>33.4G/100G</b> <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	<b>0.0G/100G</b> <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				