

高效能科學計算說明會暨使用者教育訓練工作坊 2023
NSTCCore User Training Workshop 2023

Introduction of NSTC Core Computing & Storages Services

Introduction of NSTCCore Computing Service

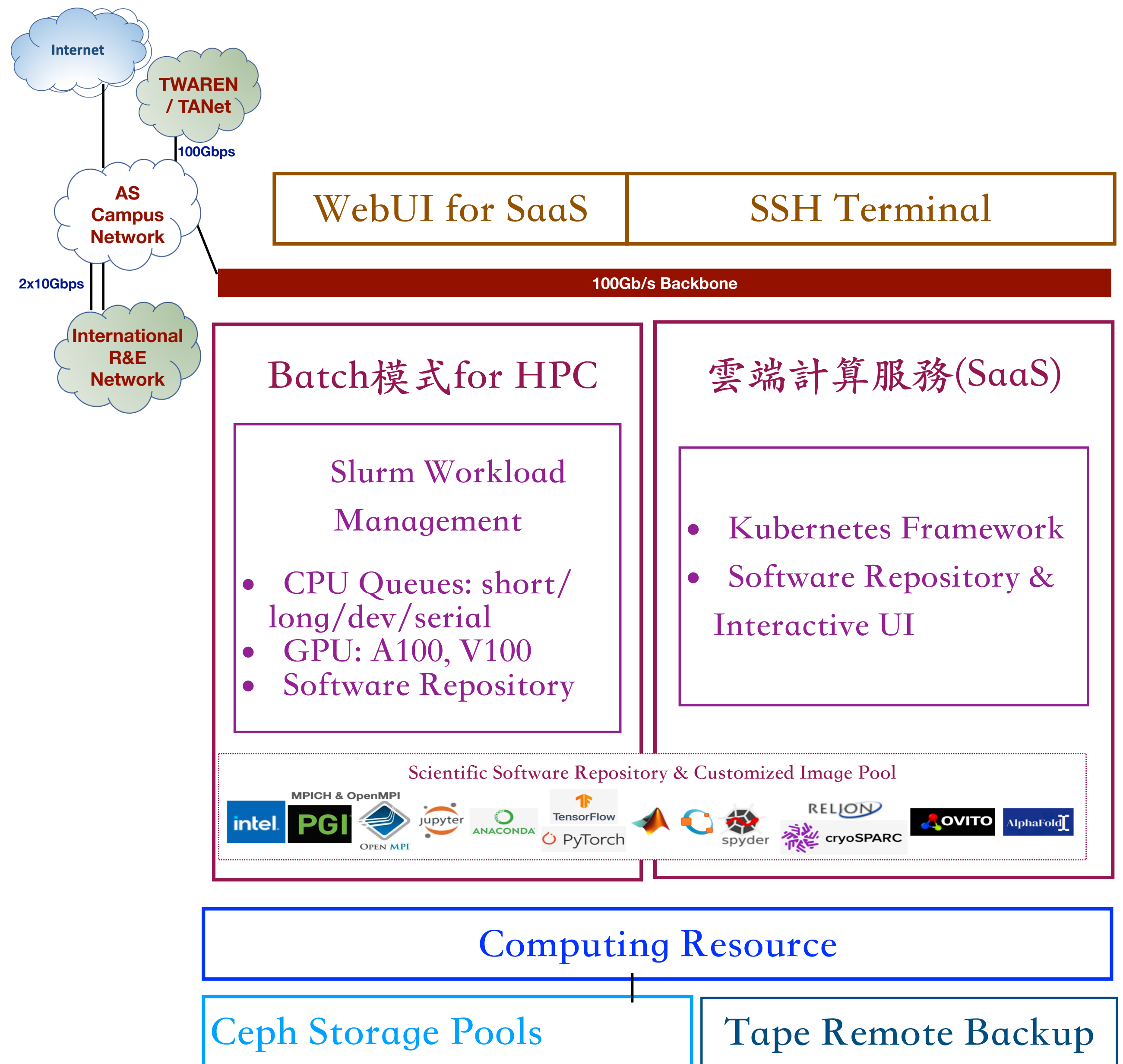
- Computing Service
- Storage Service
- Technical Support
- User Management

	2023.08~2023.11	2023.12~2024.09	2024.09~2025.08	2025.08~2026.06	
CPU	2976 Cores *Current Resources	1792 Cores *New + 768 Cores *AMD Rome	3584 Cores *New + 768 Cores *AMD Rome	5376 Cores *New + 768 Cores *AMD Rome	*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	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 2023.7

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

- Computing Nodes

- CPU

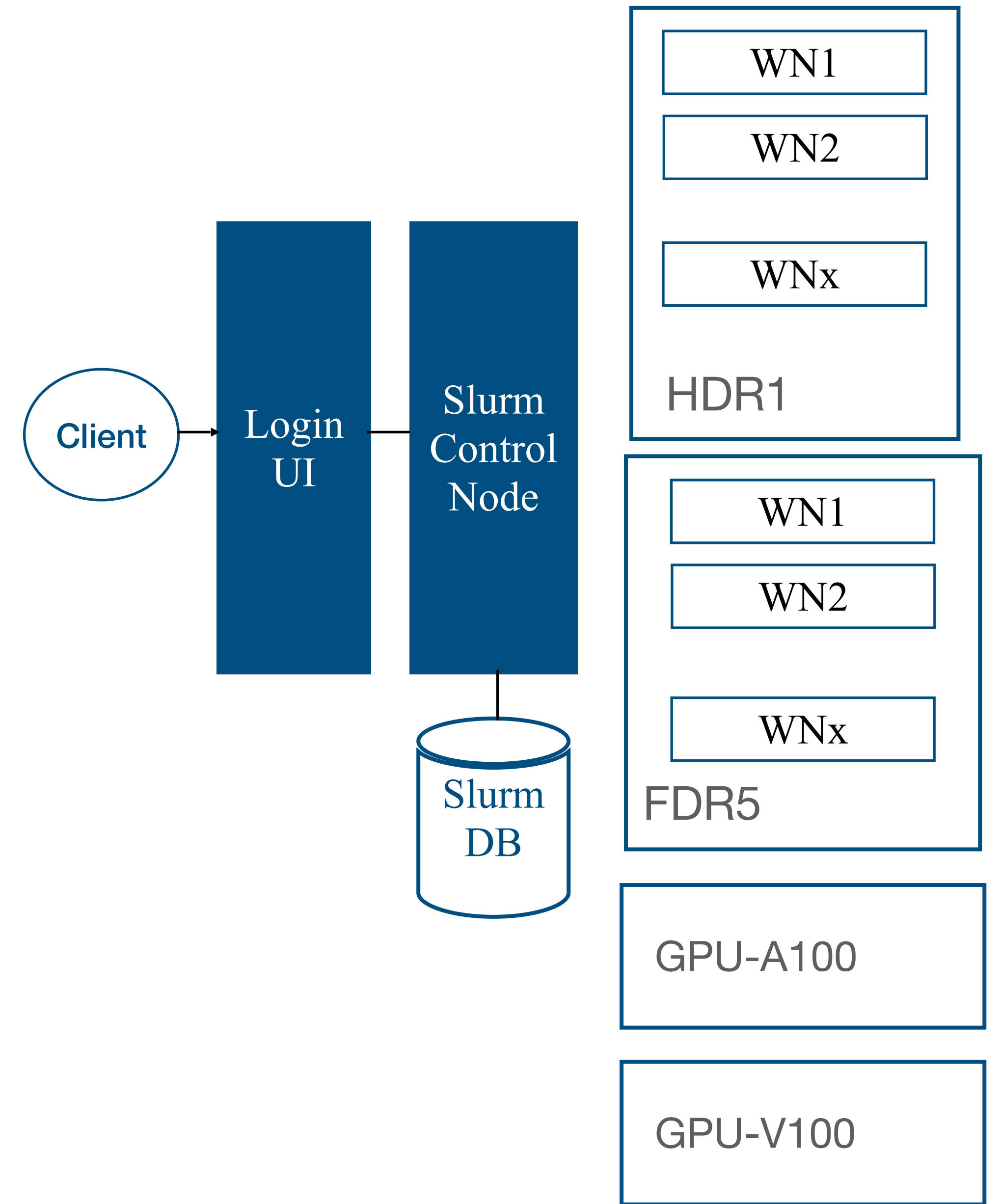
Cluster	CPU	Nodes	Cores-Per-Node	Cores	RAM(GB)	Inter-connection
FDR5	Intel® Xeon® CPU E5-2650 v4@2.20GHz	92	24	2208	128	IB:FDR, Eth:10Gbps
HDR1	AMD Rome 7662 @2.0GHz	6	128	768	1536	IB:HDR, Eth:100Gbps

- GPU - A100 、 V100

- Jobs Working Space:

- Ceph Cloud Filesystem
- Worker Node Local Disk

- [HDR1] SSD 1TB & [FDR5] NO SSD



Slurm System Architecture

Batch Jobs Computing Service - Slurm

System Spec

- OS : CentOS 7
- Login (SSH) : dicos-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
- 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}

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

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 *purchase by the end of 2023

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-ui.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: <http://canew.twgrid.org/ApplyAccount/groupcreate.php>
 - User Account: <http://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
 - 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, 00:12 AM	Jul. 06, 2023, 04:27 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)		
<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