User Training Workshop for NSTCCore Computing Service & AI Applications

(30 October, 2024)

Introduction of NSTCCore Computing & Storages Services

https://nstccore.twgrid.org

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Introduction of NSTCCore Computing Service

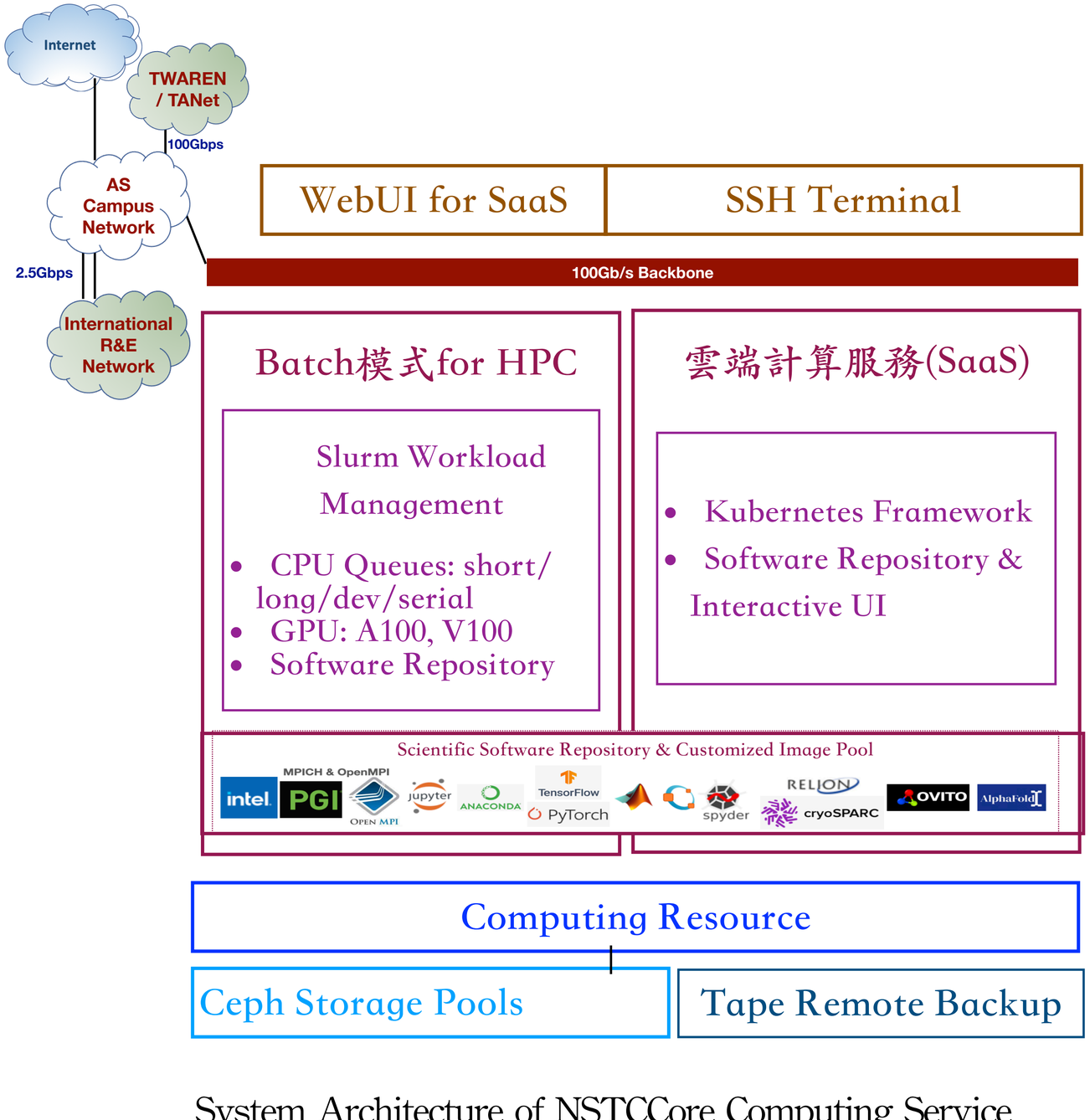
- Computing Service
- Storage Service
- Technical Support
- User Management

	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 (2024. 12) + 2688 Cores *AMD Rome + Genoa + 256 Cores *Intel-G4	3840 Cores *New + 2688 Cores *AMD Rome + Genoa + 256 Cores *Intel-G4	＊後續計算量計核狀能依畫定況決定
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 *Buy-in 3TB every year	9	
Tape (PB)	4 *Buy-in every year	8 *Buy-in 4TB every year	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

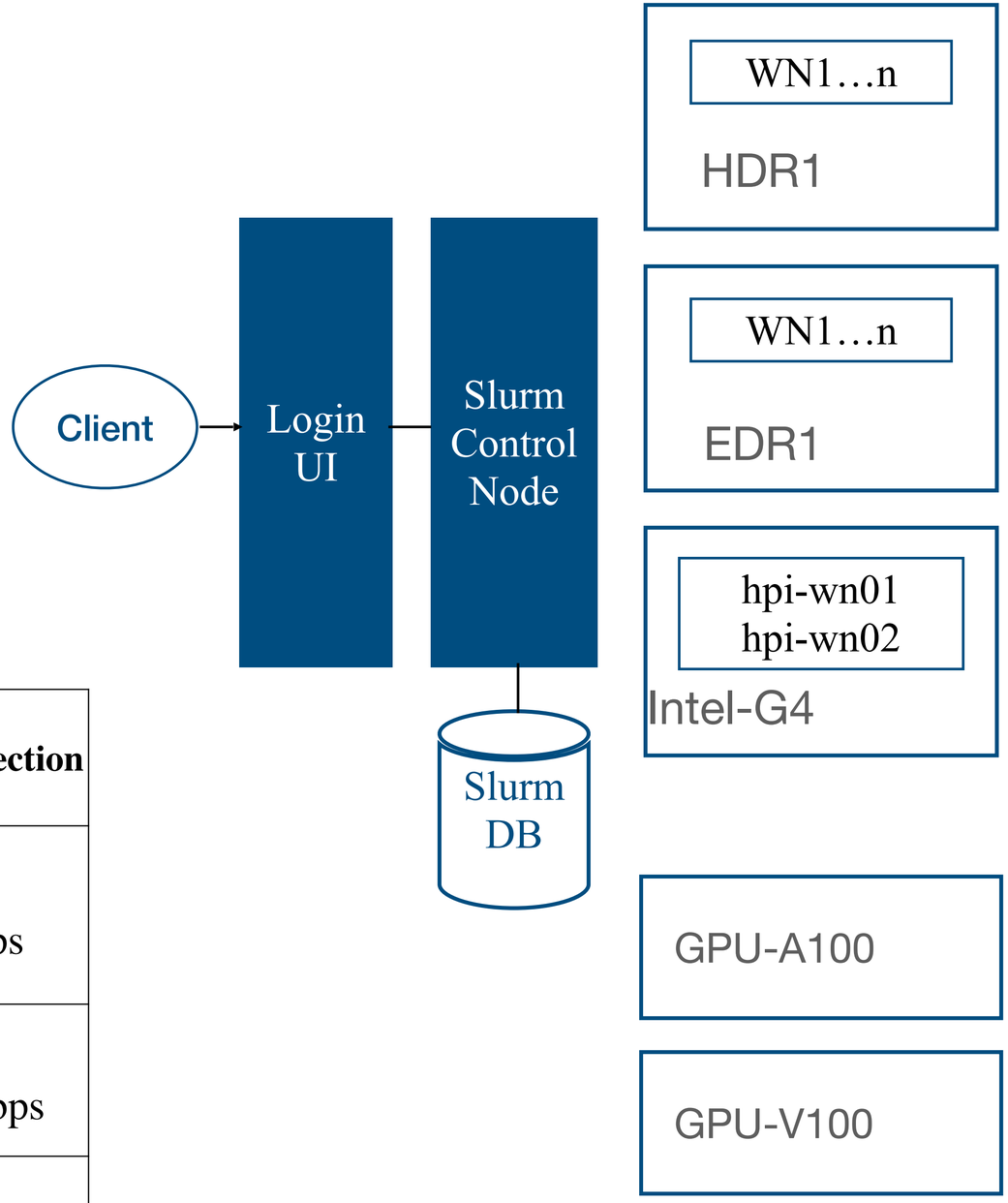


System Architecture of NSTCCore Computing Service

Batch Jobs Computing Service

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

Cluster	CPU	Nodes	Cores-Per-Node	Cores	RAM(GB)	Inter-connection
Intel-G4	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}
    (*will be available in 2025)
- 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 2025

SaaS for Virtualized Computing Service

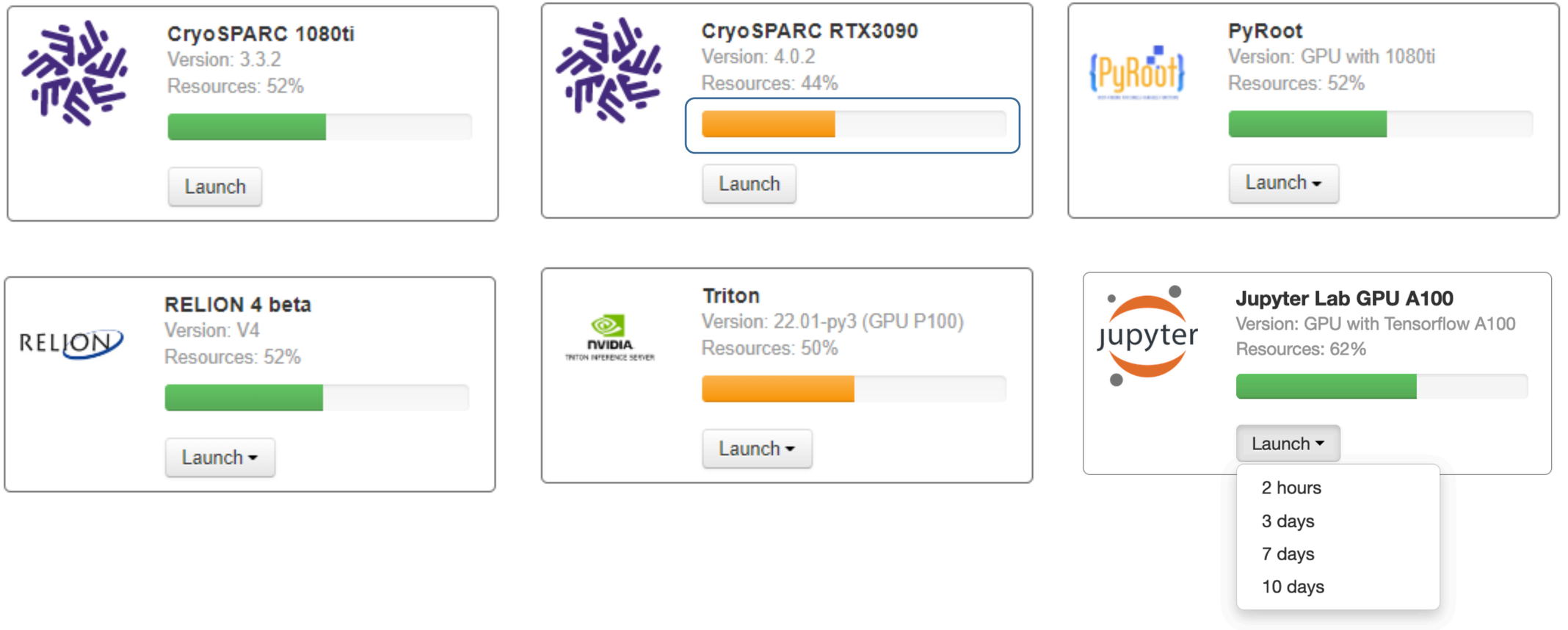
Scientific Software Repository

- 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/



Pricing for Computing Service

CPU計算服務				
機器名稱	機器規格	計費單位(Per Core/Board-Day) 價格(NTD)	國內非學術單位使用者	國外學術單位使用者
intel-g4	Intel(R) Xeon(R) Gold 6448H	1.4	加計 50%	加計 50%
EDR1	AMD Genoa 9654 @2.4GHz	1.2		
HDR1	AMD Rome 7662 @2.0GHz	1		
GPU計算服務				
A100	NVIDIA A100	120	加計 50%	加計 50%
RTX4090	NVIDIA RTX-4090	60		
RTX3090	NVIDIA RTX-3090	40		
RTX3090 (Dedicated for ASCEM user)	NVIDIA RTX-3090	40		
V100	NVIDIA V100	35		
P100	NVIDIA P100	8		
1080Ti	NVIDIA GTX-1080Ti	1		
儲存與擷取服務				
--	$1000 NTD/TB-Year		加計 20%	加計 50%
--	$3 NTD/TB-Day			
資料傳輸				
--	目前未納入計費			
進階服務				
--	依據所需人時計算。額外需開發之軟體、系統或使用介面等，將另按工時計費(每 168 man-hr 為 NT$ 120,000)			

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 2025

Tape as Backup and Preservation Service will be available soon

- /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.
  - 2-factor authentication will be implemented from 2025 January

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** Latest Update: 2023-07-31 00:50:03
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** Latest Update: 2023-07-31 00:50:03
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)

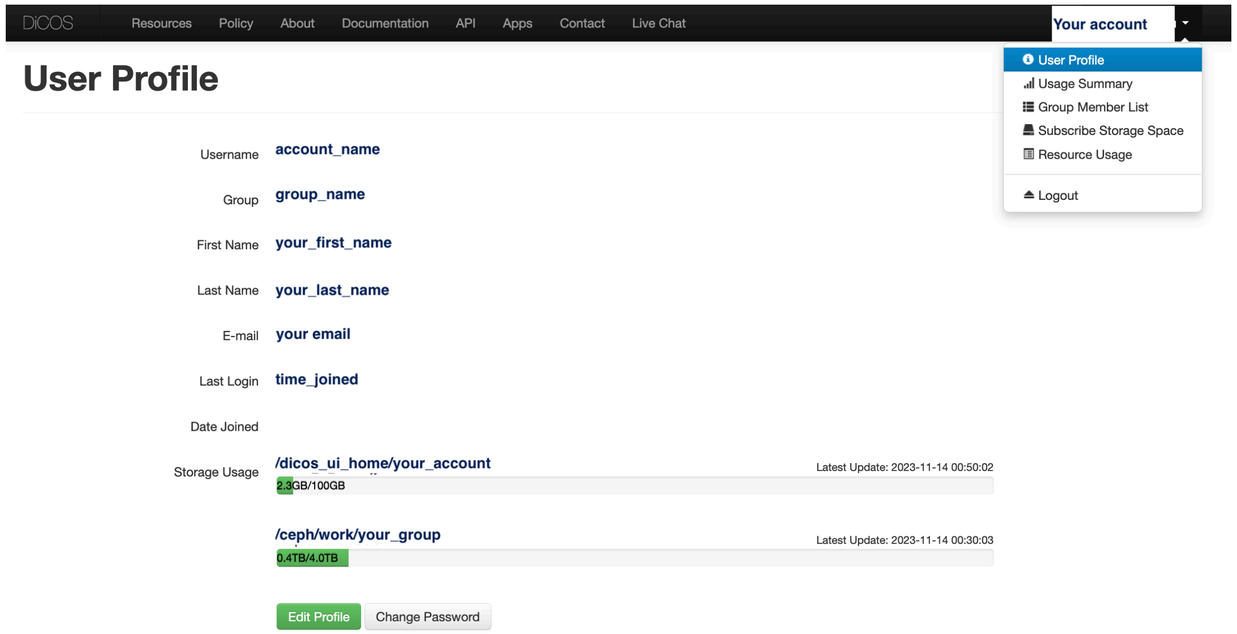
用量異常回報(submit issue)

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)
☐	relion311rtx3090	3							151	6,320		
☐	jupyterlabtf24gpu3090	2							11	474		
☐	matlab	2									0	6
☐	jupyterlabgpu26a100	1	1	519								
☐	openaccp100	1					11	282				
☐	FDR5 slurm	2			0	0						
☐	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
☐	EDR1 slurm	140	7,220	0

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
☐	jupyterlabcpu	4					14	0				