國科會
高效能核心科學計算中心
(NSTCCORE)

https://nstccore.twgrid.org

嚴漢偉 Eric Yen

中央研究院 物理所 網格中心

2026. 1. 13

NSTCCore @TPS2026

- **Seeking for advice, comment and discussion**
  - **In order to improve the service and quality**
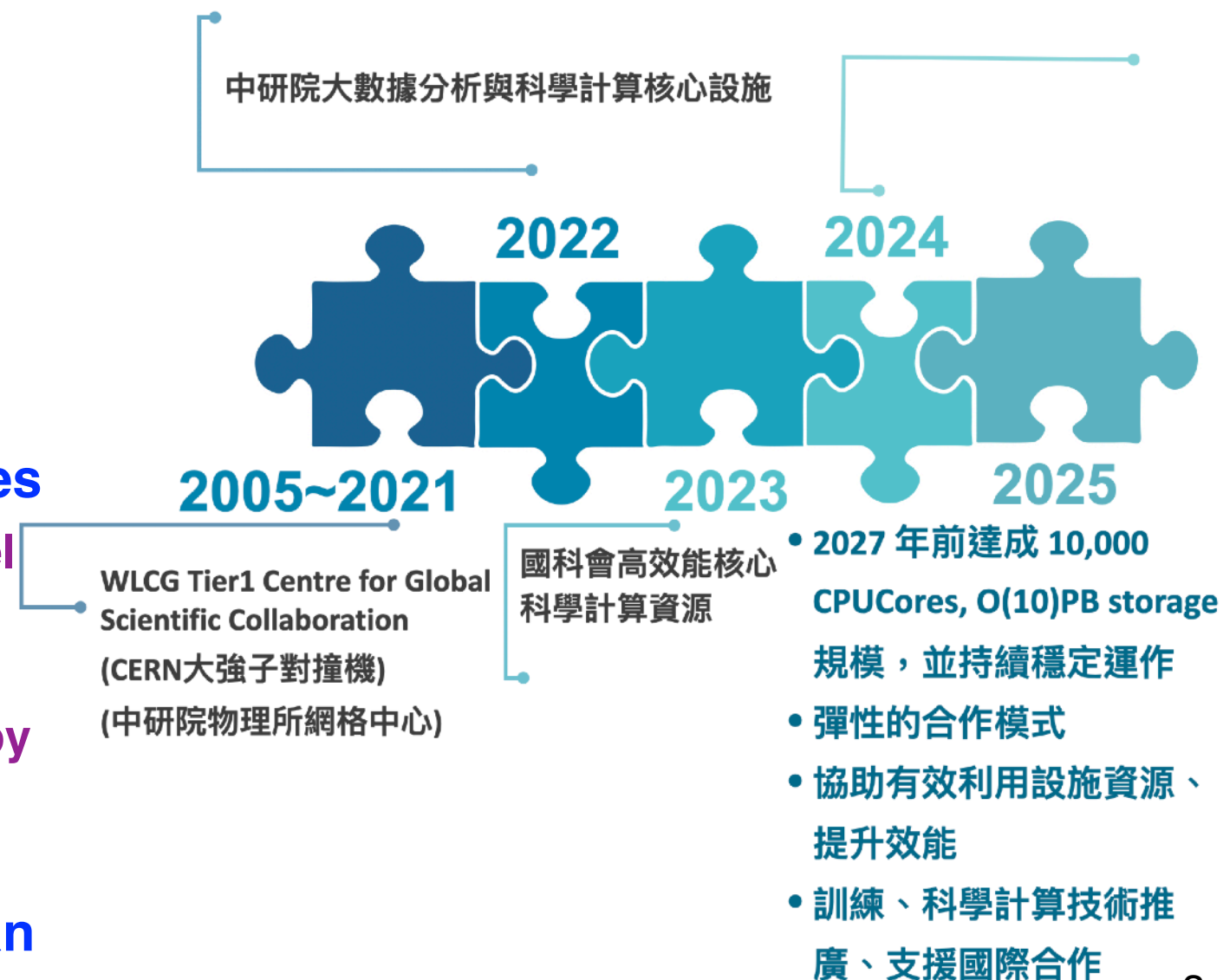- **Technical details could be explained at Booth #7**

https://indico4.twgrid.org/event/70/

4:00 PM	→ 4:10 PM	一、NSTCCore 計劃簡介 NSTCCore Project Overview
		Convener: Prof. Song-Ming Wang (ASGC)
4:10 PM	→ 4:30 PM	二、資源與服務概況 Overview of Resources and Services
		Convener: Prof. Eric Yen (ASGC)
4:30 PM	→ 5:25 PM	三、交流與討論 Discussion and Exchange
		Convener: Mr Felix Lee (ASGC)
5:25 PM	→ 5:30 PM	四、問卷調查 Questionnaire ¶

Mid-Scale Scientific Computing Services for Accelerating Discovery & Innovation

- **Funded by NSTC, June 2023 - May 2026**
  - **Jointly supported with the core facility funded by Academia Sinica since 2023**
- **Reliability & Efficiency are the top priority**
- **Serving as your computational research partner, so that scientific groups could focus on sciences**
- **Flexible and customized services: resource arrangement, workflow integration, performance improvement, etc.**
- **Resource scale: providing services utilizing O(10,000) CPUCores, O(100) GPUs and O(10)PB Disk storage resources**
  - **Able to support O(1,000) CPUCores parallel computing, multiple GPUs and big data analysis**
  - **Affordable cost and lower than operating by your own**
- **Aligning with NCHC, and enhancing the advanced computing ecosystem in Taiwan**

User-Oriented Services
24x7x365

中研院大數據分析與科學計算核心設施

2022   **2024**

2005~2021   **2023**   **2025**

WLCG Tier1 Centre for Global Scientific Collaboration (CERN大強子對撞機) (中研院物理所網格中心)

國科會高效能核心 科學計算資源

- 2027 年前達成 10,000 CPUCores, O(10)PB storage 規模，並持續穩定運作
- 彈性的合作模式
- 協助有效利用設施資源、提升效能
- 訓練、科學計算技術推廣、支援國際合作

3

Research Infrastructure Keeps Advancing With Requirements of Multiple Disciplinary Scientific Communities

From 2006, we have been supporting user communities in multiple disciplines to make better use of available scientific computing resources with efficiency.

Services are jointly provisioned by ASGC Core Facility (SCALE, 大數據分析與科學計算核心設施)
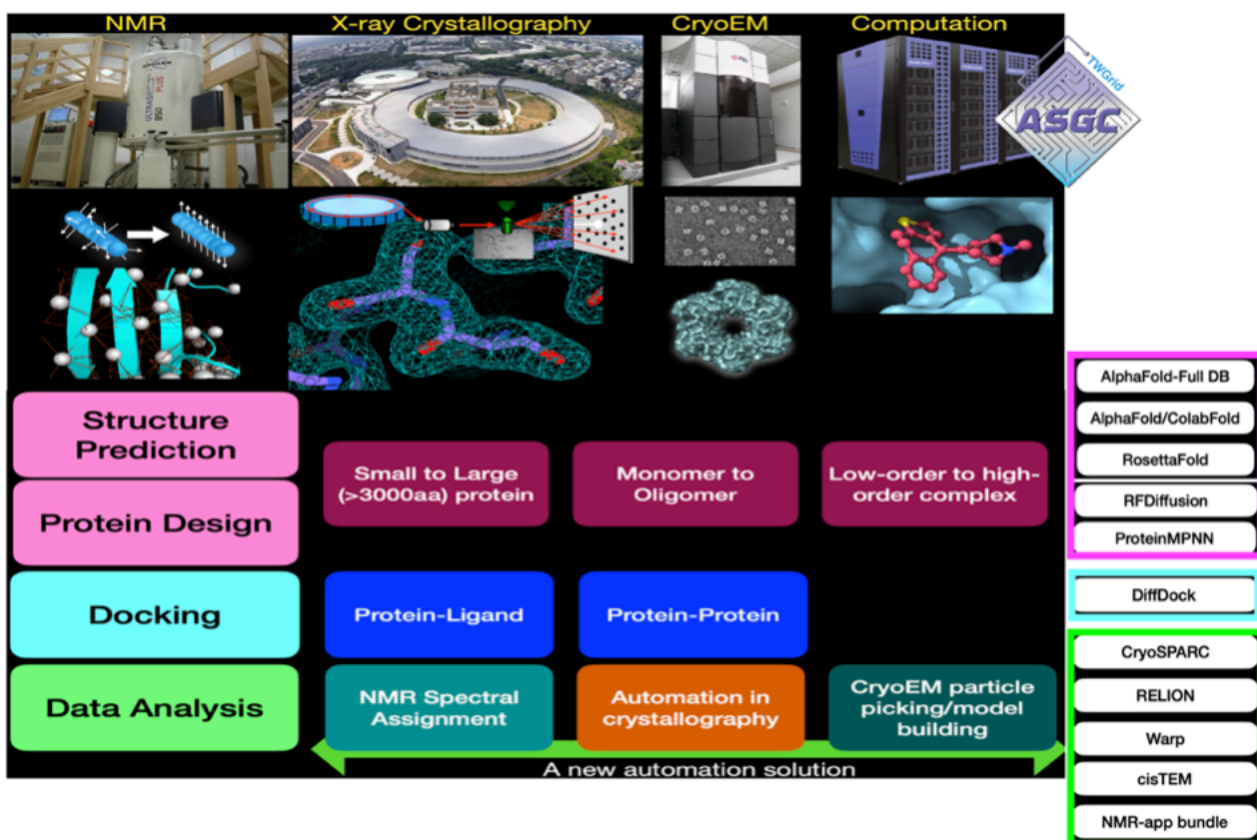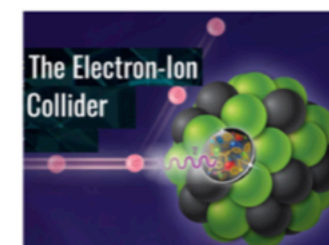
Neutrino/MHEP

Quantum Materials Physics

Physics of Active & Living Matter

Astrophysics

Earth Science

CryoEM

Bioimaging

Drug Discovery

Computational Chemistry

Biodiversity & Ecology

Computing & Storage Resources

CPU Cluster	Spec	CPU Cores	GB RAM/ Core	Nodes	Performance (TFLOP/Core)	Network	Onboard Date
EDR	AMD Genoa 9645	1,920	8	10		100Gb/HDR	Feb 2026
EDR1	AMD Genoa 9654	3,840	8	20	1.1	100Gb	Mar 2024, Dec 2024
Intel-G4	Intel Xeon 6448H	512	8	4	1	100Gb	Sep 2024

GPU Cluster	Spec	GPU	Architecture	Nodes	CPU Cores	Server RAM (GB)	CPU	Network	Onboard Date
B6000	RTX 6000 96GB	16	Blackwell	2	32	1,536	Intel 6517Px2	200Gb	Jan 2026
L40S	L40S 48GB	4	Ada Lovelace	1	32	768	AMD 9374x1	10Gb	Dec 2024
4090	RTX 4090 24GB	16	Ada Lovelace	2	40	1536	Intel 4416x2	10Gb	Jul 2024
3090	RTX 3090 24GB	56	Ampere	7	32	1024	AMD 7302x2	100Gb	Dec 2020
A100	A100 NVL 80GB	24	Ampere	3	64	512	AMD 7542x2	100Gb, NVL	Jun 2020
V100	Tesla V100 32GB	48	Volta	6	24	768	Intel 6126x2	10Gb, NVL	Dec 2018
P100	Tesla P100 16GB	16	Pascal	4	24	128	Intel 2650x2	10Gb, IB-FDR	Dec 2017

Storage	Capacity (TB)	System	Price	Remarks
Ceph File System	12,000	Online storage managed by Ceph distributed file system, with (8, 3) erasure coding	1,000 per TB-year	+3PB by end of Feb 2026
Tape Lib System	10,000	LTO9 (18TB/Tape)	300 per TB-year	Service from 2025

Scientist Could Focus on Scientific Questions

- **Utilizing high-performance computing service by affordable cost 筆電價格即可使用整年高規格計算資源**
  - **100CPUCore-Yr < NTD$51,100**
  - **1TB-Yr Disk = NTD$1,000**
  - **1xA100 (80GB RAM) GPU-Yr = NTD$ 43,800**
- **Free quota for new every new user: NT$ 200**
  - **新使用者可有 NT$ 200 免付費測試使用額度**
- **若有特殊或急迫需求，請逕洽本團隊**
- **Storage System：**
  - **Free: 3TB shared space/group, 100GB/ user**
  - **Tape Storage: NT$300/TB-Year**
- **Welcomed to share your requirements and questions**

ASGC Service Architecture - Scalable Science Cloud

- **Integrating data, algorithm and computing**
- **Scientific workflow implementation with integrated compute, storage and network resources**
- **Persistent services: Analysis facility, Web portals**
- **New resource and new services online yearly, based on users requirements**
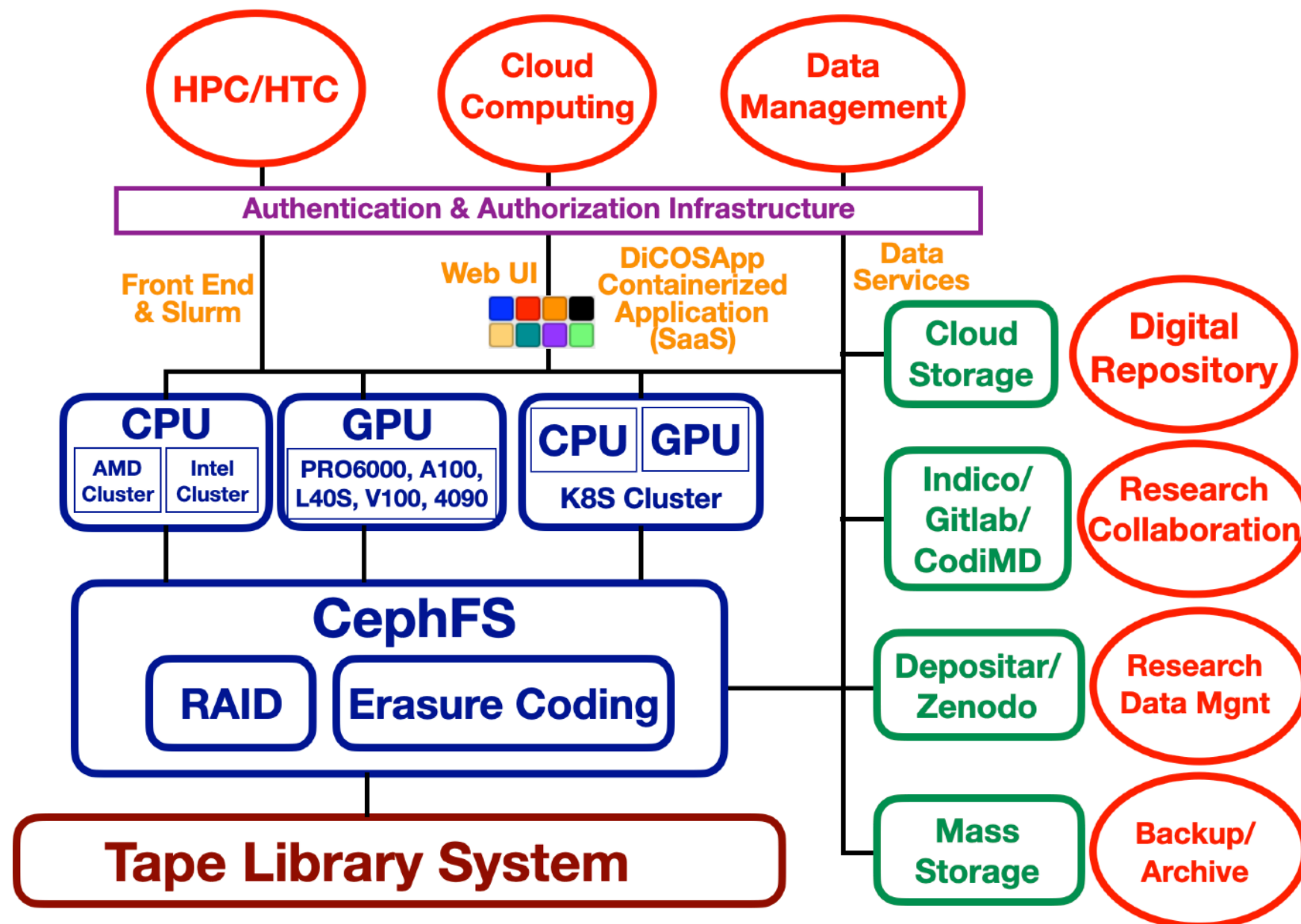
Data & Storage Services - CephFS

- **Ceph distributed storage system - O(10)PB scalable data pool**
- **High performance - 4.2GB/s throughput, 1.5K op/s rd, 2K op/s wr**
- **Reliability - Erasure coding (8, 3), with 462 OSDs, 51 hosts and multiple MDS & MONs**
- **Scalability - from O(10)TB in 2012 to 17PB in 2025**
- **Data transmission and local backup supported**
- **New Services in 2026: data transfer, cloud storage and tape backup**
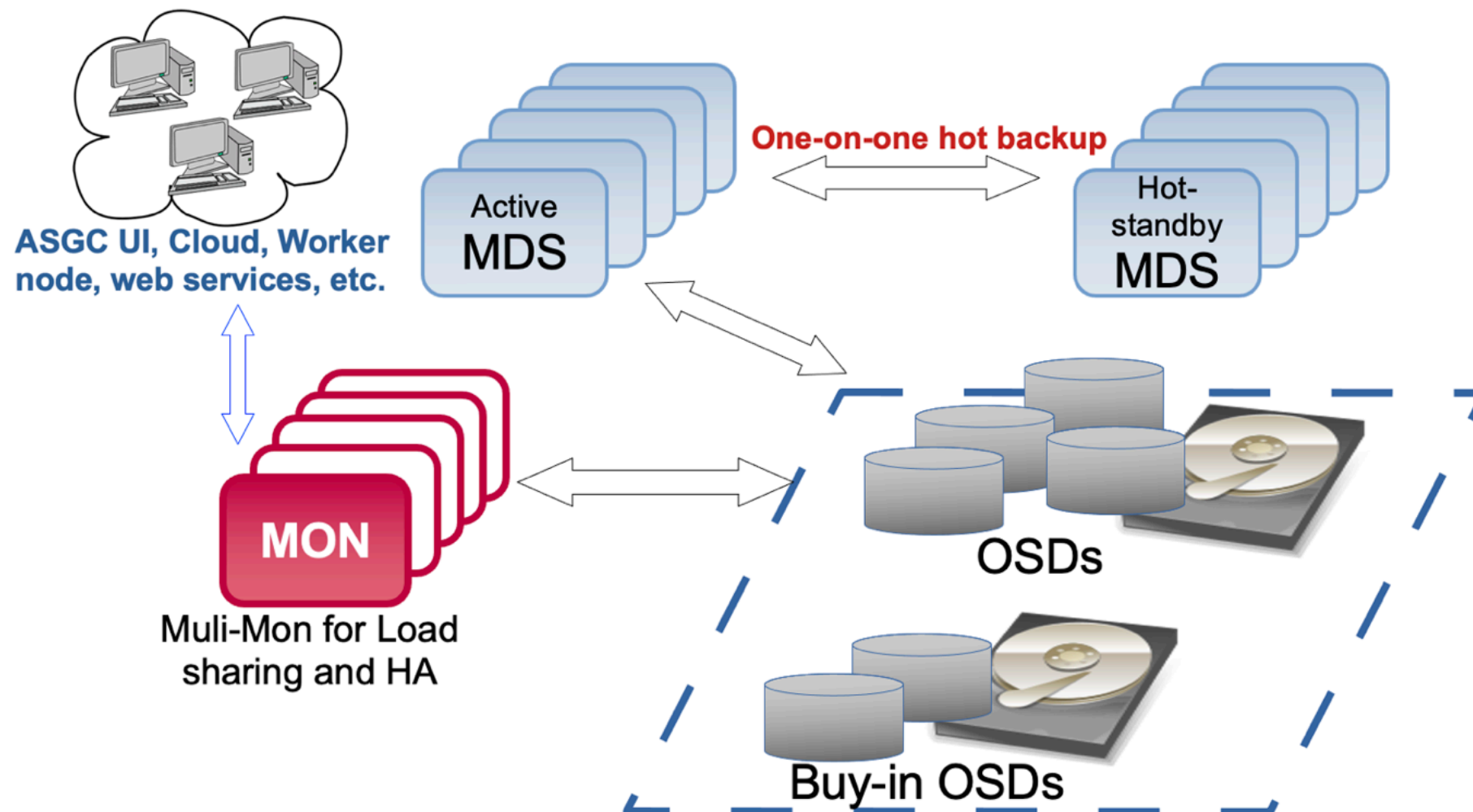
Computing Services: Optimization of Application and System Efficiency
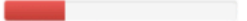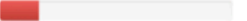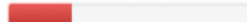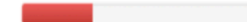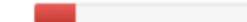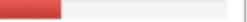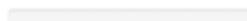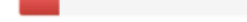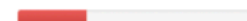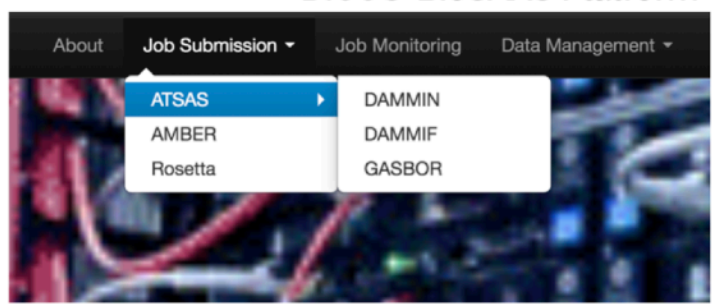
- **HTC/HPC & Cloud Computing Platform**
- **Integration of computing model and software**

- **Research data workflow and management**
- **Information security**
- **Application efficiency**
- **Customized IaaS, Paas, and SaaS**

HPC platform
Slurm System Architecture
Batch Jobs

Software-as-a-Service Web-based Cloud Platform
DiCOSApp SaaS Architecture
Interactive Jobs

70+ Applications are available

User — SSH — HTTP

Slurm DB | Slurm Control Node | Login UI | SLURM Job | Browser | DiCOS Web Server | Kubernetes API Server | Image Repository | Pod

Scientific Software Repository & Customized Image Pool

MPICH & OpenMPI — intel — PGI — OPEN MPI — jupyter — ANACONDA — TensorFlow — PyTorch — spyder — RELION — cryoSPARC — OVITO — AlphaFold

EDR1 | Intel-G4 | A100 | V100 — Ceph Cloud File System — CPU | A100 | 4090 | 3090 | P100

73+ Web Applications Provided (Software-As-a-Service)

Application	Version / Resources
CryoSPARC 32 P100	Version: 3.2, Resources: 83%
CryoSPARC 1080ti	Version: 3.3.2, Resources: 29%
CryoSPARC RTX3090	Version: 3.3.2, Resources: 26%
spyder cpu/eman2	Version: , Resources: 17%
Octave	Version: V5.2, Resources: 29%
Transfer Data	Version: , Resources: 86%
CryoSPARC RTX3090	Version: 4.0.2, Resources: 26%
CryoSPARC RTX3090	Version: 4.1.1, Resources: 26%
CryoSPARC RTX3090	Version: 4.4.1, Resources: 26%
cisTEM	Version: , Resources: 86%
Ovito	Version: , Resources: 86%
OpenACC	Version: GPU P100, Resources: 83%
AlphaFold	Version: GPU with A100, Resources: 75%
AlphaFold (Full DB)	Version: GPU with A100, Resources: 75%
IMOD	Version: GPU with 1080ti, Resources: 29%
Triton	Version: 22.01-py3 (GPU P100), Resources: 83%
AlphaFold	Version: GPU with RTX3090, Resources: 26%
AlphaFold	Version: GPU with V100, Resources: 17%
RoseTTAFold	Version: GPU with rtx3090, Resources: 26%
Dynamo	Version: GPU with 1080ti, Resources: 29%
MATLAB	Version: R2018b on GPU V00, Resources: 17%
Jupyter Lab	Version: CPU with Tensorflow v1, Resources: 86%
Jupyter Lab gpu 3090	Version: GPU with Tensorflow 3090, Resources: 26%
Jupyter Lab GPU 1080ti	Version: GPU with Tensorflow v2, Resources: 29%
RFDIFFUSION	Version: 2023 on GPU V00, Resources: 17%
diffdock	Version: 2023 on GPU V00, Resources: 17%
EvoDiff	Version: V100, Resources: 17%
Jupyter Lab GPU V100	Version: GPU with Tensorflow V100, Resources: 17%
Jupyter Lab GPU A100	Version: GPU with Tensorflow A100, Resources: 75%
Jupyter Lab Cryocare GPU	Version: GPU with 1080ti, Resources: 29%
QIIME2	Version: Genome, Resources: %
Scipion3	Version: P100, Resources: 83%
Phenix	Version: , Resources: 86%
Jupyter Lab GPU A100	Version: GPU with Tensorflow v2.6, Resources: 75%
MorphoGraphX	Version: GPU with P100, Resources: 83%
Deepmd-kit	Version: GPU with A100, Resources: 75%
Deepmd-kit	Version: GPU with V100, Resources: 17%
MAML	Version: GPU with A100, Resources: 75%
Warp	Version: rtx4090, Resources: 700%
MAML	Version: GPU with V100, Resources: 17%
PVserver	Version: 5.8.0 (GPU 1080TI), Resources: 29%
Paraview Client	Version: 5.8.0, Resources: 86%
R studio	Version: 10 CPU Cores, Resources: 54%
PyRoot	Version: GPU with 1080ti, Resources: 29%
qiskit	Version: , Resources: 86%
NVIDIA CUDA-Quantum A100	Version: , Resources: 100%

- **Web Portal**
- **Application over Cloud**
- **Jupyterlab**
- **Web Terminal**

LabVIEW Run-Time Engine	Version: 2019

DiCOS-BioSAXS Platform

About | Job Submission ▾ | Job Monitoring | Data Management ▾

ATSAS ▶	DAMMIN
AMBER	DAMMIF
Rosetta	GASBOR

Flexible Collaboration Model: User-Driven, Service Oriented

- **Pay-as-you-go**
- **Resource Integration: Collocation & Buy-In**
- **Service Hosting**
- **Reservation**
- **Experiment & Collaboration support**

- **Advanced Service: Web Application and portal, efficiency tuning, workflow optimization, customization, hands-on training**
- **User Engagement：weekly User Meeting, User Committee, dissemination & outreach**
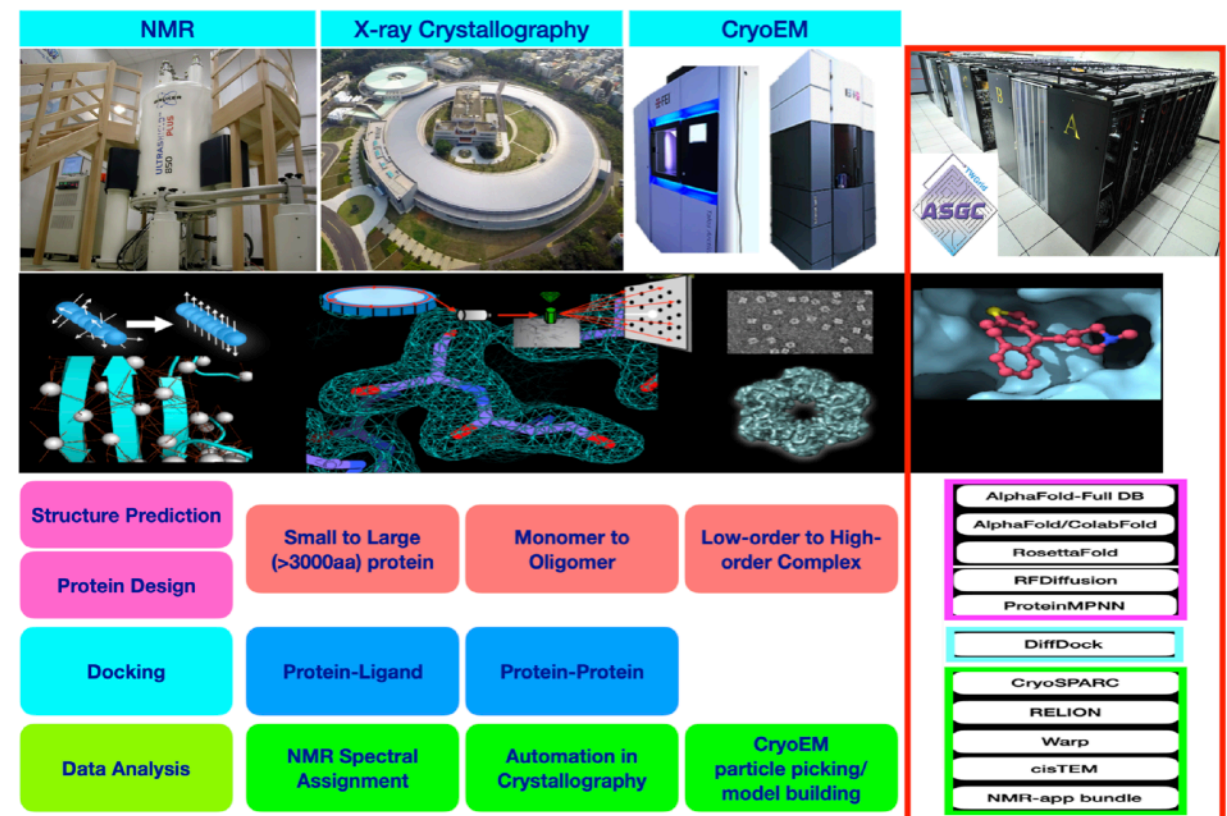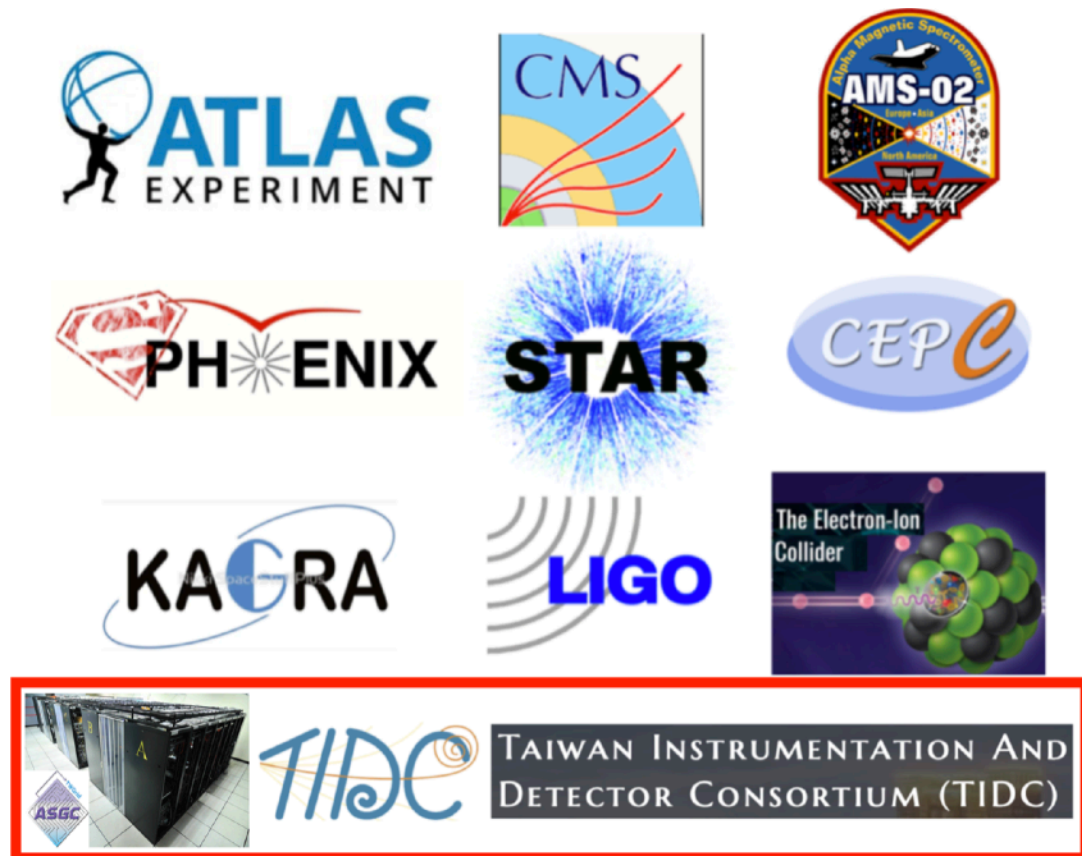
Services of ML-Enabled Data Analytics

- **ML/AI application platform service - SW library, HW, integration and application development management (e.g, MLflow, Triton)**
  - Build up customized ML platforms for user specified projects - Deploy <u>ML packages ready environment</u> in order to help ML development smoothly and provide on-demand computing power
  - Upkeep of the application framework
  - Workflow and data pipeline integration: tracking, model serving, packaging, model registry, evaluation & tracing
  - Efficiency Improvement
  - Inference-as-a-Service (incl. Model repository): e.g., Triton-based services

- **Potential use cases**
  - Users who bring existing source code - ASGC could help to setup a virtual environment and confirm source code running normally
  - Share and reuse of trained/verified models
  - MLOps over the cloud

- **Approaches**
  - Supporting Kubernetes/Jupyter lab for development purpose
    - Create Kubernetes/Jupyter lab environment with user specified ML packages ready.
    - Support on-demand scalable CPU/GPU computing power.
  - Supporting containerized environment (e.g, Docker image) for deployment purpose
    - Create takeout images in Docker format as an option for user who wants to train/predict model
    - Docker images could be downloaded from ASGC server and deployed on users' Docker Desktop on Windows/Linux.

Capacity Building

User Community

Simulation, analysis and transformation for scientific discovery & innovation
Access to required computational service and resource
Integration of data/experiment facility with computing facility

Research Infrastructure

Scalability & Elasticity
System Efficiency
Federation of Distributed resources
Access Federation

Application & Platform Service

SaaS, PaaS, IaaS
Analysis Facility
AI-enabled computing
Workflow integration
Extended beyond domain boundary

Reliability & Efficiency
Trust
Optimization & Sustainability

Enhancing User Community Engagement

- **Discipline-oriented or user community-oriented collaboration is essential**
- **Training, dissemination and outreach**
- **Improving communication and response**
- **Supporting user access and application efficiency**
- **Understanding user requirements and experiences**
- **Facilitating capacity building of users and NSTCCore**
- **Training and workshop/conference: 250+ participants in 2025**
- **Weekly user meeting: 2:30pm, Wednesday**

Basic	• 30min – full day • Get access, details of using compute, data and SaaS services, w/o hands-on, User Forum
Thematic	• 1 hrs – full day • Discipline-based Data analysis • ICT topics: GPU Computing, AI, CPU Trends
Domain-Specific Workshop	• 30min – 3hrs • Supporting hands-on, w/o ASGC service introduction
Conference	• e-Science, community-specific workshop, core technology • ISGC (International Symposium on Grids & Clouds, since 2002) • HEPiX, CHEP (Computing in High Energy Physics) • APAN (Asia Pacific Advanced Network)

Training, Dissemination, and Outreach
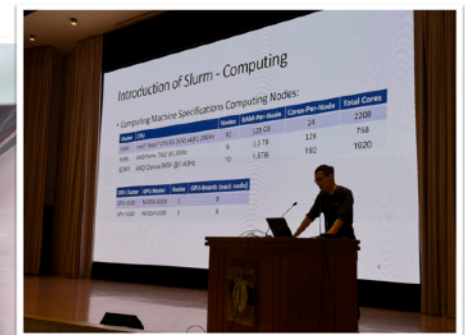
International Symposium on Grids & Clouds (ISGC, annually since 2002)

Access to NSTCCore Services

- **Two-Factor Authentication enabled from January 2025**
- **Free $200 Credits for 1-month Trial**
- **Free 3TB shared disk storage per group, and 100GB per user**

- **Group Resource Usage and Payment Management**
- **Member accounts management support**
  - **Members list**
  - **Abnormal member usage report**
  - **Member's usage review**

PI

Users

Fill Group Application Form → DiCOS Admin Approved → Notify PI when Group Setup Done

Fill in Application Form → Confirm E-mail Address → Wait for Group PI Approve → Start to use DiCOS Service

Group Account

PI's User Account

User Account

User Account

1. Register under your PI's Group
2. **Your PI's approval**

- Group Accounts
  - https://canew.twgrid.org/ApplyAccount/groupcreate.php

- User Accounts
  - https://canew.twgrid.org/ApplyAccount/ApplyAccount.php
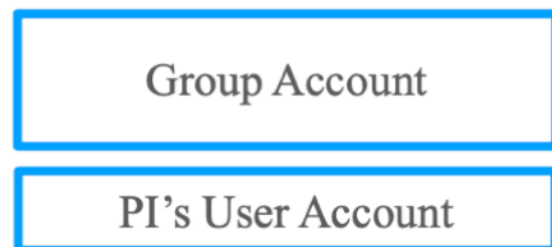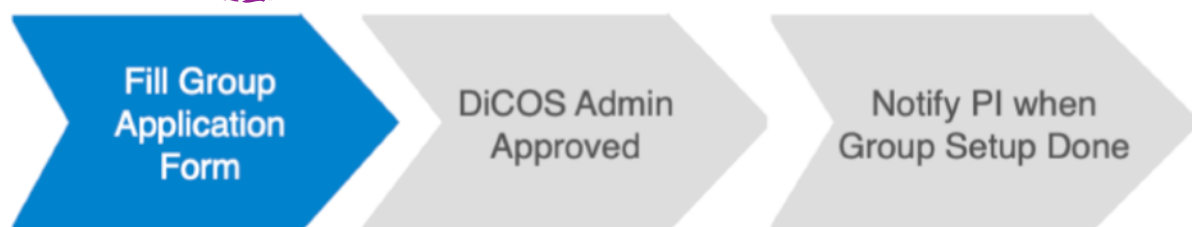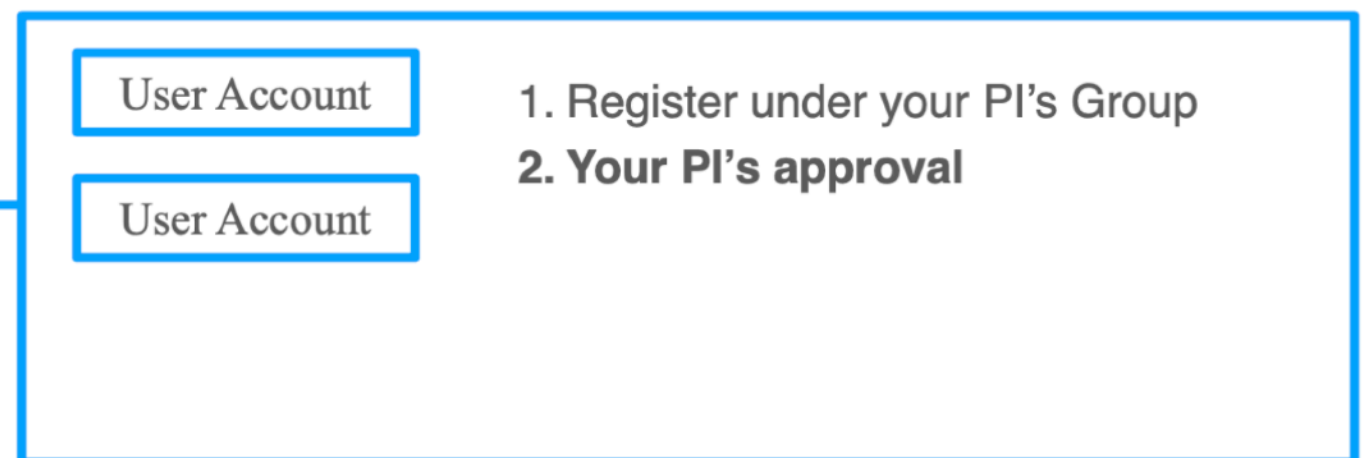
Group Management

- **Members management**
  - **Members list**
  - **Abnormal member usage report**
  - **Member's usage review**

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	Dec. 08, 2023, 00:00 AM	True	Apr. 23, 2013, 00:00 AM	Jul. 24, 2023, 03:22 AM	0.0G/100G Latest Update: 2023-07-31 00:50:03
etomo	etomo etomo	etomo@twgrid.org	Aug. 09, 2025, 00:00 AM	True	Dec. 23, 2020, 09:19 AM	Jan. 22, 2021, 10:16 AM	0.0G/100G Latest Update: 2023-07-31 00:50:03
felixlee	Felix Lee	felix@twgrid.org	Oct. 24, 2023, 00:00 AM	True	Mar. 05, 2013, 00:00 AM	Jul. 27, 2023, 07:29 AM	436.3G/100G Latest Update: 2023-07-31 00:50:03

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)										

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
總計	單價SRU=NT$2	183	7,756	(183+7,756)*2=15,878

- 儲存資源使用統計(STORAGE USAGE OF GROUP) − 預估使用費(INITIAL COST): NT $417

帳號(ID)	名稱(name)	儲存空間用量(storage(TB))	預估費用(Initial Cost Estimation)	說明(note)
ASGC	Group	0.0	0.0	Group使用空間
chiong	CHAN-HIN IONG	0.0	0.0	User使用空間
jyou	Jingya You	0.0	0.0	User使用空間
rudy	陳侑廷	0.0	0.0	User使用空間
thwu	Tsung-Hsun Wu	4.9	408.3	User使用空間

NCHC Collaboration

- **Collaboration Model**
  - **Workload distribution Principle: large-scale vs high-throughput**
  - **Quarterly meeting for milestones**
- **Starting from**
  - **Federated IdM - easy access to both sites using the same account (better to be user's home institute SSO account)**
  - **Home directory and data consistency**
  - **Faster access to required services and finish processing efficiently**
- **Challenge**
  - **Security governance - requirements and policy**
  - **Unique UID for each user**
  - **Data & storage consistency**
  - **Compatible Software and environment**
  - **Services**

Addressing Challenges for Sustainability

- **Target: growing Users x Service x Resource, with reliability and efficiency**
- **Maximize the effectiveness of budget from AS and NSTC**
- **Short of advanced GPU resource: budget, scientific computing support are key issues**
- **Data Center reliability**
  - **Power system upgrade**
  - **Energy efficiency**
  - **Upgrade for higher power consumption & liquid-cooling computing hardware in the near future**
  - **Deployment & R/D on Intelligent monitoring & control**
- **High and increasing electricity cost**
- **Improving system efficiency**
  - **Improving users' experience, utilization, and reducing the waiting time**
- **HR & Capacity building: enhancing professional skills according to user needs and ICT progress**
  - **Have to catch up/support evolving needs of scientific computing and AI applications**
  - **Hard to have backup HR for key technologies**
  - **User support needs more investment**
  - **Uncompetitive ecosystem**
- **Pricing strategy**
  - **Baseline: covering power consumption (including data center operation)**
  - **Will rely mainly on data services and advanced services**
  - **Expect NSTC to approve 使用費留用**

NSTCCore Services 聯絡資訊

- **Core Facility Services**
  - **https://nstccore.twgrid.org**
  - **https://scale.grid.sinica.edu.tw/index.php**
- **ASGC Web Site: https://www.twgrid.org**
- **Access to ASGC Resources**
  - **https://dicos.grid.sinica.edu.tw/**
- **Contact point: DiCOS-Support@twgrid.org**

- **Gentle Reminder**
  - **Please include ASGC (Academia Sinica Grid-computing Center) in the acknowledgement when research outcomes that relied on ASGC resources, services or expertise are presented in your research.**

Unit Cost of Electricity Is 15.8% Higher in 2025

- **Electricity unit cost in 2025 (monthly average) is 4.01/kWh, which is 48.2% higher comparing to 2022**
- **Both facility and cooling power usage decrease by > 20% in 2023 and 2024**
- **The power usage in 2025 keeps having 2.7% drop**
- **PUE (2025) is 1.58, which maintains the same level as in 2024 (1.56)**