



**NSTC** 國家科學及技術委員會  
National Science and Technology Council



# 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. 7

# Program Today

**2:00 PM** → 2:20 PM 一、NSTCCore 計劃簡介 NSTCCore Project Overview

Convener: Prof. Song-Ming Wang


**2:20 PM** → 2:40 PM 二、NSTCCore 服務與合作 NSTCCore Services and Collaboration

Convener: Prof. Eric Yen (ASGC)

**2:40 PM** → 3:10 PM 三、SLURM 計算服務 SLURM Computing Service

- SLURM 執行工作操作
- SLURM 參數介紹
- 多核心程式編程及操作 Multi-Core Jobs

Convener: Ms Yi-Ru Chen (ASGC)


 Introduction on Slur...

**3:10 PM** → 3:30 PM Break

**3:30 PM** → 4:00 PM 四、虛擬化SaaS雲端計算服務 - DiCOSApp Virtualized SaaS Cloud Computing Service – DiCOSApp

- 計算資源
- 服務架構
- 軟體部署

Convener: Ms Ming-Jyuan Yang (ASGC)

 DiCOSApps.pdf

**4:00 PM** → 4:30 PM 五、資料服務 Data Service

- 資料傳輸
- 資料操作

Convener: Ms Ming-Jyuan Yang (ASGC)

 Storage & Data Tran...

**4:30 PM** → 5:00 PM 六、使用者經驗分享 & 綜合討論 User Experience Sharing & Discussion

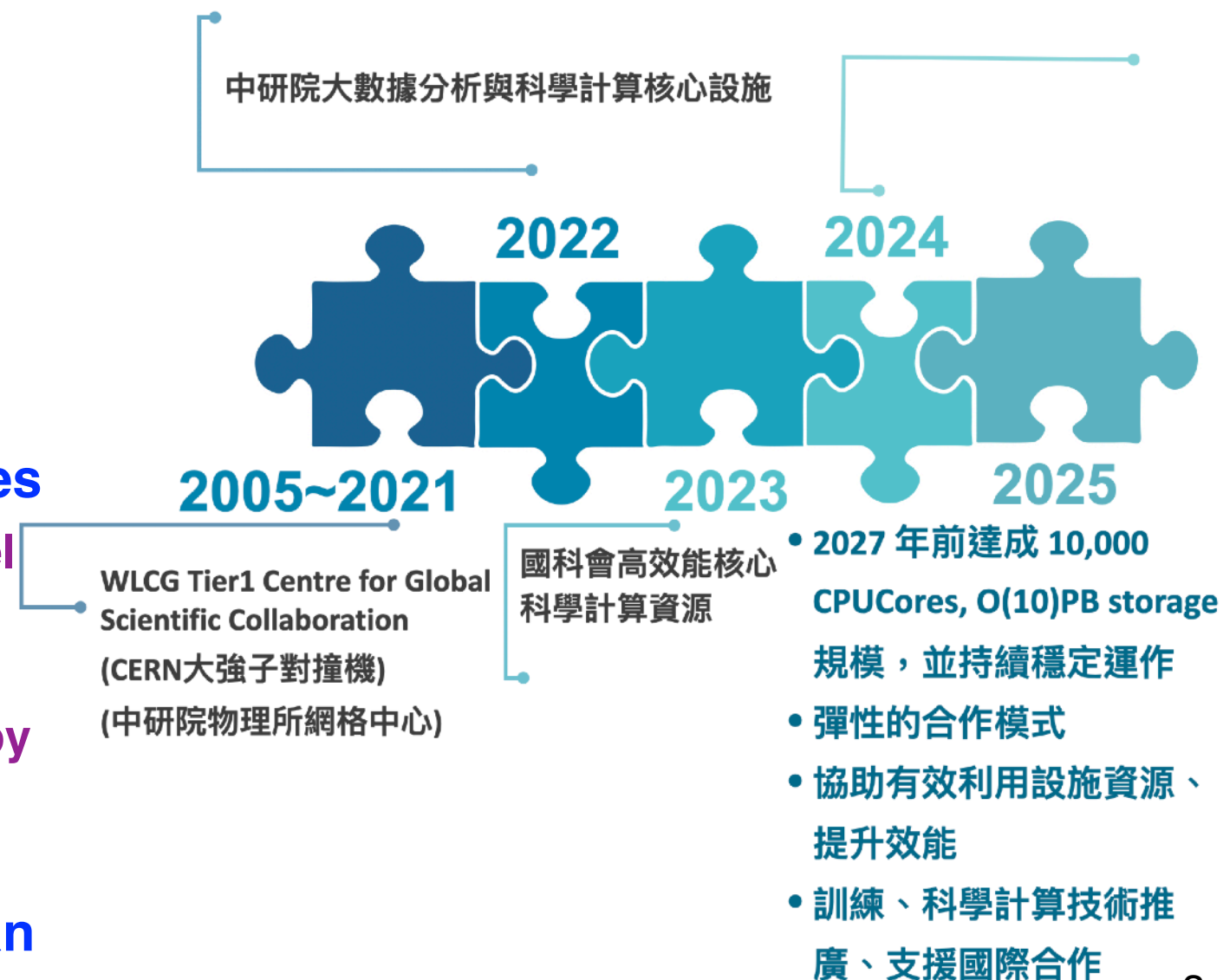
Convener: Mr Felix Lee (ASGC)

 HTcondor\_tut Screenshot

# Mid-Scale Scientific Computing Services for Accelerating Discovery & Innovation

- **Funded by NSTC, June 2023 - May 2026**
  - In association with the core facility supported by Academia Sinica
- **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) CPU Cores, O(100) GPUs and O(10)PB Disk storage resources**
  - **Able to support O(1,000) CPU Cores 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**

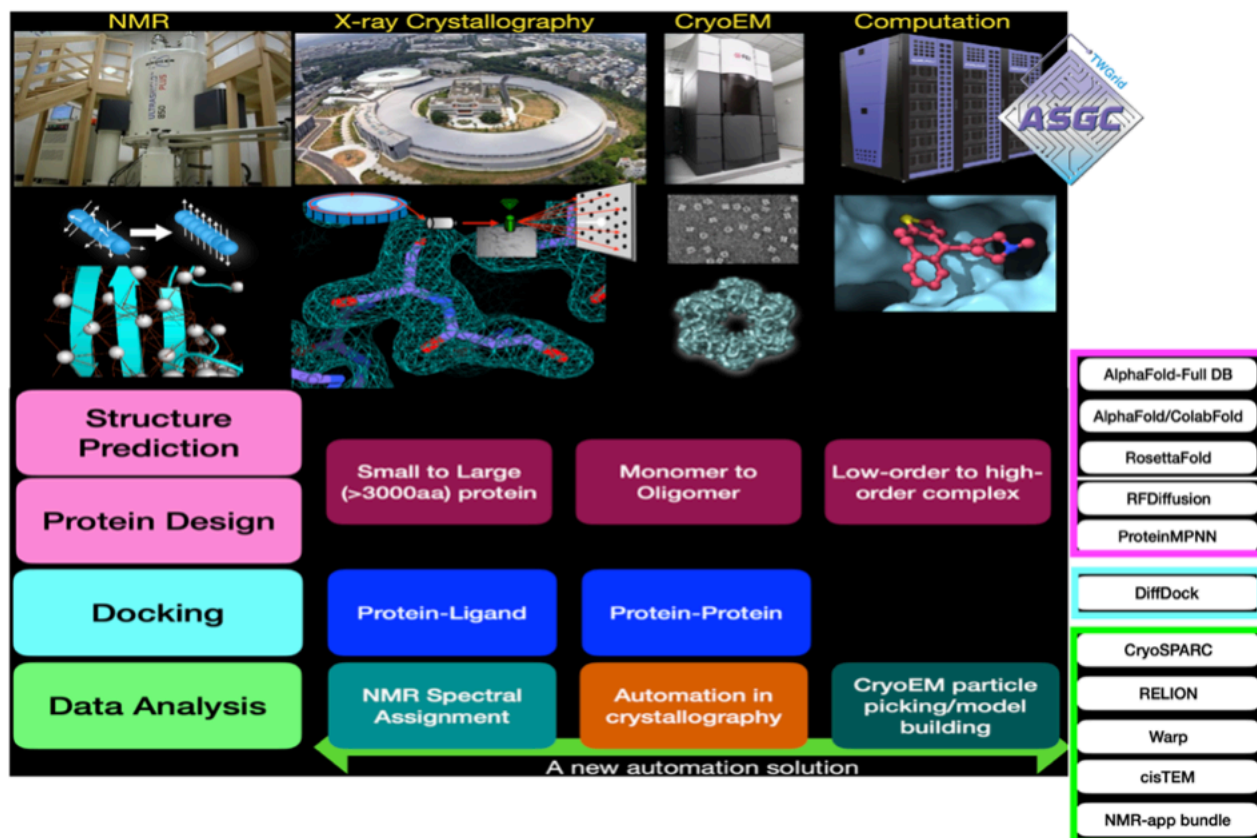
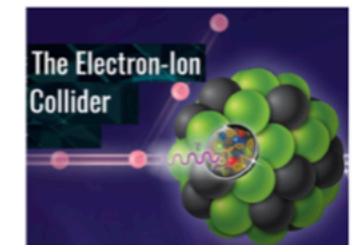
## User-Oriented Services 24x7x365



# 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

CryoEM

Quantum Materials  
Physics

Bioimaging

Physics of Active & Living Matter

Drug Discovery

Astrophysics

Computational Chemistry

Earth Science

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

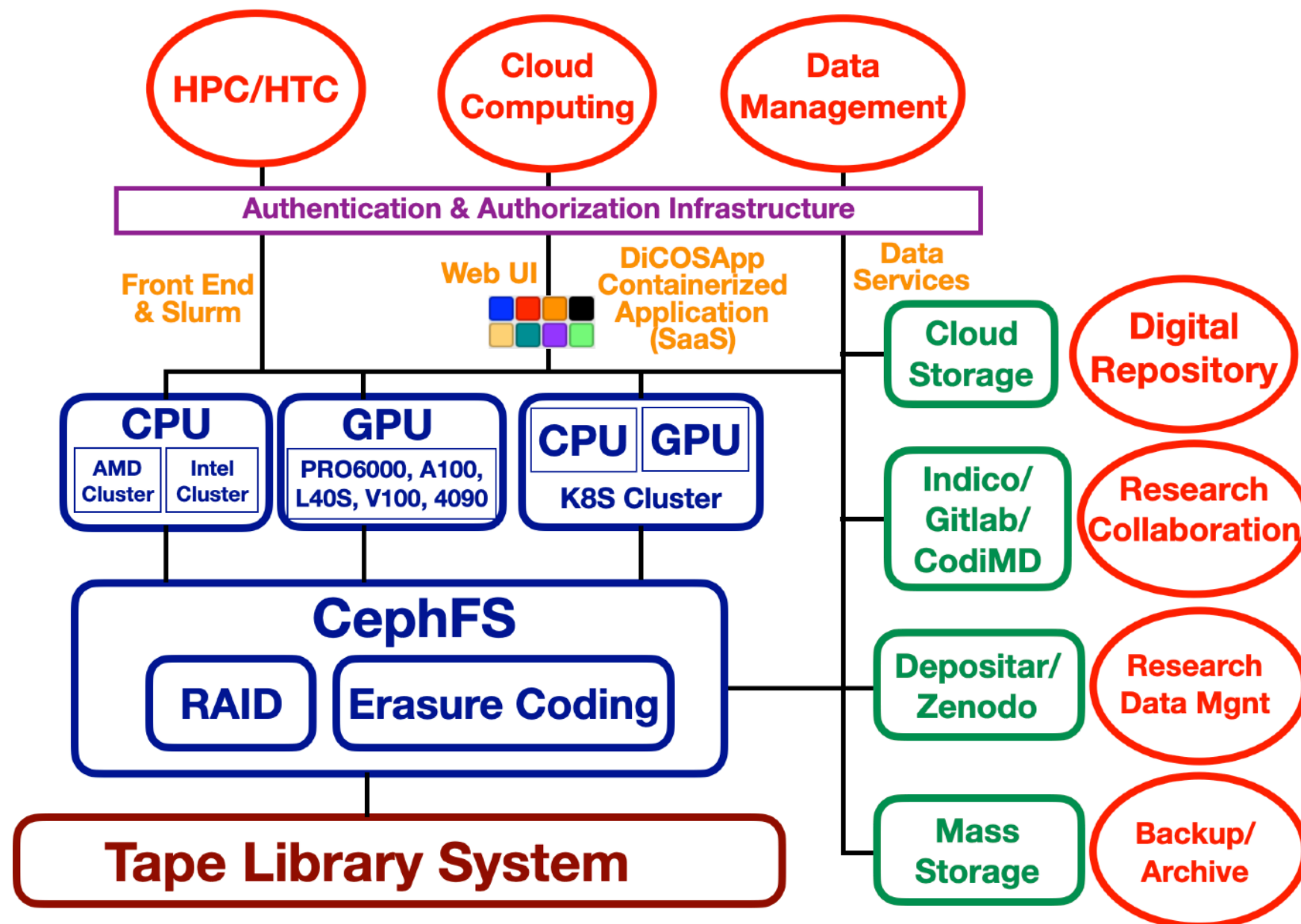
Storage	Capacity (TB)	System	Price	Remarks
Ceph File System	12,000	Online storage managed by Ceph distributed file system, with (8, 3) erasure coding	1,000 per TB-year	+3PB by end of Feb 2026
Tape Lib System	10,000	LTO9 (18TB/Tape)	300 per TB-year	Service from 2025

# 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

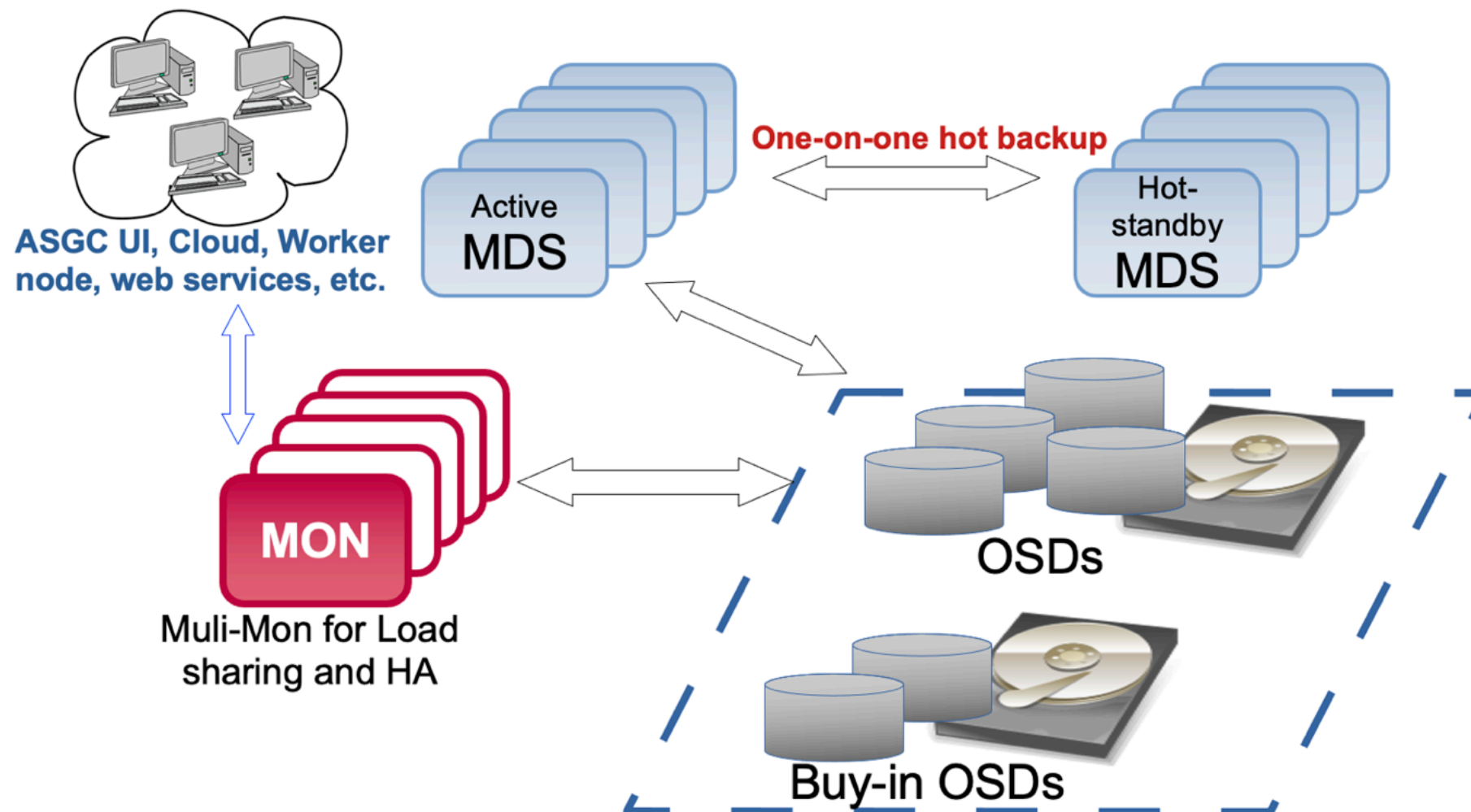
# ASGC Service Architecture - Scalable Science Cloud

- 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



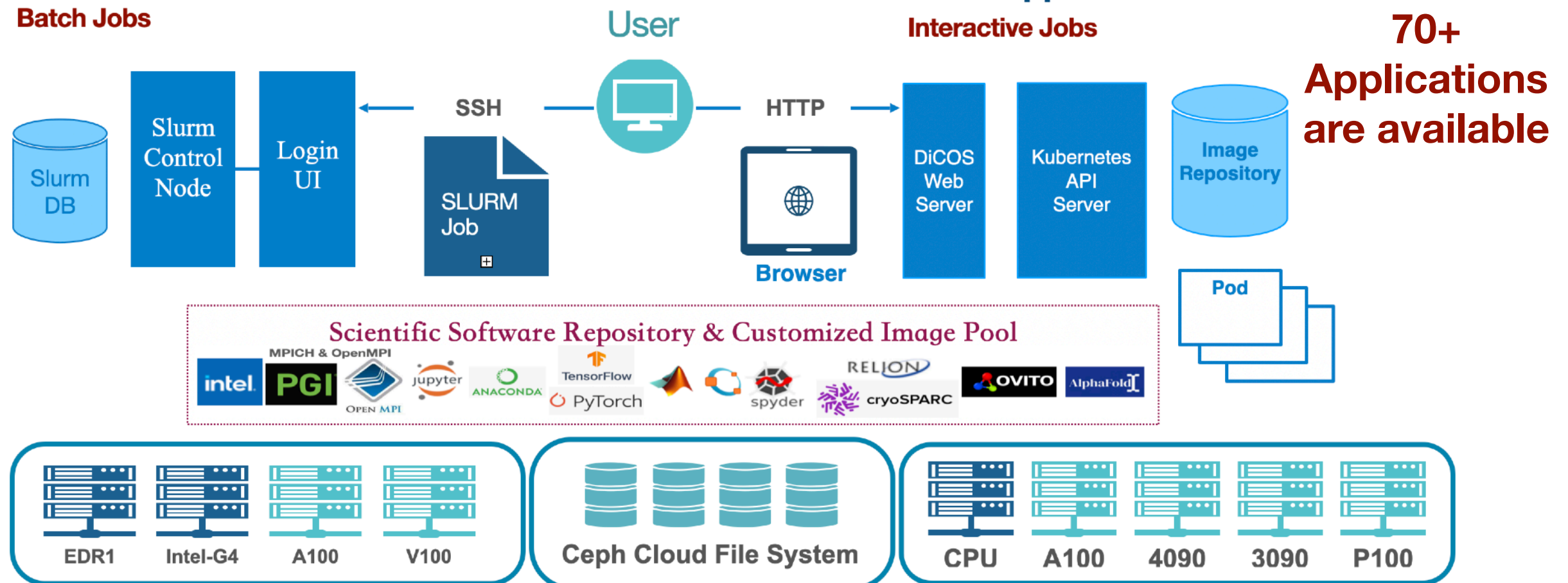


# Computing Services: Optimization of Application and System Efficiency


































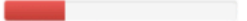

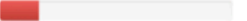

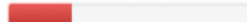

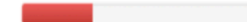

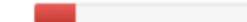





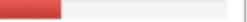













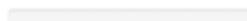











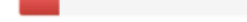
















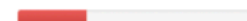




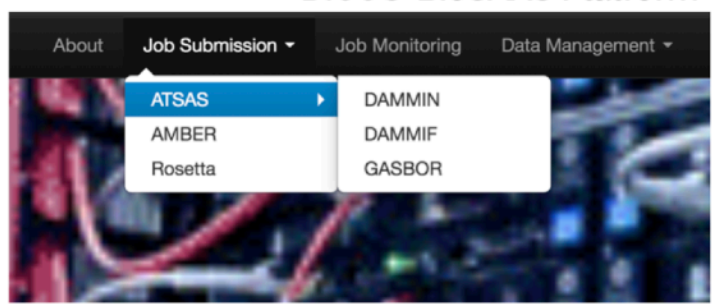
- HTC/HPC & Cloud Computing Platform
- Integration of computing model and software
- Research data workflow and management
- Information security
- Application efficiency
- Customized IaaS, PaaS, and SaaS

**HPC platform**  
**Slurm System Architecture**  
**Batch Jobs**

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



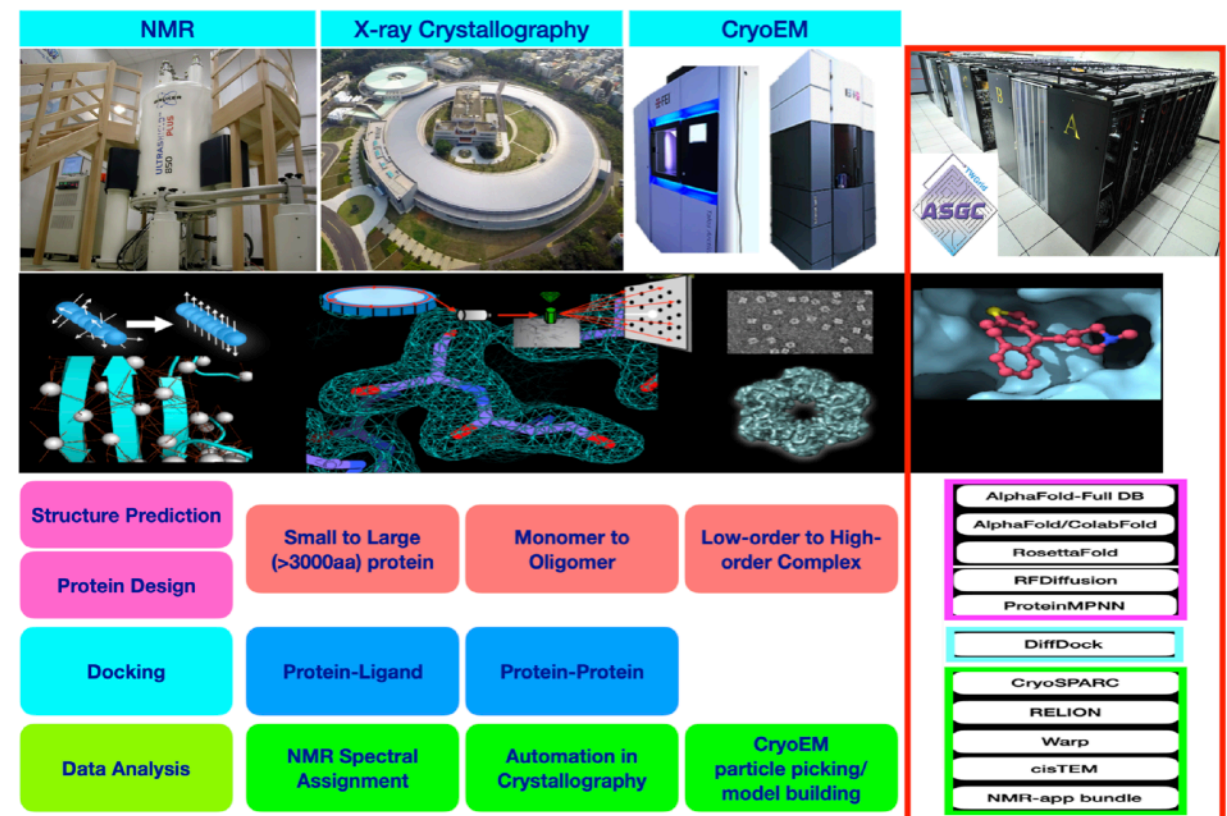
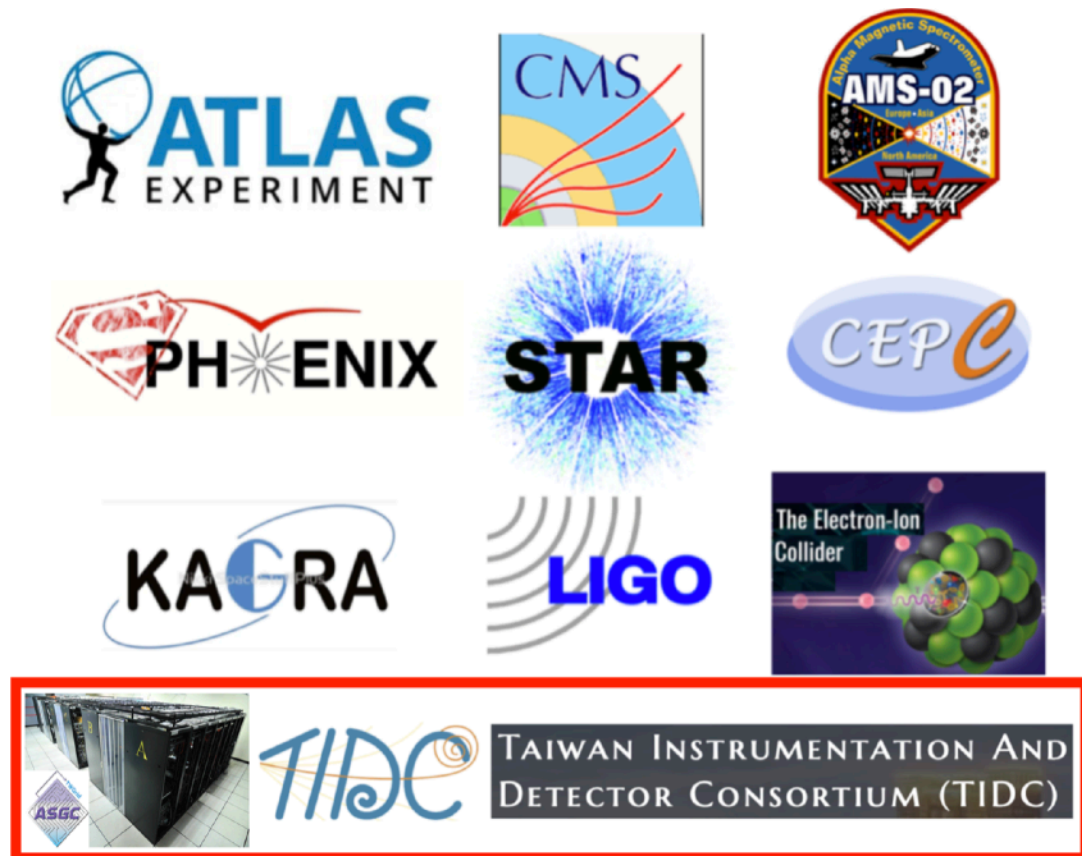
# 73+ Web Applications Provided (Software-As-a-Service)

 <b>CryoSPARC 32 P100</b> Version: 3.2 Resources: 83%  <a href="#">Launch</a>	 <b>CryoSPARC 1080ti</b> Version: 3.3.2 Resources: 29%  <a href="#">Launch</a>	 <b>CryoSPARC RTX3090</b> Version: 3.3.2 Resources: 26%  <a href="#">Launch</a>	 <b>spyder cpu/eman2</b> Version: Resources: 17%  <a href="#">Launch</a>	 <b>Octave</b> Version: V5.2 Resources: 29%  <a href="#">Launch</a>	 <b>Transfer Data</b> Version: Resources: 86%  <a href="#">Launch</a>
 <b>CryoSPARC RTX3090</b> Version: 4.0.2 Resources: 26%  <a href="#">Launch</a>	 <b>CryoSPARC RTX3090</b> Version: 4.1.1 Resources: 26%  <a href="#">Launch</a>	 <b>CryoSPARC RTX3090</b> Version: 4.4.1 Resources: 26%  <a href="#">Launch</a>	 <b>cisTEM</b> Version: Resources: 86%  <a href="#">Launch</a>	 <b>Ovito</b> Version: Resources: 86%  <a href="#">Launch</a>	 <b>OpenACC</b> Version: GPU P100 Resources: 83%  <a href="#">Launch</a>
 <b>AlphaFold</b> Version: GPU with A100 Resources: 75%  <a href="#">Launch</a>	 <b>AlphaFold (Full DB)</b> Version: GPU with A100 Resources: 75%  <a href="#">Launch</a>	 <b>IMOD</b> Version: GPU with 1080ti Resources: 29%  <a href="#">Launch</a>	 <b>Triton</b> Version: 22.01-py3 (GPU P100) Resources: 83%  <a href="#">Launch</a>	 <b>AlphaFold</b> Version: GPU with RTX3090 Resources: 26%  <a href="#">Launch</a>	 <b>AlphaFold</b> Version: GPU with V100 Resources: 17%  <a href="#">Launch</a>
 <b>RoseTTAFold</b> Version: GPU with rtx3090 Resources: 26%  <a href="#">Launch</a>	 <b>Dynamo</b> Version: GPU with 1080ti Resources: 29%  <a href="#">Launch</a>	 <b>MATLAB</b> Version: R2018b on GPU V00 Resources: 17%  <a href="#">Launch</a>	 <b>Jupyter Lab</b> Version: CPU with Tensorflow v1 Resources: 86%  <a href="#">Launch</a>	 <b>Jupyter Lab gpu 3090</b> Version: GPU with Tensorflow 3090 Resources: 26%  <a href="#">Launch</a>	 <b>Jupyter Lab GPU 1080ti</b> Version: GPU with Tensorflow v2 Resources: 29%  <a href="#">Launch</a>
 <b>RFDIFFUSION</b> Version: 2023 on GPU V00 Resources: 17%  <a href="#">Launch</a>	 <b>diffdock</b> Version: 2023 on GPU V00 Resources: 17%  <a href="#">Launch</a>	 <b>EvoDiff</b> Version: V100 Resources: 17%  <a href="#">Launch</a>	 <b>Jupyter Lab GPU V100</b> Version: GPU with Tensorflow V100 Resources: 17%  <a href="#">Launch</a>	 <b>Jupyter Lab GPU A100</b> Version: GPU with Tensorflow A100 Resources: 75%  <a href="#">Launch</a>	 <b>Jupyter Lab Cryocare GPU</b> Version: GPU with 1080ti Resources: 29%  <a href="#">Launch</a>
 <b>QIIME2</b> Version: Genome Resources: %  <a href="#">Launch</a>	 <b>Scipion3</b> Version: P100 Resources: 83%  <a href="#">Launch</a>	 <b>Phenix</b> Version: Resources: 86%  <a href="#">Launch</a>	 <b>Jupyter Lab GPU A100</b> Version: GPU with Tensorflow v2.6 Resources: 75%  <a href="#">Launch</a>	<ul style="list-style-type: none"><li>• Web Portal</li><li>• Application over Cloud</li><li>• Jupyterlab</li><li>• Web Terminal</li></ul>	
 <b>MorphoGraphX</b> Version: GPU with P100 Resources: 83%  <a href="#">Launch</a>	 <b>DeepMD-kit</b> Version: GPU with A100 Resources: 75%  <a href="#">Launch</a>	 <b>DeepMD-kit</b> Version: GPU with V100 Resources: 17%  <a href="#">Launch</a>	 <b>MAML</b> Version: GPU with A100 Resources: 75%  <a href="#">Launch</a>	 <b>LabVIEW Run-Time Engine</b> Version: 2019  <a href="#">Launch</a>	
 <b>Warp</b> Version: rtx4090 Resources: 700%  <a href="#">Launch</a>	 <b>MAML</b> Version: GPU with V100 Resources: 17%  <a href="#">Launch</a>	 <b>PVserver</b> Version: 5.8.0 (GPU 1080Ti) Resources: 29%  <a href="#">Launch</a>	 <b>Paraview Client</b> Version: 5.8.0 Resources: 86%  <a href="#">Launch</a>		
 <b>R studio</b> Version: 10 CPU Cores Resources: 54%  <a href="#">Launch</a>	 <b>PyRoot</b> Version: GPU with 1080ti Resources: 29%  <a href="#">Launch</a>	 <b>qiskit</b> Version: Resources: 86%  <a href="#">Launch</a>	 <b>NVIDIA CUDA-Quantum A100</b> Version: Resources: 100%  <a href="#">Launch</a>	 <p>DiCOS-BioSAXS Platform</p> <p>About Job Submission Job Monitoring Data Management</p> <p>ATSAS AMBER Rosetta DAMMIN DAMMIF GASBOR</p>	

# Flexible Collaboration Model: User-Driven, Service Oriented

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

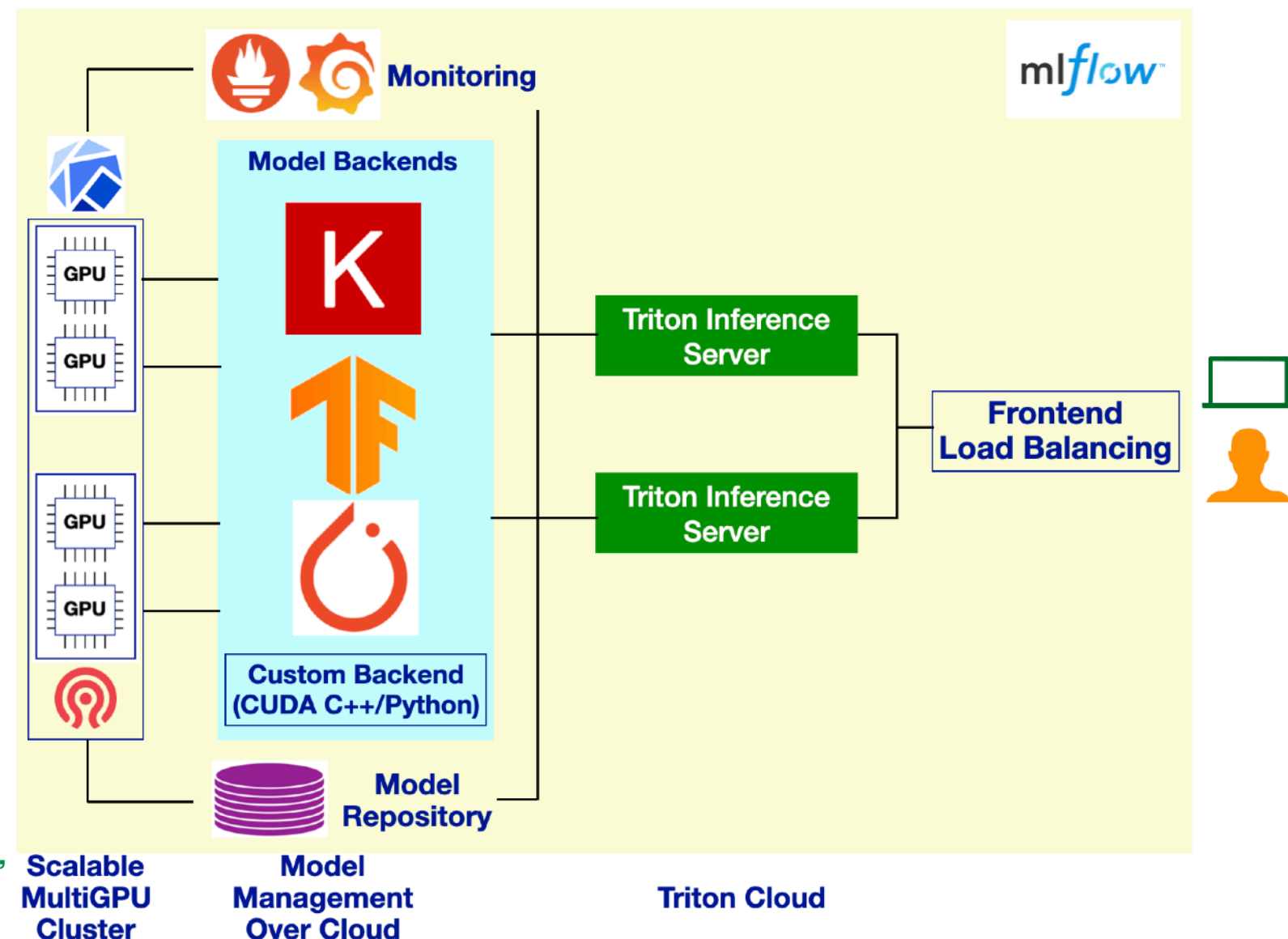
- Advanced Service: Web Application and portal, efficiency tuning, workflow optimization, customization, hands-on training
- User Engagement : weekly User Meeting, User Committee, dissemination & outreach



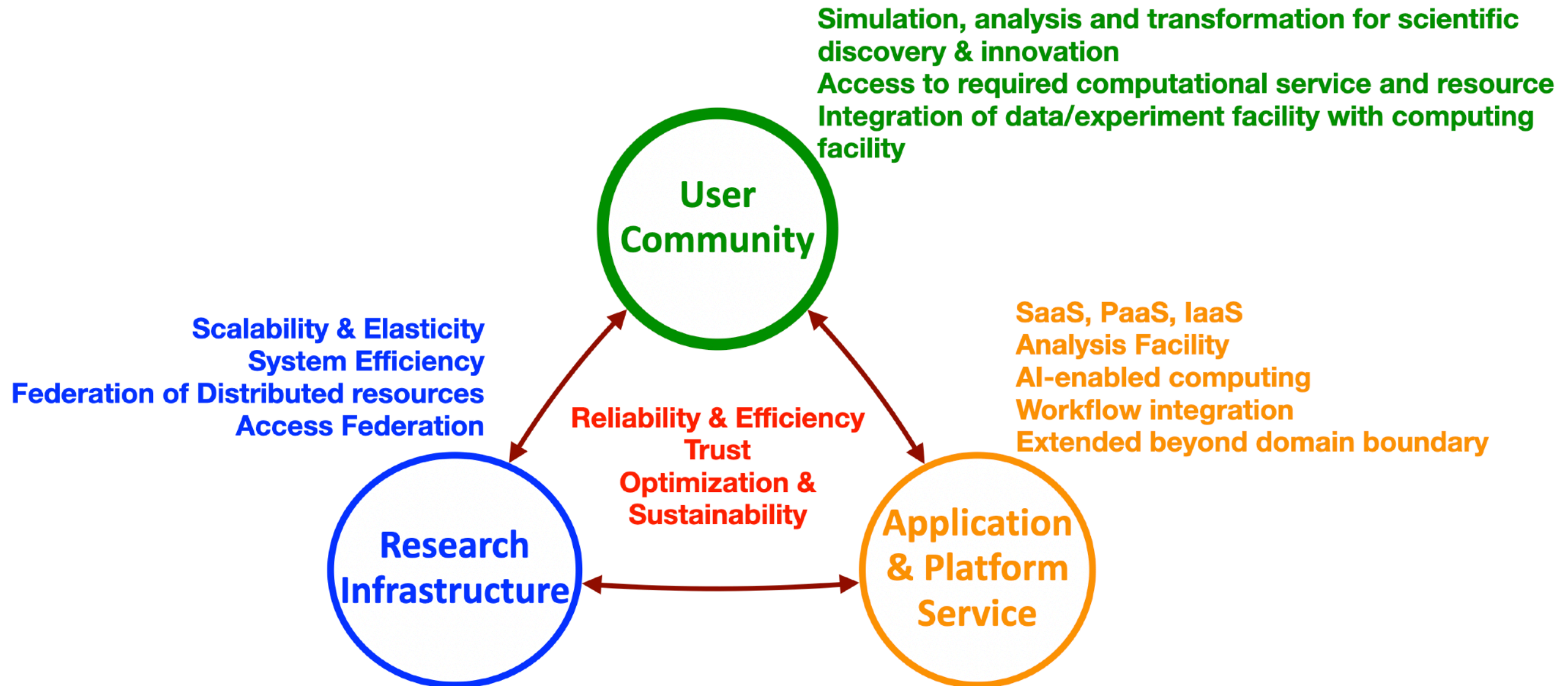


# Services of ML-Enabled Data Analytics

- **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 ML packages ready environment 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





# Enhancing User Community Engagement

- 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

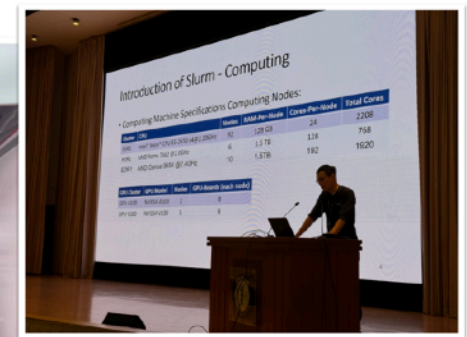
## Domain-Specific Workshop

- 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



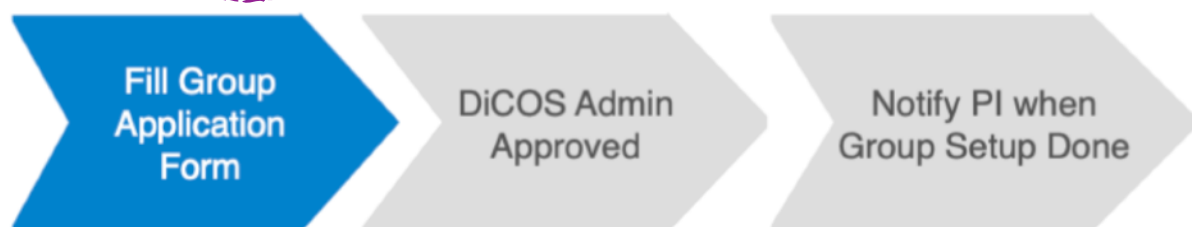
International Symposium on Grids & Clouds (ISGC, annually since 2002)



# Access to NSTCCore Services

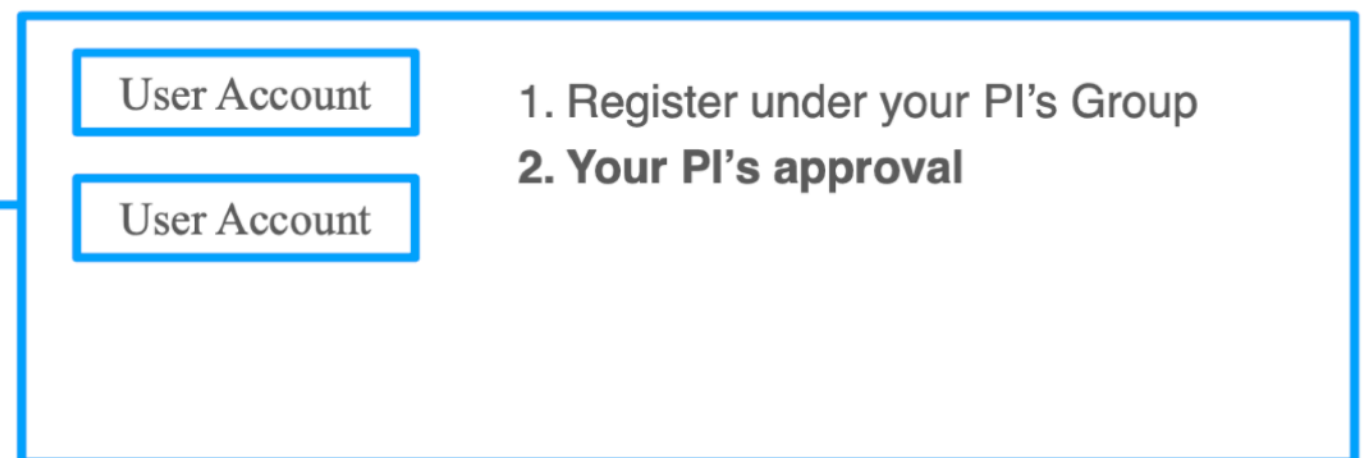
- Two-Factor Authentication enabled from January 2025
- Free \$200 Credits for 1-month Trial
- Free 3TB shared disk storage per group, and 100GB per user

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



## • 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)											

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	Dec. 08, 2023, 00:00 AM	True	Apr. 23, 2013, 00:00 AM	Jul. 24, 2023, 03:22 AM	0.0G/100G <small>Latest Update: 2023-07-31 00:50:03</small>
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 <small>Latest Update: 2023-07-31 00:50:03</small>
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 <small>Latest Update: 2023-07-31 00:50:03</small>

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

# 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](mailto: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.