User Committee Meeting
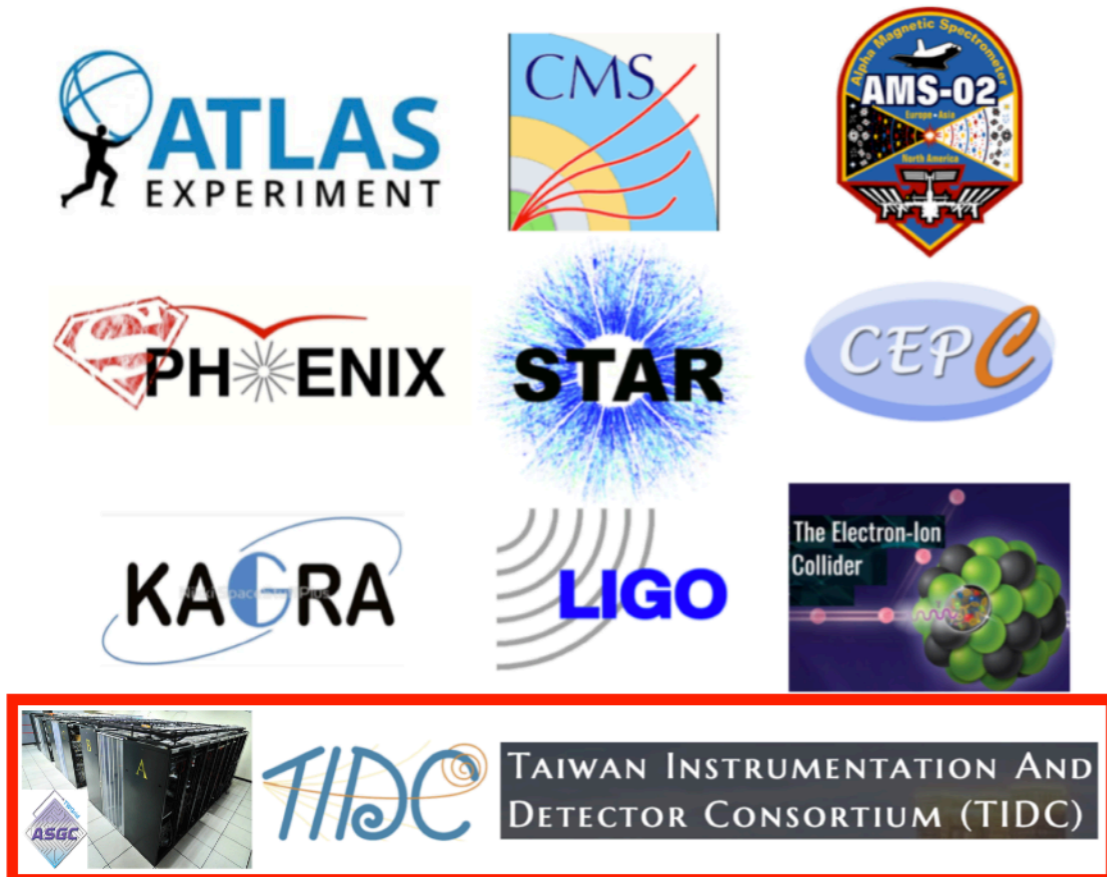
https://indico4.twgrid.org/event/62/

Eric Yen

**Academia Sinica Grid Computing Centre (ASGC)
Taiwan**

08 Jan. 2025

ASGC - Accelerating Discovery & Innovation Your Computational Research Partner

- **WLCG Tier Centre - building capacity by participating the development & deployment of the world largest and advanced distributed cloud research infrastructure**
  - **WLCG is moving towards O(1000)PB scale in RUN4**
- **Core Facility - computing arms of HEP experiment, research facility and research communities, based on WLCG core technologies**
 - **Also part of the research infrastructure**

Achievement (I)

- **Sustained growth of users, utilization, reliability and satisfaction in 2024**
    - **174 PI Groups, 595 users from 25 Institutes in Taiwan**
    - **Finished 4.94M CPU jobs, and 52.8K GPU Jobs, with 99%+ reliability**
    - **26+ supported research publications**
    - **Demands of advanced GPU keeps growing in 2024 - 20% utilization growth in high usage situation**
    - **CPU usage has increase of 333% in 2024**
- **Gaining trust of users/ building collaboration with user communities**
    - **Customized services: just like tailored-made services in the cloud/ serving as the computing arm**
- **Onboarding new hardware and retiring legacy ones for power saving and performance improvements: 5,760 CPUCores, 210 GPUBoards, 12PB Disk, 4PB Tape**
    - **New procured HW (1,920 + 256 CPUCores, 2.5PB Disk Storage) had been available on 20 Dec 2024**
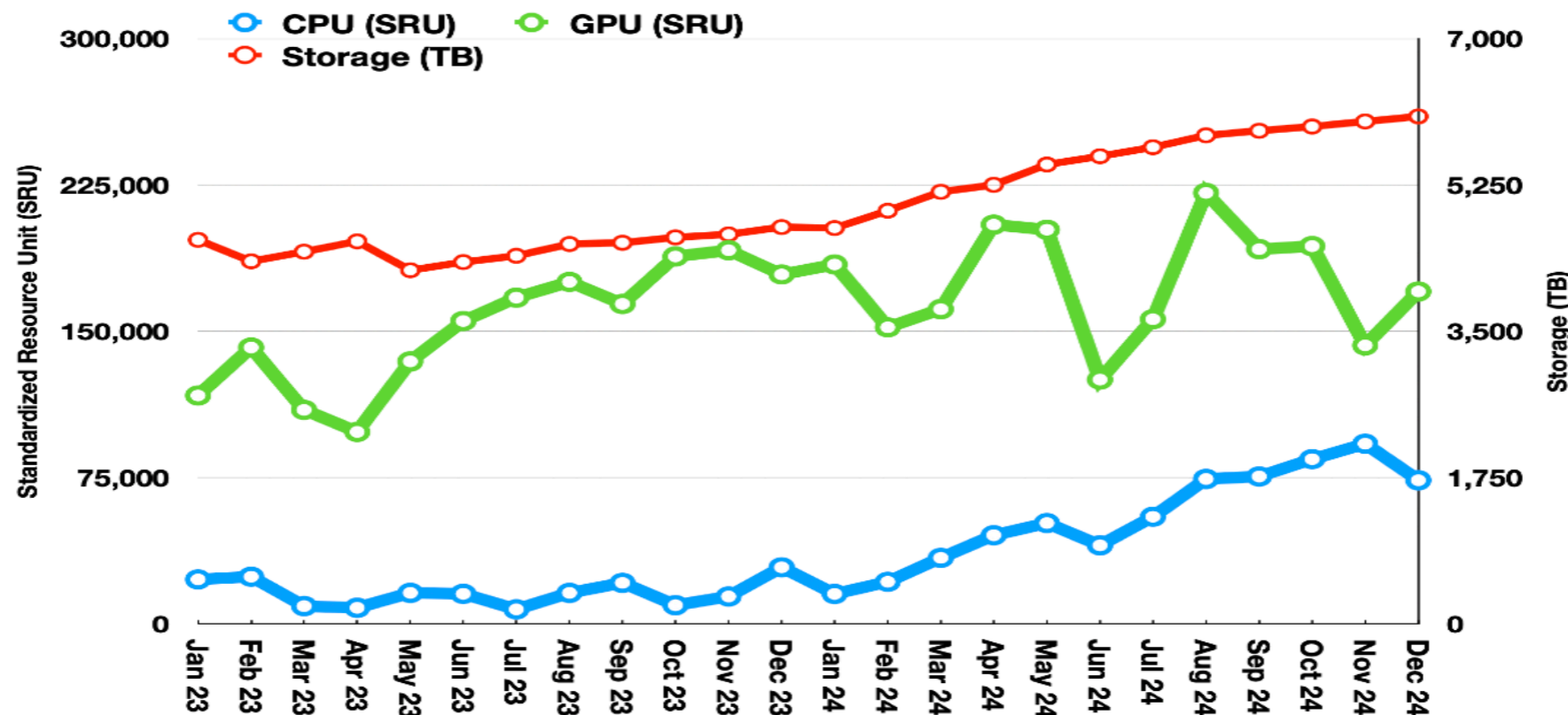
Achievement (II)

- **Persistent capacity building**
  - **Improved research application efficiency, service accessibility, resource utilization, system efficiency, etc.**
  - **Training: 300+ participants**
    - **4x training a year (basic + thematic, with hands-on)**
    - **Hands-on training support for IBMS, NPAS and Telescope Array ML Workshop**
    - **Thematic/ community-oriented training on-demand: e.g, AI applications, HEP data analysis**
  - **Core technology and international collaboration: annual ISGC event (~100 participants, 5-day event)**
  - **Attending 15th Thematic CERN School of Computing on Machine Learning 2024 in Croatia (supported by AS)**
- **Efficiency (& power saving): Power consumption reduced 20% in two years straight from 2023**
- **OS Migration from CentOS7 to AlmaLinux9: All online resource are AL9 from 1 Jan 2025**
- **Security: ISO27001, annual audit by AS (ITS), Vulnerability test**
- **Customized Services and Collaborations: NMR Cloud data analysis, AlphaFold/RosettaFold,**
- **New Services from Jan 2025: 2-factor authentication, Password renew schedule, DiCOSApps, Tape archival & backup**
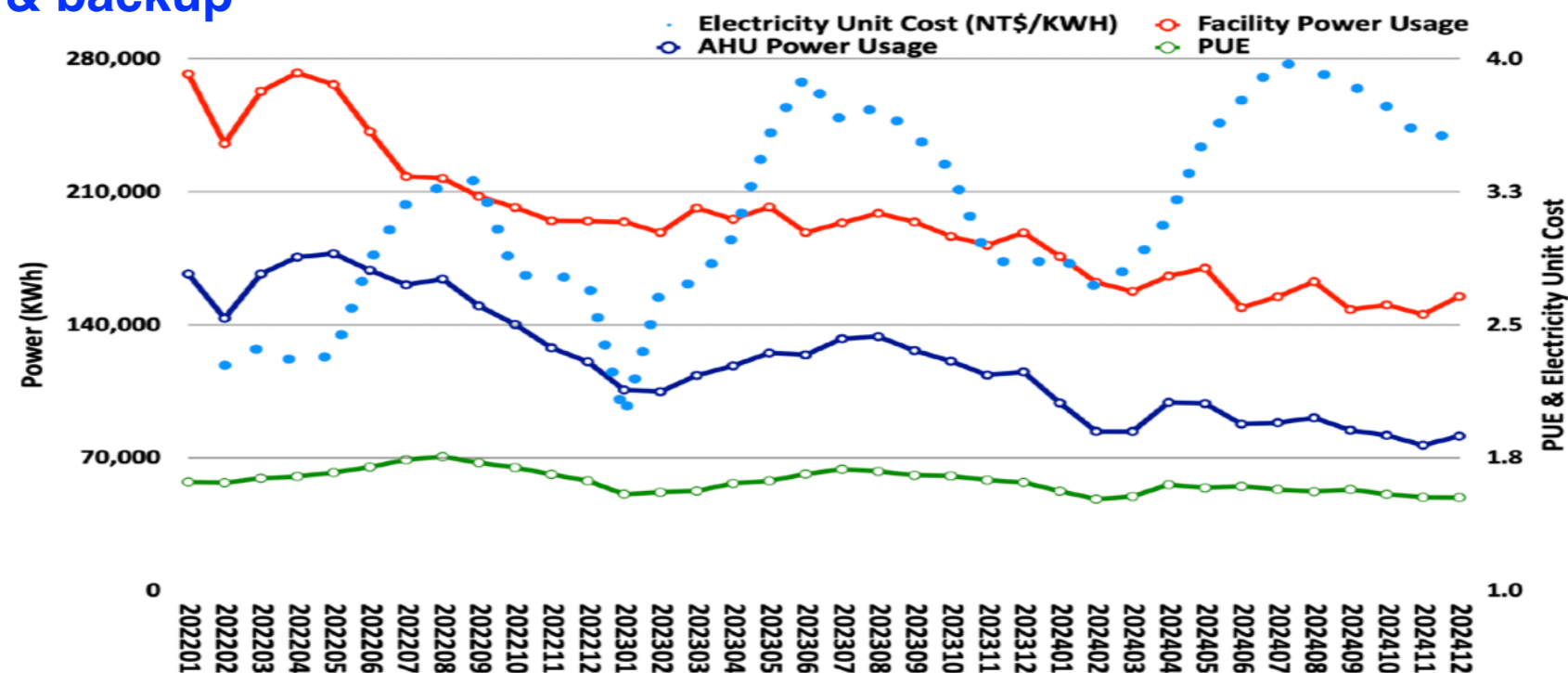
Challenges & Opportunities

- **Advance computing services and Advocate for the widespread use of computational thinking to improve researches and applications**
- **Reliability and Efficiency are the keystones**
- **Both service and capacity have to be evolved constantly with users' needs. Simply cycle provisioning is far from enough.**
- **Sustainability is the primary long-term goal**
  - **Flexible collaboration model is the key:**
    - **Support and engagement of broader user communities**
    - **Trust**
  - **Continuous development of the capacity of both users and ASGC**
    - **Advanced AI-enabled big data analysis**
    - **High-performance computing system and cloud services**
    - **DC & network infrastructure**
    - **GPU disadvantage**
  - **Advanced services**
  - **Infrastructure, computing resource and human resource have to grow with the requirements and evolutionary services**
- **User has the equal liability for Resource management**
  - **Education, criteria, and alleviation approach will be enforced by ASGC (service provider)**

Action Plans in 2025

- **Broader user community engagement**
  - **Earth science, life science, etc.**
- **Enhanced resilience & efficiency of storage system**
  - **Moving dark data to Tape: KAGRA, Soundscape, Earthquake, Satellite images, etc.**
  - **Kick off tape backup services**
- **AI-enabled big data analytics: extending from development platform and software/program integration**
- **Gaining certification of ISO27001 + ISO27017 (for Cloud Service)**
- **HW procurement and retirement plan**
  - **Another 2,176+ CPUCores (higher than AMD Genoa) and GPUs (L40S or higher-end) online**
  - **3PB+ disk and 4PB+ tape on board**
  - **1080ti retirement**
- **Capacity Building: another 4x training events, ISGC2025**
  - **GPU Computing, AI application, ASGC Core Technology (distributed Cloud, BDA, AAI, data repository), etc.**
- **Effective communication**
  - **Contact point**
  - **Responsive**
  - **Information service**
  - **Weekly user meeting**
- **Call for collaboration - flexibility and R&D oriented**
  - **AI-enabled BDA for research applications and new services**
  - **Efficiency**
  - **Security - intelligent monitoring and responses**

6

ISGC 2025

AI and Hybrid Quantum - Shaping Tomorrow's Scientific Breakthroughs

- **16-21 March 2025, Academia Sinica, Taipei, Taiwan**
- **ISGC is a collaboration platform for e-Science hosted by ASGC from 2002**

- **Keynote & Plenary Speakers**
  - **Ilkay Altintas (SDSC, US)**
  - **Daniele Bonacorsi (UniBol, IT)**
  - **Simone Campana (CERN, CH)**
  - **Michael Dowling (U. Regensburg, DE)**
  - **David Groep (NIKHEF, NL)**
  - **Danny Hsu (AS, TW)**
  - **Yeu-Hwang Hwu (AS, TW)**
  - **Dieter Kranzlmueller (LRZ, DE)**
  - **Yusuke Oda (NII, JP)**
  - **Ping Yeh (Google)**
  - **(NVIDIA)**
  - **Gergely Sipos (EGI)**

- **Workshops**
  - **17 March - Security Workshop (Nikhef, EGI-CSIRT)**
  - **18 March - Hybrid Quantum Computing Workshop (LRZ/DE, ASGC)**
  - **19 March - AI Masterclass (U. Bologna/IT)**
  - **20 - 21 March - Environmental Computing Workshop (LRZ/DE and ASGC)**
- **Asia Country Updates (AU, CN, ID, JP, TH, TW, + KR, SG, PH)**
- **Sessions (based on submitted abstracts)**
  - **AI, Physics Applications, Life Science Applications, Earth Science Applications, Humanities & Social Sciences, Infrastructure Cloud & Virtualization, Converging HPC Infrastructure, Data Management, Networking & Security**
- **https://indico4.twgrid.org/event/51/**

Hybrid Quantum Computing Workshop @ISGC2025

- **Date & Time: 9am - 5pm, 18 March**
- **Objectives: status update and get ready for the paradigm shift**
  - **Understanding the Realization of quantum advantages**
  - **Review and sharing of Requirements & experiences of quantum computing applications**
  - **Probing the development of hybrid quantum computing, hardware, software, applications and collaborations**
- **Plenary Sessions (2x Sessions in the morning)**
  - **LRZ/DE, Google, NVIDIA and Prof. Danny Hsu**
- **Talks in afternoon sessions**
  - **Quantum ML (TW), Quantum GNN for HEP data analysis (TW), QC education and promotion (EntangleTech, TW)**
  - **Open Quantum Initiative (OQI)**
  - **Discussion with computational fluid dynamics community (earth science)**
- **More contributions related with hybrid/quantum computing in ISGC**
  - **Qiskit-symb**
  - **Mass spectra prediction & analysis: ML and QC perspectives**
  - **Distributing the simulated annealing workload for quantum unfolding in HEP**
  - **Quantum error mitigation through autoencoder**
  - **Simulation of a neuromuscular control using a quantum computer**

Discussion

- **Comments from the Committee**
- **Term of this committee members: Jan 2025 - Dec 2026**
- **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.**
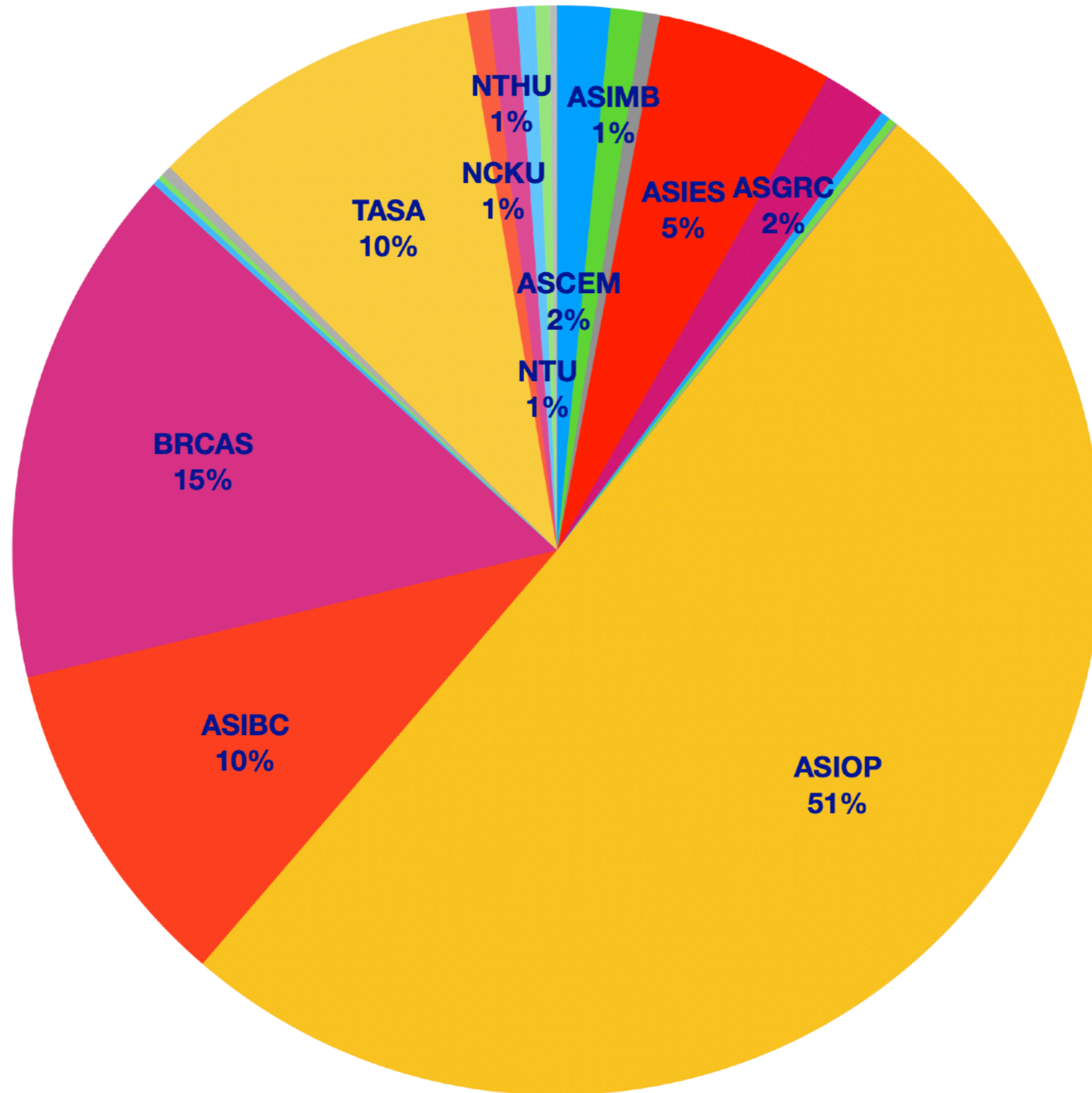
Supplementary Information

Funding Support & Primary Expenditure

	2023		2024		2025	
Funding Support	**AS-CF**	**NSTCCore (2023.6.1-)**	**AS-CF**	**NSTCCore (2024.6.1-)**	**AS-CF**	**NSTCCore (2025.6.1-)**
業務費	3,500,000	5,154,400	3,500,000	7,659,200	4,000,000	
設備費	4,850,000	19,000,000		18,127,000		
管理費		845,600		1,213,800		
Total	8,350,000	25,000,000	3,500,000	27,000,000	4,000,000	
Usage Fee	3,867,219		4,983,416			
Primary Expenditure						
Electricity	11,679,926		915,886			
HR	7,855,346		8,721,810		10,100,498	
Operation	3,000,000		3,000,000			
Facility	23,850,000		18,127,000			

Computing Resource Usage

CPU (2024)

- IBMS 3%
- NCU 2%
- IAMS 9%
- NTHU 8%
- ASICOB 4%
- ASIOP 28%
- NYCU 14%
- ASRCAS 2%
- ASIPMB 7%
- ASIAA 15%
- ASGC 4%
- CryoEM 4%

GPU (2024)

- IBMS 2%
- IIS 2%
- ASGRC 1%
- TMU 3%
- CCU 3%
- ASIOP 25%
- NYCU 12%
- ASRCAS 3%
- NTU 1%
- IBC 4%
- ASIPMB 1%
- CITI 7%
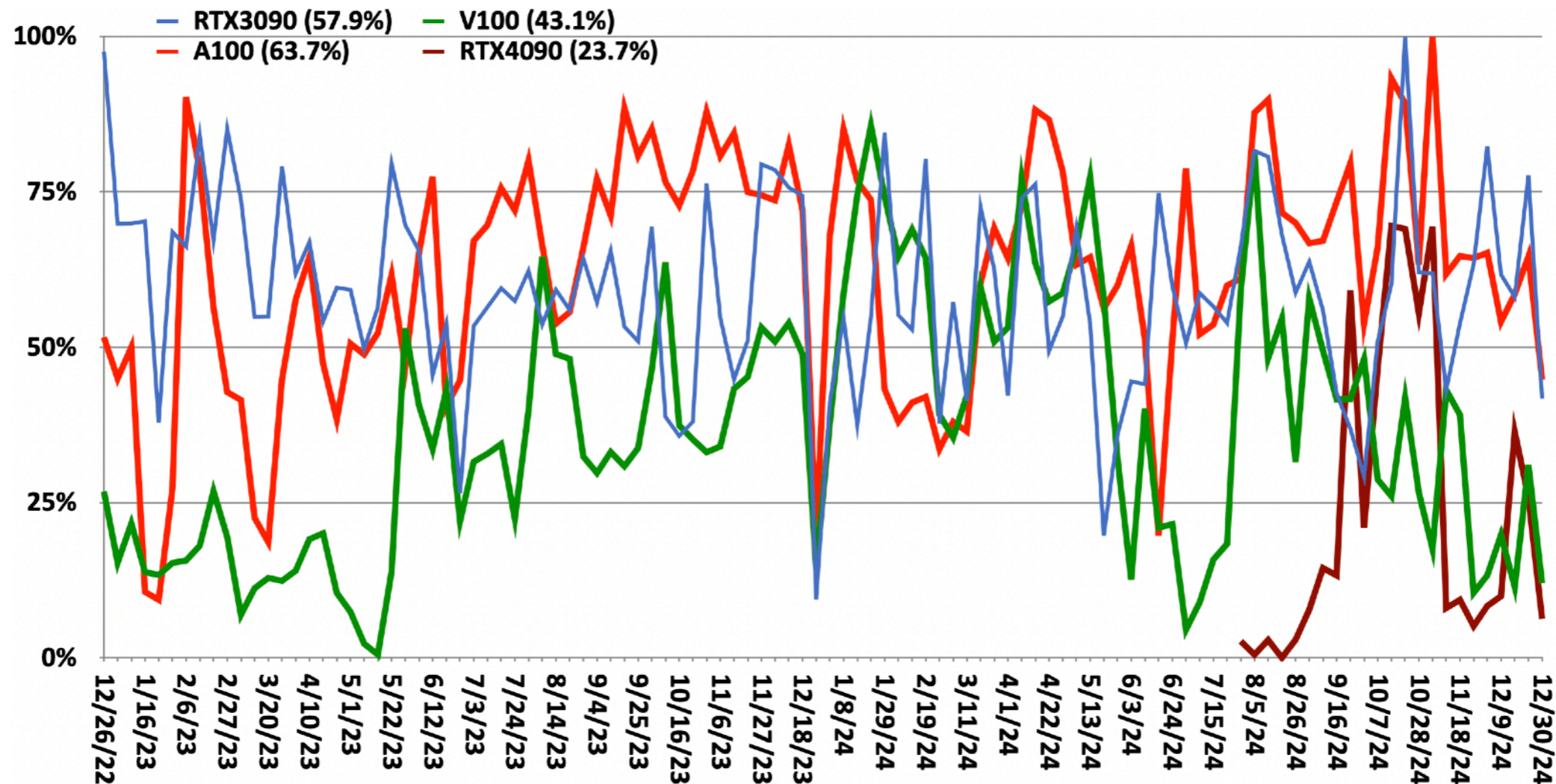- ASIAA 4%
- ASGC 2%
- CryoEM 30%

12

Disk Storage Usage (TB)

GPU Resource Usage in 2024

- **GPU demand keeps growing in 2024: <u>20%</u> utilization growth comparing to 2023 under high usage situations**
  - **Diversified user communities**
  - **Not just AI model training and development, scientific computing also requires large amount of high-end GPU resource**
- **Users can hardly access to the most advanced GPU like H100 - Urgent action is needed before being GPU disadvantaged**
  - **Unaffordable usage cost, not mentioning the acquisition of powerful enough high-end GPUs**
  - **Long waiting queue for competing the rare resources for the academic**
- **A100 servers @ASGC with large embedded GPU memory (80GB) and interconnection bandwidth (NVLink) becomes the alternative**
  - **Congested jobs/requests for limited A100 servers (24 boards in 3 servers) has been since 2023**
    - **A100, 3090 are almost saturated - average utilization in 2023&2024 are around 60%. Users were forced to choose less advanced V100. Usage of V100 in 2024 has grown by 1.4 times (average utilization is about 45%). Even the primitive GPUs (P100 & 1080ti) are also highly utilized.**
    - **Although newly procured 4090 (8 boards only) served as the substitute in time**
- **More investment in advanced GPU is needed, for both AI development as well as scientific computing**

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

Application	Version	Resources
CryoSPARC 32 P100	3.2	83%
CryoSPARC 1080ti	3.3.2	29%
CryoSPARC RTX3090	3.3.2	26%
spyder cpu/eman2		17%
Octave	V5.2	29%
Transfer Data		86%
CryoSPARC RTX3090	4.0.2	26%
CryoSPARC RTX3090	4.1.1	26%
CryoSPARC RTX3090	4.4.1	26%
cisTEM		86%
Ovito		86%
OpenACC	GPU P100	83%
AlphaFold	GPU with A100	75%
AlphaFold (Full DB)	GPU with A100	75%
IMOD	GPU with 1080ti	29%
Triton	22.01-py3 (GPU P100)	83%
AlphaFold	GPU with RTX3090	26%
AlphaFold	GPU with V100	17%
RoseTTAFold	GPU with rtx3090	26%
Dynamo	GPU with 1080ti	29%
MATLAB	R2018b on GPU V00	17%
Jupyter Lab	CPU with Tensorflow v1	86%
Jupyter Lab gpu 3090	GPU with Tensorflow 3090	26%
Jupyter Lab GPU 1080ti	GPU with Tensorflow v2	29%
RFDIFFUSION	2023 on GPU V00	17%
diffdock	2023 on GPU V00	17%
EvoDiff	V100	17%
Jupyter Lab GPU V100	GPU with Tensorflow V100	17%
Jupyter Lab GPU A100	GPU with Tensorflow A100	75%
Jupyter Lab Cryocare GPU	GPU with 1080ti	29%
QIIME2	Genome	%
Scipion3	P100	83%
Phenix		86%
Jupyter Lab GPU A100	GPU with Tensorflow v2.6	75%
MorphoGraphX	GPU with P100	83%
Deepmd-kit	GPU with A100	75%
Deepmd-kit	GPU with V100	17%
MAML	GPU with A100	75%
LabVIEW Run-Time Engine	2019	
Warp	rtx4090	700%
MAML	GPU with V100	17%
PVserver	5.8.0 (GPU 1080Ti)	29%
Paraview Client	5.8.0	86%
R studio	10 CPU Cores	54%
PyRoot	GPU with 1080ti	29%
qiskit		86%
NVIDIA CUDA-Quantum A100		100%

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

DiCOS-BioSAXS Platform

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

ATSAS ▸ | DAMMIN
AMBER | DAMMIF
Rosetta | GASBOR

Collaboration Model

- **Pay-as-you-go: using existing resource and services**
- **Buy-In: joint procurement with ASGC by PI's fund and the procured hardware is shared to all NSTCCore users managed by ASGC**
  - **Contributor would have priority to the resource and deducted usage fee**
  - **Examples: IOP, TIDC**
- **Facility collocation without sharing to all users at this moment (for AS institute only)**
  - **Example: ASIAA, IOC (joint procurement) and IOP**
- **Service Collocation: providing shared services developed by user group(s)**
  - **Examples: Depositar - Research Data Management System developed by IIS/AS**
- **Engagement with other Core facility: e.g., ASCEM, Data Science**
- **Advanced or Customized services: analysis workflow integration**
  - **Shared or common service first**
  - **CryoEM - integration of CryoEM facility and data analysis facility**
- **Exclusive Mode (for least-performance CPU nodes or special needs): by request, monthly basis，<= 50% capacity. For now, only FDR5 and QDR6 are applicable.**

CECAM-TW Will Be Inaugurated in 2025

- **Our mission: promotion of fundamental research on advanced computational methods and their application to important problems in frontier areas of science and technology.**

- **Core Activities**
  - **International events such as workshops, schools, conferences, lectures (15-25/y at HQ)**
  - **Research activities (method development and applications for material and life sciences)**
  - **Collaboration with other EPFL centers**
  - **Swiss and European projects (OSSCAR, Lhumos, BIONT, MDDB, MultiXscale)**
  - **Education and dissemination**
  - **Berni J. Alder Award for exceptional contributions to the field of microscopic simulation of matter (every three years)**
  - **Coordination of the CECAM network**

- **CECAM-TW Node Director: Dr. Jer-Lai Kuo (IAMS)**

- **Consortium: IAMS, RCAS, IoC, IoP and NCTS-Physics, local universities & institutes.**

- **Hands-on training (supported by ASGC)**

- **https://www.cecam.org/**

Service Pricing

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
CPU計算服務				
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)			

ASGC Team

	Name	Jobs
1	李宏德 Felix	Technical Lead, System Design
2	吳宗訓 Tsung-Hsun	DiCOSApp, User Support, Deputy Lead
3	尤靖雅 Jing-Ya	User Support
4	楊明娟 Mandy	System Development
5	林建宏 Chien-Hung	Networking
6	朱子豪 Laspha	Security, Authentication Services
7	張力中 Li-Chung	Fabric
8	褚昶銓 George	Data Center Operation and Efficiency
9	楊翔宇 Patrick	Storage System
10	陳怡如 Jennifer	Batch System
11	林澂蓁 Alice	WLCG Operation
12	廖慧如 Nereid	General Support
13	黃佩華 Vicky	ISGC, Dissemination & Outreach

中研院網格中心 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**