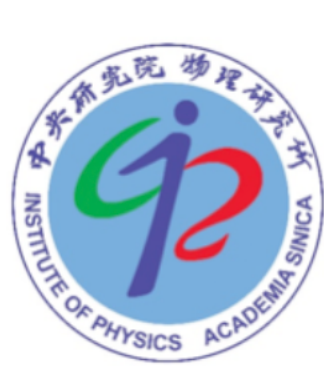




ML/AI Application Support of ASGC

Eric Yen and Felix Lee

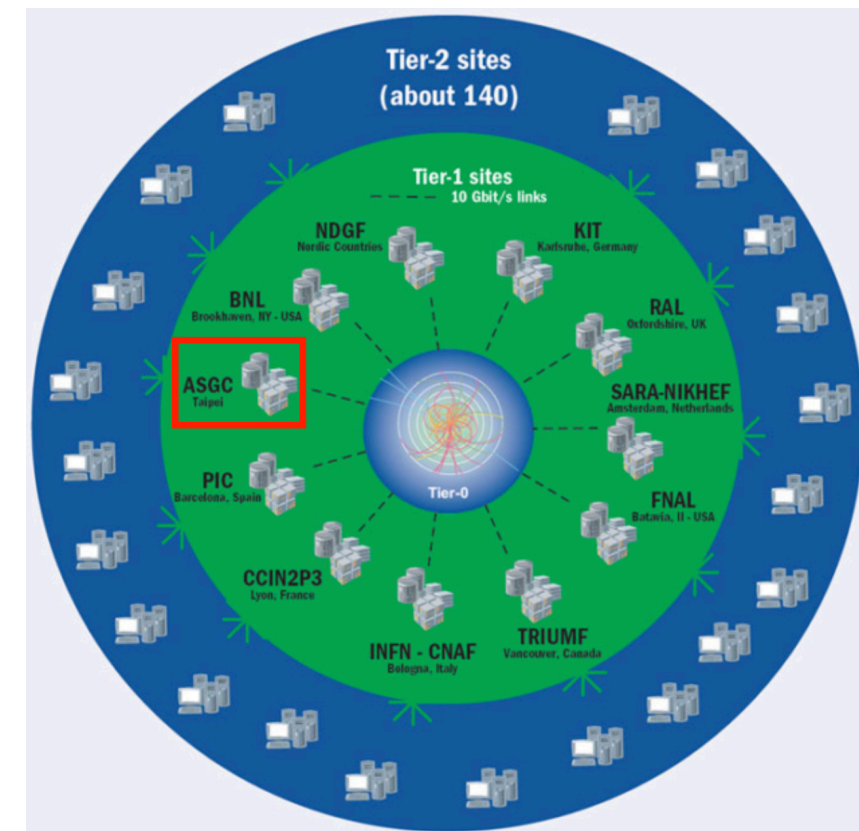
Academia Sinica Grid Computing Centre (ASGC)

AS-IOP Machine Learning Workshop

22 April 2022

ASGC Mission

- Founded as a WLCG Tier-1 Centre in 2005 and jointly develop & deploy advanced, worldwide distributed cloud infrastructure for WLCG
- Enhancing science-enabling capabilities by advanced research infrastructure and big data analytics
 - Building capacity of large-scale distributed cloud for efficient big data analysis and scientific computing of Academia Sinica
 - The research infrastructure, application and services are improved progressively along with growing scientific applications of various disciplines
 - ML-enabled data analysis framework is also upgraded
- System efficiency optimization: power, thermal, application, operation, system, etc.
- ASGC will become a Core Facility for ML-enabled big data analysis and scientific computing from 2023

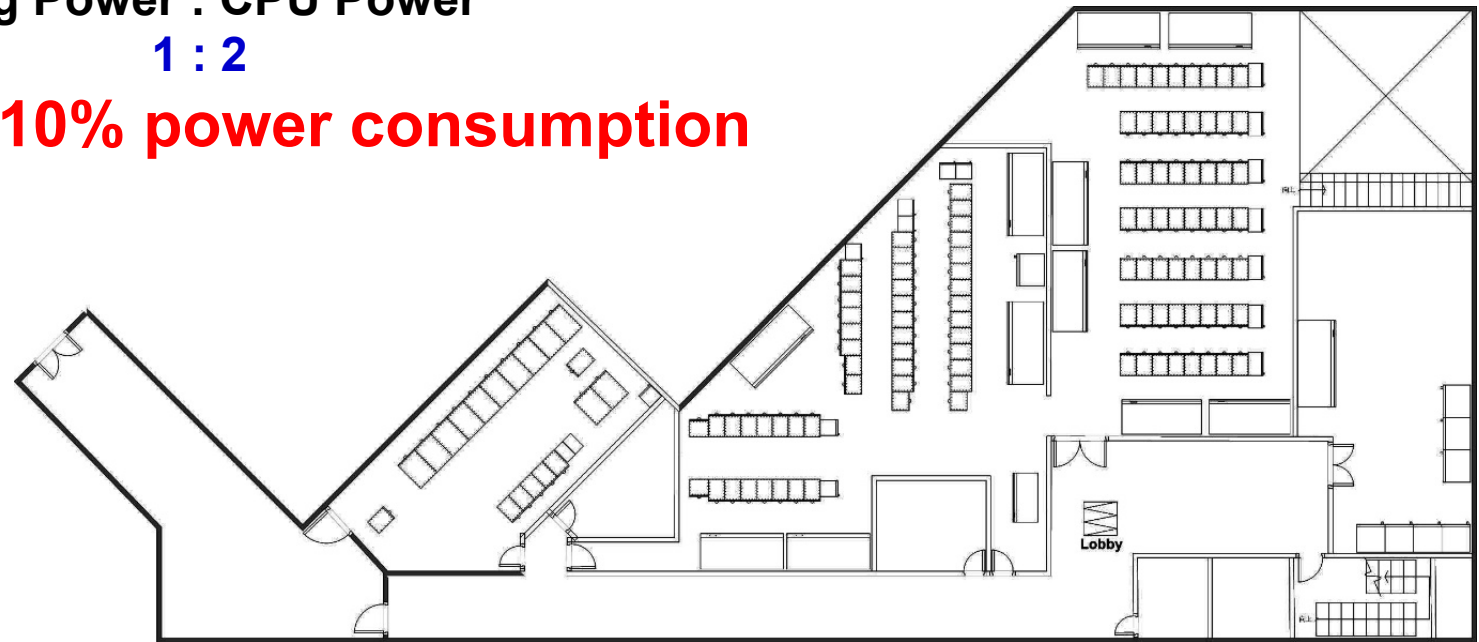


ASGC Resources

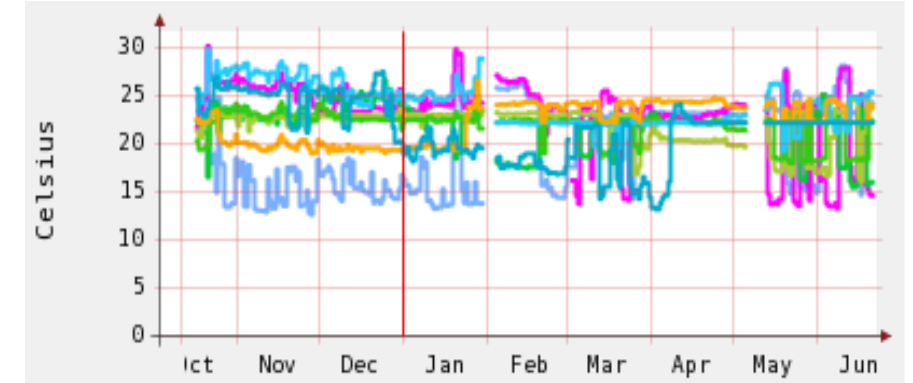
Cooling Power : CPU Power

1 : 2

No UPS to save 10% power consumption



- **Total Capacity**
 - 2MW, 400 tons AHUs
 - 112 racks in ~ 800 m²
- **Resources (2021)**
 - 13,652 CPU Cores
 - 192 GPU Cards
 - A100 Server *2 (8 GPU Card for each) are available in 2021
 - 24 PB Disk Storage
 - 2x10Gb links to CERN and primary NRENs worldwide
- WLCG Tier-1 Center since 2005
- Supporting HPC & HTC in Academia Sinica by distributed cloud operating system (DiCOS)
 - Usage > 1M CPUCore-Days in 2015
 - Usage > 2M CPUCore-Days in 2019
 - GPU usage is growing exponentially from 2017
- R&D on system efficiency optimization by intelligent monitoring & control

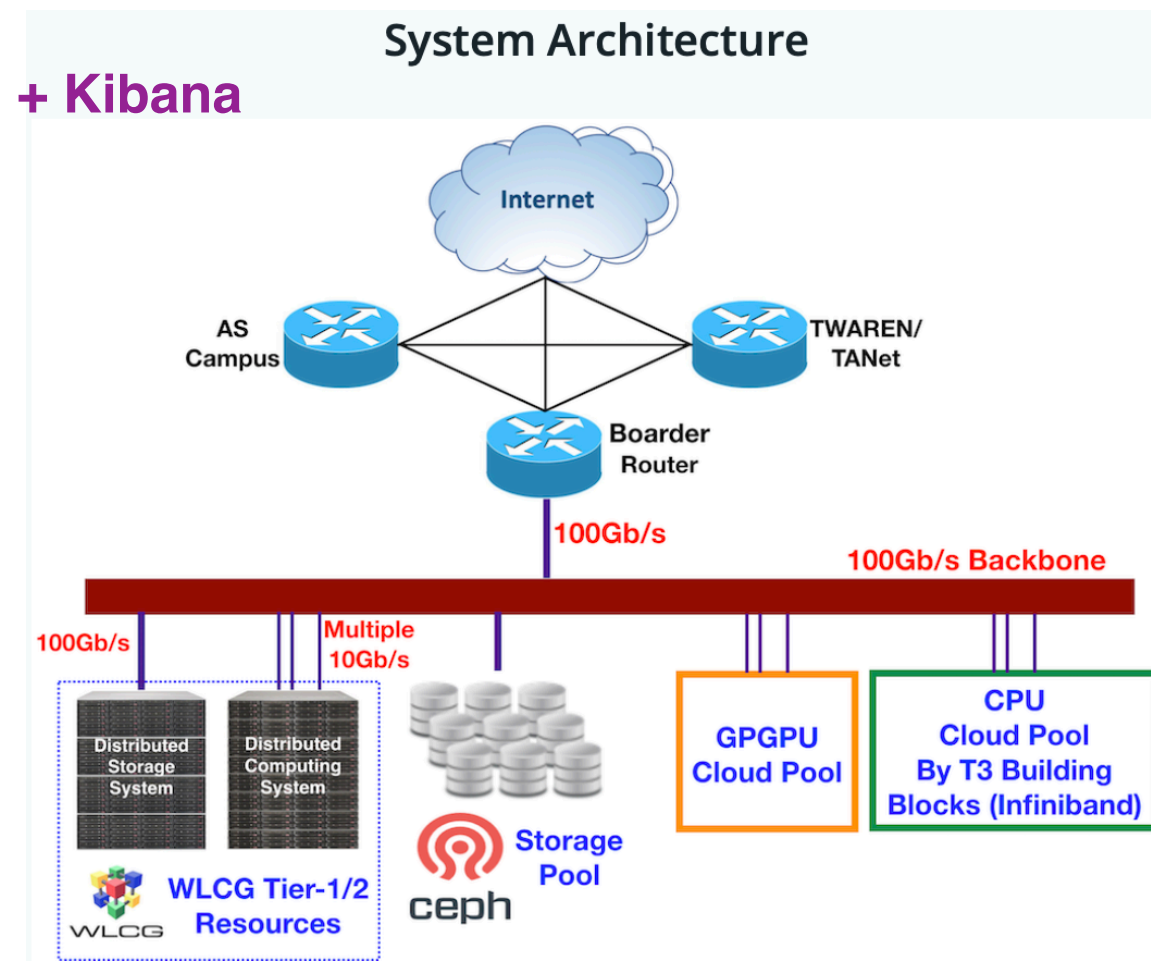


Monitoring the power consumption and temperature of every piece of equipment every 10 seconds.

All software used are open-source codes developed by ASGC and an international collaboration led by CERN

ASGC Science Cloud Infrastructure (DiCOS)

- **OpenStack Cloud:** for core services and on-demand worker nodes
 - Separate regions for scalability
 - Multiple cells/Region for various configurations and capabilities
 - e.g. GPU, Neutron Compute, Nova Compute, ...
 - Single hypervisor type: KVM
 - #hypervisors: 100+
 - #VMs: 500+, dynamic provisioning
 - Networking: flat and segmented
- **Containerized Resources managed by Kubernetes framework**
 - User cluster:
 - batch, interactive GUI jobs: remote Jupyterlab, virtual desktop
 - GPU Cloud
 - Core Services: distributed cloud cores; Elasticsearch + Kibana
- **Storage system: Ceph-based**
 - OpenStack services (RBD): 1.5PB
 - Users: CephFS (7+PB)
 - Cloud Storage (DropBox-like) services: 2TB/user
 - Accessible from user home directory
- **UI: Web UI/Terminal; JupyterLab**
- **Operation and management**
 - Source control: Gitlab
 - Puppet-based deployment of components
 - HELM

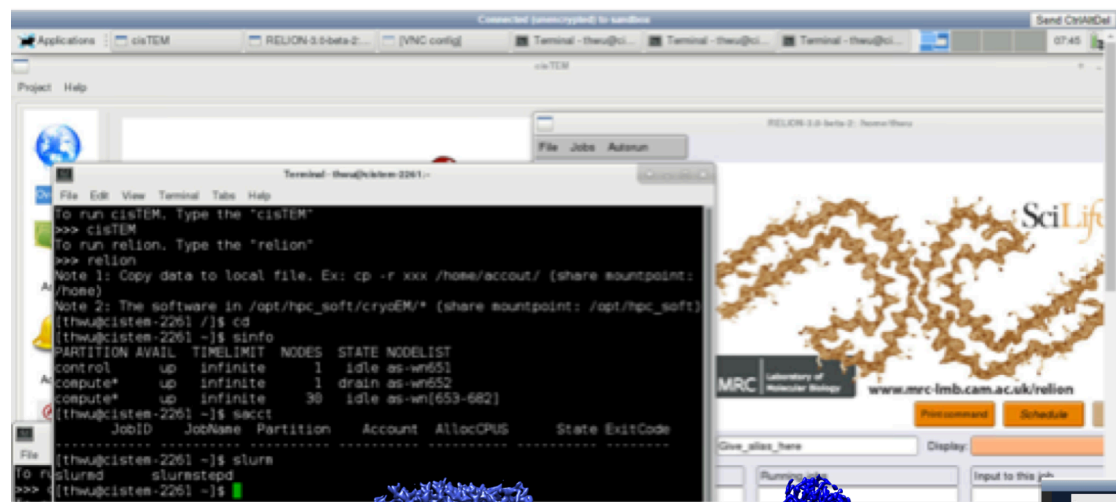


DiCOS for ML

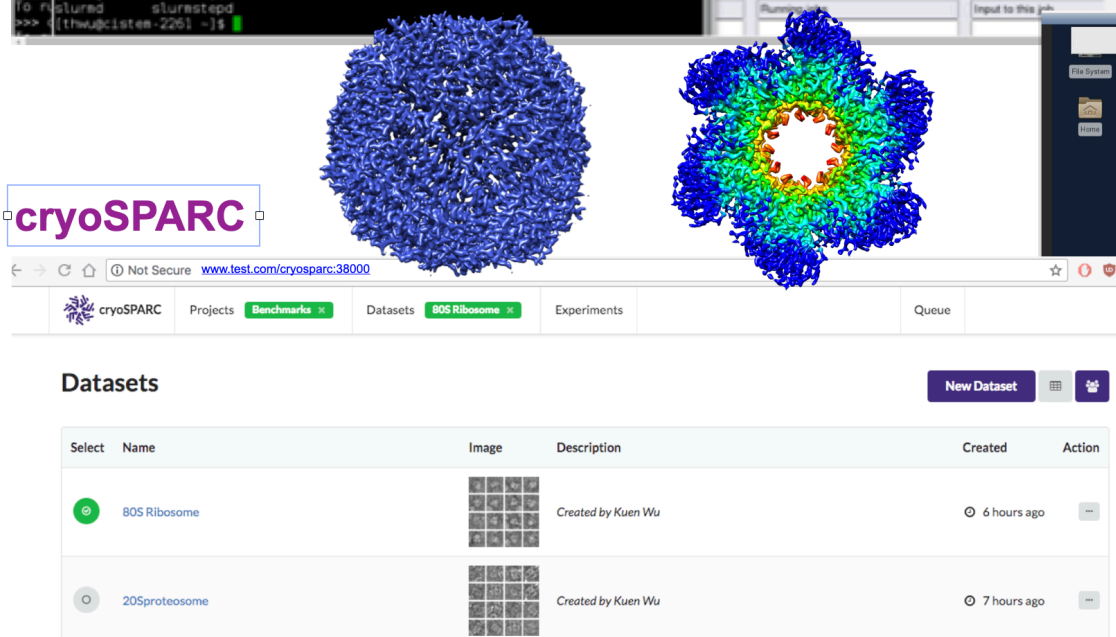
- **DiCOSAPP (Interactive jobs) - user-oriented, Web-based computing environment or application portal**
 - Jupyterlab (Jupyter notebooks)
 - PyTorch
 - Tensorflow2.x & Keras
 - Triton inference server
 - Cloud storage attached (2TB/user)
 - GPU: GTX-1080, RTX-3090, P100, V100(32G), A100(80G)
 - MPI/CPU Cluster resource is also accessible
- **Batch jobs**
 - through DiCOS command line UI or web terminal :
 - Queue: ANALY_TAIWAN_TWGRID_ML_V100
 - The system environment is the same as Jupyterlab
 - GPU: V100

Supporting Cryo-EM Applications by DiCOS

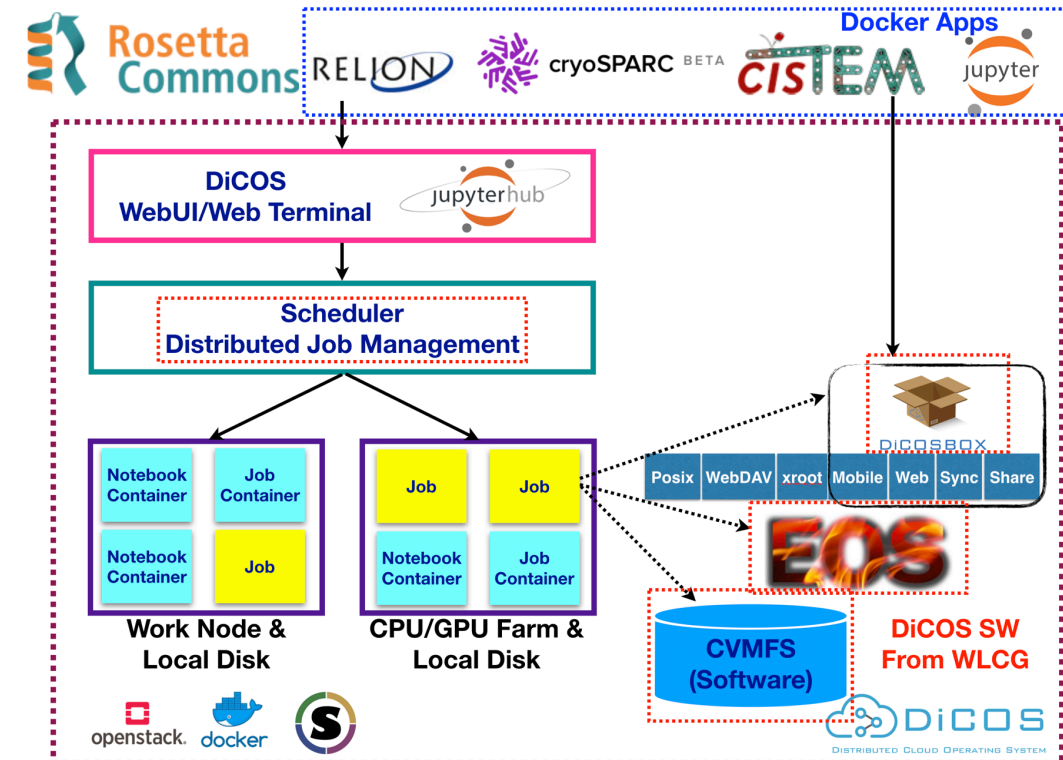
- Primary GPU (single precision) and CPU (300-600 threads) users, ~5-10TB input/job
- ASGC Contributions: providing high-performance big data analysis and processing for multiple user groups concurrently in AS, with customized workflow
 - Integration of analysis pipeline over ASGC distributed cloud infrastructure, through Relion, CryoSparc and cisTEM
 - Computing (CPU, GPU, cluster), storage, networking, and web portal
 - Software and computing workflow setup, upgrade, maintenance and system operation
 - Shorten latency between ASCEM and analysis facility: on-the-fly processing & transmission
 - Web /JupyterLab UI development
 - Efficiency optimization: analysis workflow and applications
 - Extending from CryoEM to tomography
 - ASCEM IT & Security operation support
 - Data access from EMPIAR
 - New resource/tools provisioning: RosettaFold, AlphaFold



cisTEM



- Load dataset
- Align movies
- CTF estimation
- Particle picking
- 2D class
- Ab-initio model
- Auto refinement
- Bayesian Polish
- Local resolution



AlphaFold2 Use Case

- AlphaFold: AI tool which could predict 3D shape of proteins from genetic sequence with accuracy
- Comparison of running on Google Colab and ASGC V100 server
 - 240min vs 15min for one simulation;
 - Length of amino acid: 900 vs 2000
- Research Applications
 - Large-scale screening for protein-protein interactions: ~15,000 protein
 - Could be finished in ONE month by ASGC V100. Or, shorter time by 2xV100
 - Only Top10 candidates shall be confirmed their structures through CryoEM experiments afterwards
 - ~200K NTD\$ cost for consumables would be saved
- ASGC Support
 - Develop ease-of-use AlphaFold2 Web App
 - Support automation of large amount job submission when mutation varies
- RoseTTAFold is also available @ASGC - DL-enabled protein structure prediction service developed by U. Washington

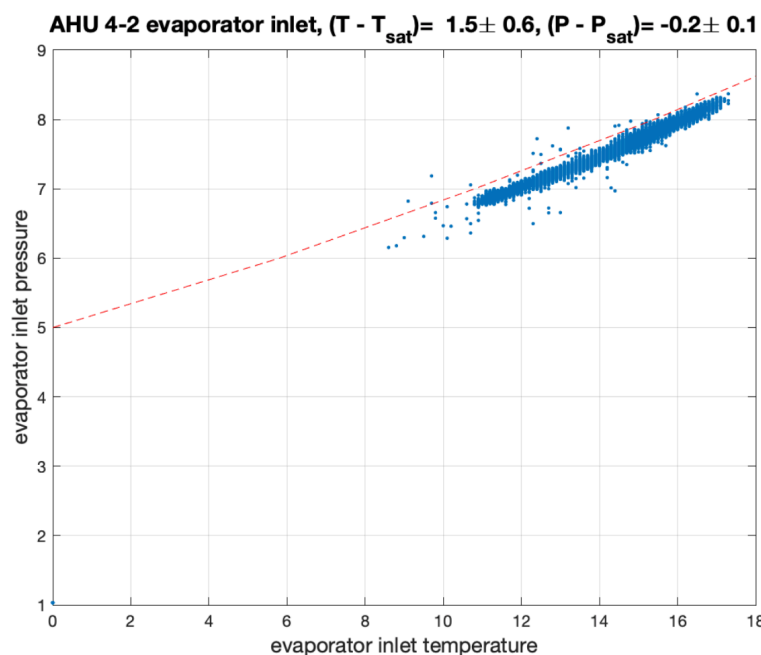
Other Use Cases

- **DeepMD-kit setup over GPU**
 - Deep learning package for many-body potential energy representation and molecular dynamics using TensorFlow
 - Support interface with LAMMPS
 - ASGC also build up Web App for DeepMD
- **NVIDIA Triton Inference Server**
 - “streamlines AI inference by enabling teams to deploy, run and scale trained AI models from any framework on any GPU- or CPU-based infrastructure.”
 - Triton environment @ASGC is available
- **Workflow, UI and analysis pipeline will be improved progressively according to users experiences and innovations**

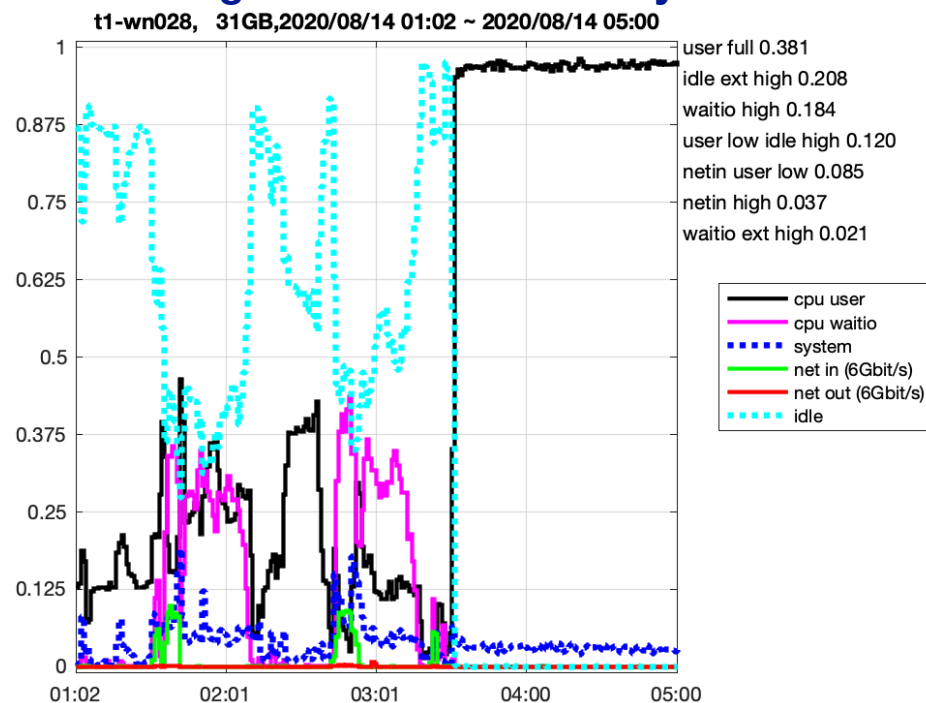
System Efficiency Optimization

- **Goals:** maximize application performance by available resources dynamically, in terms of power, thermal and system (Comp, Storage, Network, application) efficiency
- **Scope:** Power, Thermal and Distributed Cloud System management
- **Strategy:** intelligent monitoring and control assisted by ML
- **Example:** Thermal management, Compute/storage/network anomaly detection, Power saving of work nodes
- **AHU monitoring and control**
 - Detection of refrigerant operating issues and abnormal components; Efficiency optimization
 - 13 sensors x 16AHU; 18K data points/day;
 - Realtime monitoring, adjustment and diagnostics: refrigerant operating issue; abnormal components detection; efficiency tuning; ML-based automatic detection of critical problems;
- **System Anomaly Detection**
 - Classify machine status into 5 clusters daily: based on CPU-user, CPU-wio, CPU-system, CPU-idle, Network In/Out
 - >30M records/day from all systems of ASGC are covered
 - 146 events in 14 types identified during March 2020 - March 2021

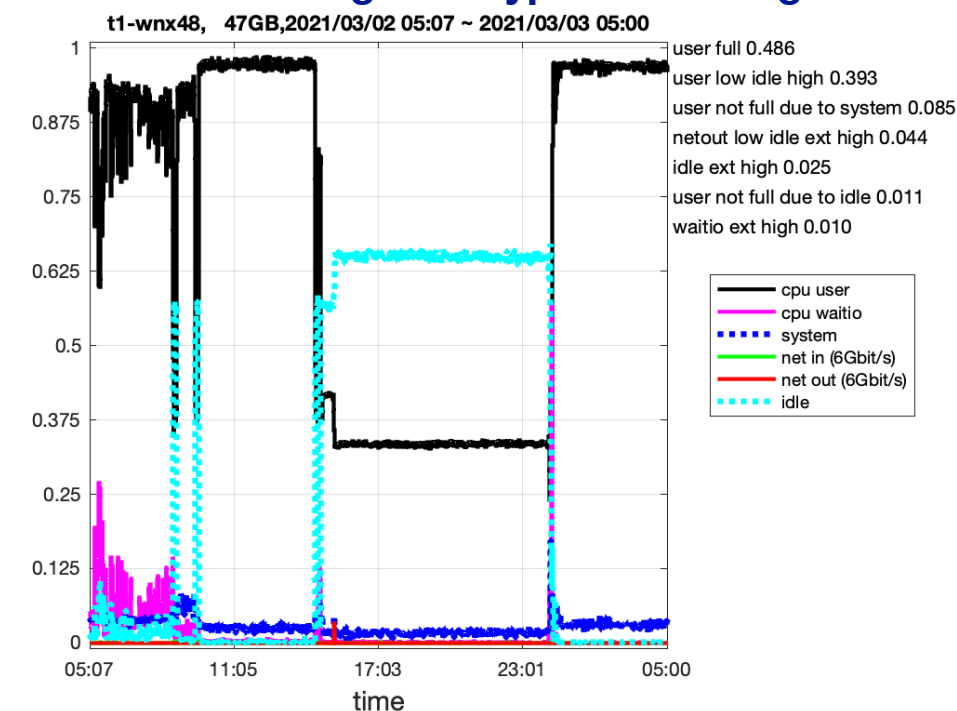
AHU Performance Monitoring



Worknode Monitoring: High ratio of WaitIO & System



Worknode Monitoring: Misconfigured hyper-threading

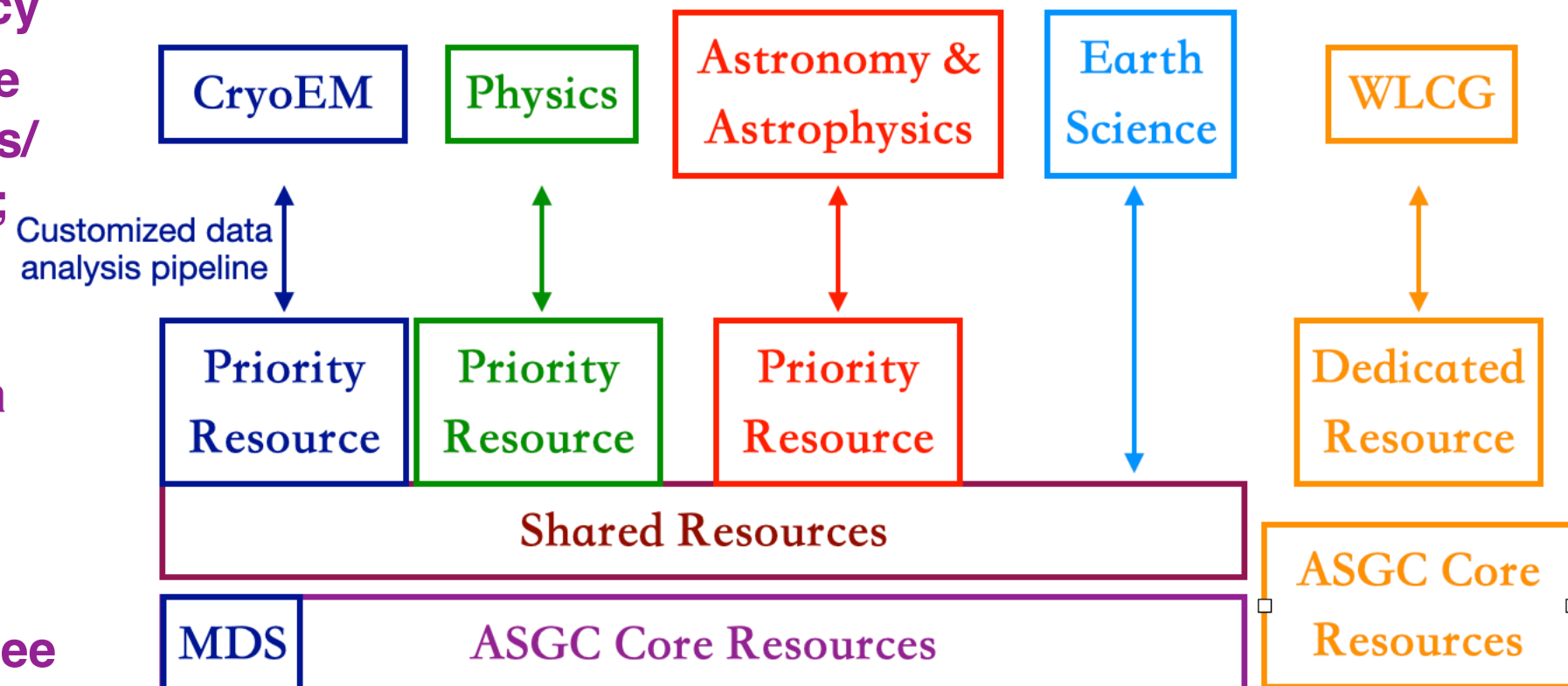


ML-Cloud

- **Research groups could focus on scientific problems solving**
- **Application environment: Research Infrastructure based**
 - HPC facility - computing + storage + network
 - Ease-to-use and customized analysis pipeline, including application and platform
 - Research data management (including tools, backup and archive)
- **Use Cases collections: reusable, reproducible, training, learning and benchmarking**
 - Based on FAIR principles
 - Coverage: data set, tools, execution environment (e.g, Jupyter Notebook), publication (e.g, documents)
- **Leveraging HPC powers**
 - To shorten training time, support pre-training by large amount of datasets, support (near) real-time applications, ...
- **Consulting services: ASGC + volunteers and invited experts**
- **Capacity building:**
 - Providing ML resources based on IOP/users needs
 - Datasets, tools, codes, algorithms, case studies, ...
 - Learning materials in all aspects
 - Training, workshop, GPU computing workshop, hackathon

Resource Policy

- **Type of resource**
 - Core resource: used for providing services
 - Shared resource: shared by all users
 - Priority resource: invested by user communities. Will be shared to other users whenever facility is free
- **Allocation Policy**
 - Once resource is not insufficient: 1) request funding support from AS (申請核心設施設備擴充); 2) invest by user communities
 - Any user community needs more resource: 1) $\leq 50\%$ of shared resource; 2) $\leq 75\%$ of total resource; 3) $\leq 25\%$ growth rate
- **Rules**
 - AUP, Privacy, Security policy
 - Shared resource: fare share basis; limit of #running jobs/PI group; limit of time (job); limit (used CPU/GPU)/user
 - Storage: quota/user; dark data purge reminder; quota review regularly (every 3 month); quota increase request
 - Reviewed by User Committee



Interactive UI

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

DiCOS

AboutJob SubmissionJob MonitoringData ManagementWikiAPIAppsTerminal

Eric YEN

DiCOS Apps

Contact us
If you have any questions, please feel free to contact us.
EmailLive Chat

CryoSPARC v2

Version:

Resources:

Launch

Jupyter Lab

Version: CPU with Tensorflow v1

Resources:

Launch

Jupyter Lab GPU

Version: GPU with Tensorflow v1

Resources:

Launch

cisTEM

Version:

Resources:

Launch

Instance list

RELION 3

Version: V3.0.8

Resources:

Launch

RELION 3.1

Version: V3.1

Resources:

Launch

LabVIEW Run-Time Engine

Version: 2019

Resources:

Launch

Jupyter Lab GPU

Version: GPU with Tensorflow v2

Resources:

Launch

CryoSPARC v2 P100

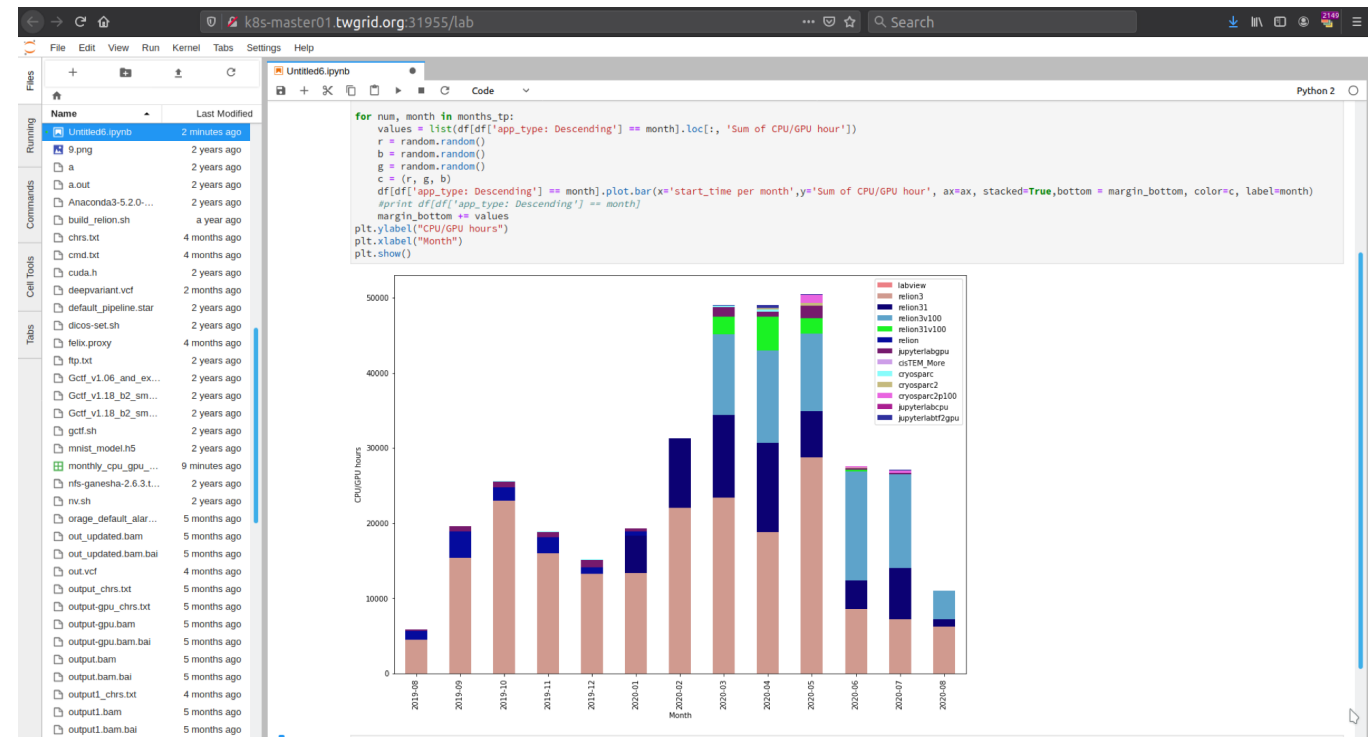
Version:

Resources:

Launch

DiCOS Web Interface

ASGC 2015 | license



k8s-master01.twgrid.org:31491

Search

cryoSPARC

ProjectsWorkspaces

Statistics

This weekThis monthTotal

Projects111

Workspaces111

Jobs000

Completed Jobs000

Change Log

Current version: v2.14.2

My Recent Jobs

P1 J1

Import Movies

Links

General Reference

Job Reference

Tutorials

Discussion Forum

EMPIAR

EMDB

Details

Job Builder

Workflows (1)

Imports (6)

Motion Correction (5)

CTF Estimation (4)

EXposure Curation (1)

Particle Picking (6)

You are looking at the new notification system! To clear this notification, open the Notification Manager tab in the Resource Manager and click 'clear' next to this notification.

DashboardProjectsResource Manager

New update available: v2.15.0

felixleeAdmin

DiCOS

AboutJob SubmissionJob MonitoringData ManagementWikiAPIContactTerminal

Felix Lee

```
[felixlee@dicos-ut02 ~]$  
[felixlee@dicos-ut02 ~]$ export X509_USER_PROXY=$HOME/.globus/felix.proxy  
[felixlee@dicos-ut02 ~]$ voms-proxy-info -all  
subject      /C=TW/O=AS/OU=GRID/CN=Felix Dteam Lee 153280/CN=proxy  
issuer       /C=TW/O=AS/OU=GRID/CN=Felix Dteam Lee 153280  
identity     /C=TW/O=AS/OU=GRID/CN=Felix Dteam Lee 153280  
type         full legacy globus proxy  
strength     2048  
path         /asgc_ut_home/felix/.globus/felix.proxy  
timeleft     120:18:56  
key usage    Digital Signature, Key Encipherment, Data Encipherment, Key Agreement  
=== V0 ans02 cern.ch extension information ===  
V0  
subject      /C=TW/O=AS/OU=GRID/CN=Felix Dteam Lee 153280  
issuer       /C=TW/O=AS/OU=GRID/CN=voms.grid.sinica.edu.tw  
attribute    /ans02.cern.ch/Role=production/Capability=NULL  
attribute    /ans02.cern.ch/Role=NULL/Capability=NULL  
timeleft     120:18:56  
url          voms.grid.sinica.edu.tw:15016  
  
[felixlee@dicos-ut02 ~]$  
[felixlee@dicos-ut02 ~]$ dicos job status  
PandaID  Name      Status  
-----  
2301292  taiwan 873059581 he4 pl1 activated  
2301290  taiwan 873059580 he4 pl1 activated  
2301288  taiwan 873059579 he4 pl1 activated  
2301286  taiwan 873059578 he4 pl1 activated  
2301284  taiwan 873059577 he4 pl1 activated  
2301282  taiwan 873059576 he4 pl1 activated  
2301280  taiwan 873059575 he4 pl1 activated  
2301278  taiwan 873059574 he4 pl1 activated  
2301276  taiwan 873059573 he4 pl1 activated  
2301274  taiwan 873059572 he4 pl1 activated  
2301272  taiwan 873059571 he4 pl1 activated  
2301270  taiwan 873059570 he4 pl1 activated  
2301268  taiwan 873059569 he4 pl1 activated  
2301266  taiwan 873059568 he4 pl1 activated  
2301264  taiwan 873059567 he4 pl1 activated  
[felixlee@dicos-ut02 ~]$
```

3:31:37 PM

ASGC Federated Resource

GPU Cluster	GPU	#Nodes	GPU RAM (GB)	CPU	Sys RAM (GB)	Inter-Connection
IOC-GPU-A100	A100*4/node	2	80	AMD		Eth: 100Gbps Shall be online in late 2022
GPU-A100	A100*8/node	2	80	AMD EPYC 7302 16C @3GHz*2	1024	IB: EDR; Eth: 100Gbps
GPU-V100	V100*8/node	6	24	Xeon 6126 12C @2.6GHz*2	768	IB: EDR; Eth: 10Gbps
GPU-P100	P100*4/node	2	11	Xeon E5-2650L v4 8C@2.2G1GHz *2	503	IB: FDR; Eth: 10Gbps
GPU-3090	3090*8/node	4+4*4	11	AMD EPYC 7302 16C @3GHz*2	1024	IB: FDR; Eth: 10Gbps
GPU-1080	1080*8/node	8	11	Xeon E5-2650L v4 8C@2.2G1GHz *2	768	IB: QDR; Eth: 10Gbps

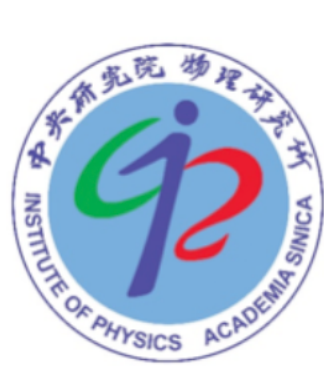
Cluster	CPU	#Nodes	#Cores	RAM(GB)/Core	Inter-connection	Remark
IOC	AMD 7H12	12	768		Eth: 100Gbps	Shall be online in late 2022
ASIAA	AMD Rome 7763 @2.5GHz *2/node	32	1,792		Eth: 10Gbps	Online in May 2022
AMD	AMD Rome 7662 @2.0GHz *2/node	6	768	6.0	IB: EDR; Eth: 100Gbps	Online in May 2022
FDR5	Intel Xeon E5-2650L v4@2.2GHz *2/	92	2,208	5.2	IB: FDR; Eth: 10Gbps	50 TFLOPS;
FDR4	Intel Xeon E5-2650L v3@1.8GHz *2/	39	936	3.9	IB: FDR; Eth: 10Gbps	11 TFLOPS;
QDR4	Intel Xeon E5-2650L v2@1.7GHz *2/	50	1,000	6.3	IB: QDR; Eth: 10Gbps	6 TFLOPS;
QDR2	Intel Xeon E5-2650L @1.8GHz *2/node	96	1,536	3.9	IB: QDR; Eth: 10Gbps	
FDR1&2	Intel Xeon E5-2650L @1.8GHz *2/node	50	1,200	3.9	Eth: 10Gbps	WLCG T1;
WLCG	Quad-Core Xeon L5408/L5500/E5-2609	360	3,172	2.0	Eth: 10Gbps	WLCG T1/T2;

ASGC Resource + IAA & IOC HW

Disk 儲存資源	Raw Space (TB)	Usable Space (TB)	說明
WLCG 全球網格 T1 & T2	13,080	9,810	2019/2020 購置。9PB 為 WLCG 2021 承諾額度。720TB 為 EOS 轉換用
科學計算+1000 (CryoEM)	8,628	6,471	提供使用者登入、計算、儲存與備份等空間
Cloud Storage	2,370	1,777.5	提供核心服務、公共服務與測試環境
總計	24,078	18,058.5	

Summary

- **Collaboration model with ASGC**
 - Upkeep of scientific computing and big data analysis system
 - Workflow integration, customization and efficiency improvement
 - Resource federation for extension of the research infrastructure
 - Facility owner has priority usage but resource has to share with AS users
 - Bring your own hardware or investment, etc.
 - Distributed cloud operation
 - Capacity building: consulting, training, workshop, hackathon, etc.
- **ASGC is turning requests into services**
- **ML-Cloud services**
- **ASGC ongoing operations are funded by AS and collaborators.**
 - Cost sharing model: pay-as-you-go
- **Test of the most advancement AMD/NVIDIA GPU (MI250x4 and Hopper)**
 - AMD provides trial accounts for AS during 13-27 May. Longer term of trial might be possible if more demands call by end of April



ASGC Services

- **ASGC Web Site: <https://www.twgrid.org>**
- **Access to ASGC Resources**
- **Contact point: DiCOS-Support@twgrid.org**