BNL, SLAC and UChicago Shared Analysis Facilities

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US ATLAS Computing Facilities Face-to-Face at SLAC
2022.11.30

Outline

- Overview of the US AFs
- Hardware at each site
- Common Capabilities
  - Identity Management
  - Batch Access
  - Jupyter Access
- Unique Features

Overview of US Analysis Facilities

US ATLAS has three shared Tier 3 analysis facilities providing software & computing

- Resources that fill gaps between grid jobs and interactive analysis on local computers
- Interactive ssh login, local batch, non-grid storage, LOCALGROUPDISK, PanDA
- GPU resources available

BNL Facility

~2000 cores, part of a larger shared pool, opportunistic access up to 40k cores

User quota: 500GB GPFS plus 5TB dCache

~200 users

SLAC Facility

~1200 cores, part of larger shared pool, opportunistic access up to 15k cores

User quota: 100GB home, 2-10TB for data

~100 users

Launched Oct 2021

UChicago Facility

~3000 cores, co-located with MWT2, opportunistic access up to 16k cores

User quota: 100GB home, 10TB for data

~170 users

Hardware specifications @SLAC

SLAC operates 3 computing environment:

- LSF/AFS based cluster and farm (to be decommissioned by Aug 2023)
  - Lots of slots. Some users still heavily using them
- Interim (SLAC Data Facility, or SDF) SLURM Cluster and Lustre storage
  - US ATLAS owns:
  - 512 AMD EYPC 7702 cores in 4 nodes. 512GB RAM on each node.
  - 64 AMD EYPC 7542 cores + 4 Nvidia A100 GPU, 1TB RAM on one node
  - ~830TB Lustre space
- SLAC Shared Scientific Data Facility (S3DF) SLURM Cluster and Weka storage
  - Available to general usage by Jan 2023
  - Major experiments such as LCLS and Vera C. Rubin are adding hardware here.
  - All US ATLAS resource in SDF will be moved to S3DF.

Hardware specifications @BNL

BNL has several storage systems and technologies available to the users

- NFS Posix home area with small quota (100 GB) on storage appliance
- Each user has dCache R/W disk space
- ATLAS users can be granted access to GPFS storage
- New Lustre storage (2 PB) available to all SDCC ATLAS users
- CERN EOS R/W access via fuse mount and CERN kerberos credentials

Two different computer clusters – Shared HTCondor pool and Institutional Cluster

- Shared pool:
  - 56k cores. ATLAS users have 2.2k core quota but able to burst much higher
  - 2 nodes dual NVidia A100-80 GPU's – MIG used to subdivide GPU's
- Institutional Cluster (6 dedicated nodes with dual P100 GPU's)

Hardware specifications @UChicago (excluding GPU)

Node Type	Number of Nodes	Processor Per Node	Cores Per Node	Memory Per Node	Storage Per Node	Notes
Hyper-converged storage & CPU	19	Two AMD EPYC 7402 CPUs at 2.8 GHz	48C/96T	512 GB DDR4 SDRAM	Two 960 GB SSDs, four 2TB NVMe and twelve 16 TB spinning disks.	3 nodes provided by, and for, UChicago ATLAS group
Fast Compute & storage	16	Two Intel(R) Xeon(R) Gold 6348 CPU at 2.60 GHz	56C/112T	384 GB DDR4 SDRAM	Ten 3.2 TB NVMe	Provided by, and for, IRIS-HEP SSL
Interactive Nodes	8	Two AMD EPYC 7402 CPUs at 2.8 GHz	48C/96T	256 GB DDR4 SDRAM	Two 960 GB SSDs	2 nodes provided by, and for, UChicago ATLAS group
Xcache Node	1	Two Intel(R) Xeon(R) Silver 4214 CPU @ 2.20GHz	24C/48T	192 GB DDR4 SDRAM	Twenty Four 1.5 TB NVMe	

Hardware specifications @UChicago GPU Nodes

Node Type	Number of Nodes	Processor Per Node	Cores Per Node	Memory Per Node	GPUs Per Node (Mem)	Storage Per Node	Notes
GPU A	2	Two AMD EPYC 7543 32-Core Processor	64C/128T	512 GB DDR4 SDRAM	Four NVIDIA A100 (40G)	One 1.5TB NVMe	MIG(4*7*5G) configured on one of the two nodes
GPU B	1	Two Intel(R) Xeon(R) Silver 4116 CPU @ 2.10GHz	24C/48T	96 GB DDR4 SDRAM	Four Tesla V100 (16G)	Three 220GB SSD	
GPU C	3	Two Intel(R) Xeon(R) Gold 6146 CPU @ 3.20GHz	24C/48T	192 GB DDR4 SDRAM	Eight NVIDIA GeForce RTX 2080 Ti (12G)	Six 450GB SSD	
GPU D	1	Two Intel(R) Xeon(R) CPU E5-2687W v4 @ 3.00GHz	24C	128 GB DDR4 SDRAM	Eight NVIDIA GeForce GTX 1080 Ti (12G)	Six 450GB SSD	

Identity management at BNL/SLAC

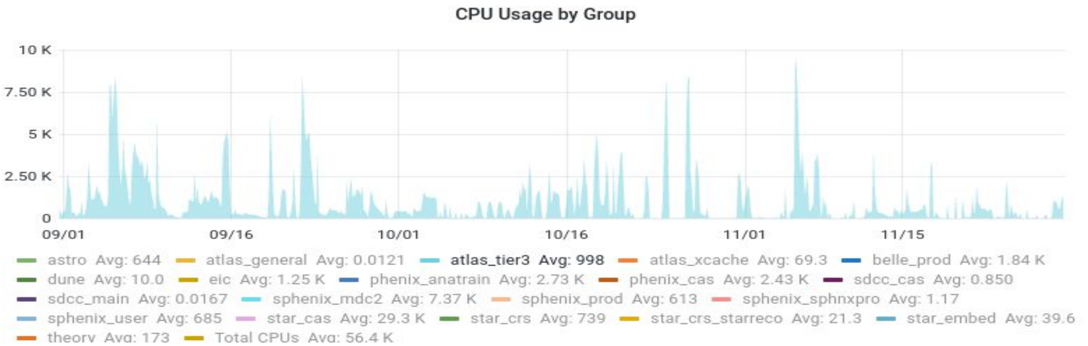
- SLAC
  - Porting NERSC IRIS to SLAC for account management
  - Experimenting Dex IdP for token based SSH access
  - Progress are slow due to effort on S3DF
- BNL
  - Interactive access requires an SDCC account
  - SDCC federated account can be created via CERN/SLAC/FNAL MFA login with a manual account verification procedure (no ssh access)
    - Documented in US ATLAS Tier 3 documentation (Link)

Account Management @UChicago

- In-house user management system (leveraging CI Connect component)
  - Users can sign up for SSH or Notebook access via globus oauth(CILogon)
- Openid connect(dex running on kubernetes)
  - Power users can access K8S directly via Dex IdP configured to utilize CILogon
- CERN IAM for atlas(oauth)
  - Coffea Casa users utilize the ATLAS IdP at CERN

Batch Access at BNL

- Users with SDCC accounts can access HTCondor batch system in the Shared Pool via the command line on the spar* nodes.
- Users with SDCC accounts wanting to run jobs on the GPU machines in the Institutional cluster can access via the command line on icsubmit* nodes.
- All users with Federated-account or SDCC account can use the jupyter-lab interface to launch jobs from the Terminal or via Dask (Shared Pool).
- All ATLAS users can direct PanDA jobs to an opportunistic PanDA queue

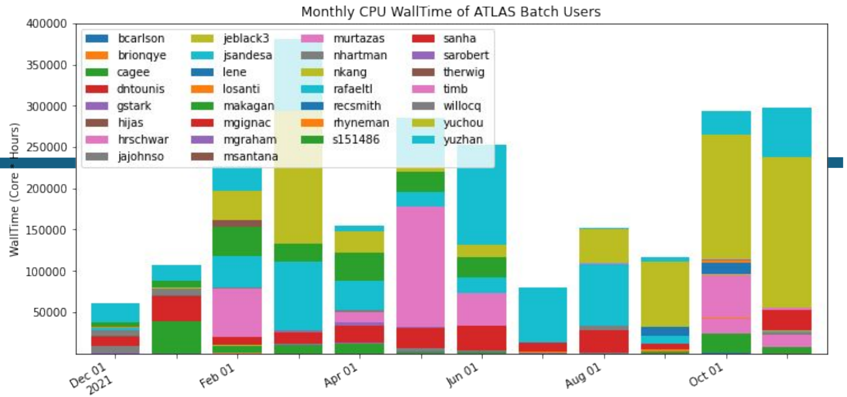


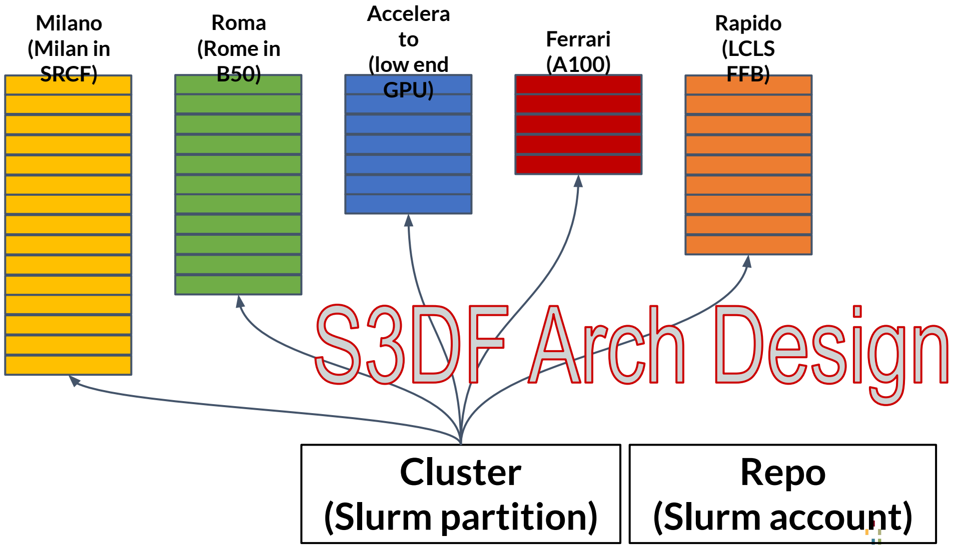
ATLAS AF batch activity for last 90 days peaks to 10k cores can be seen.
Usage very spiky – much higher than default quota – 2.2k cores.

Batch Access at SLAC

SLAC has three computing facilities

- ATLAS users currently use the two older ones
  - one uses LSF, the other uses Slurm
- Will soon migrate all users to the latest one (S3DF)
  - Slurm



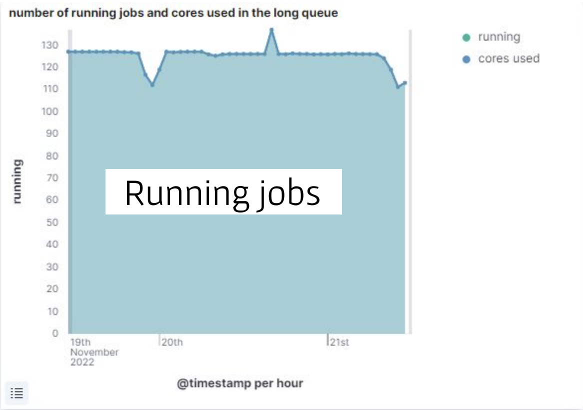


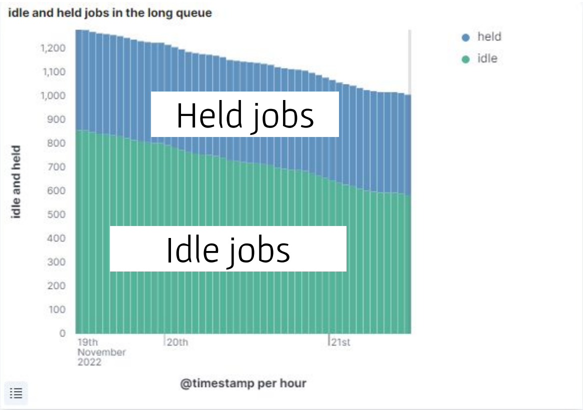
Batch access @UChicago – a synergy of cloud native Kubernetes and traditional batch system HTCondor

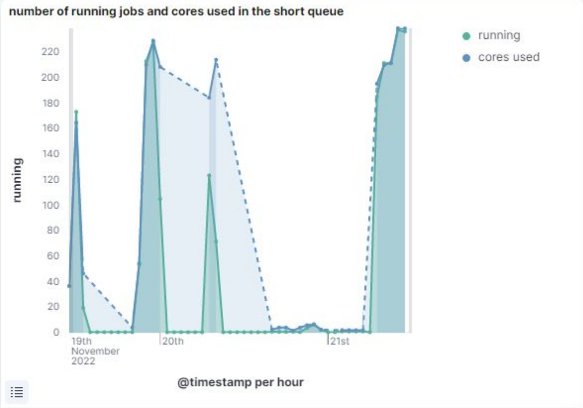
- Kubernetes is for containerized workloads and it minimizes the time and effort required to provision and manage infrastructure resources, but it has limited support for batch workloads
- HTCondor as deployments in Kubernetes
- Resource allocation at two layers
  - Kubernetes allocates resources to pods– dynamically auto scale with Horizontal Pod Autoscaling (HPA) to match demands
  - htcondor job claim resources from the htcondor pod
- Prometheus monitoring of real time resource usage
- Custom monitoring scripts and Elastic Search / kibana for HTCondor queue status monitoring

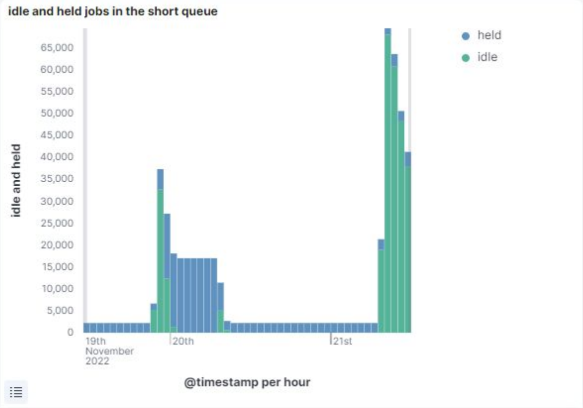
Batch Access @UChicago

- Short queue
  - Shorter walltime limit, quick turnaround
- Long queue
- MWT2 queue
  - Potential for handling bursty interactive load (Dask support in the works)

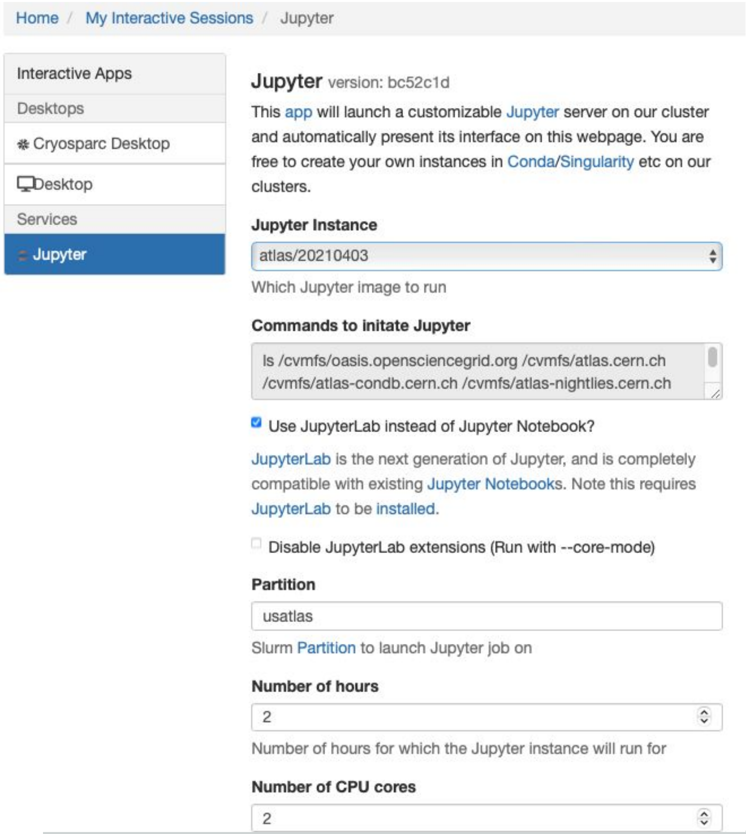








Jupyter Access @SLAC

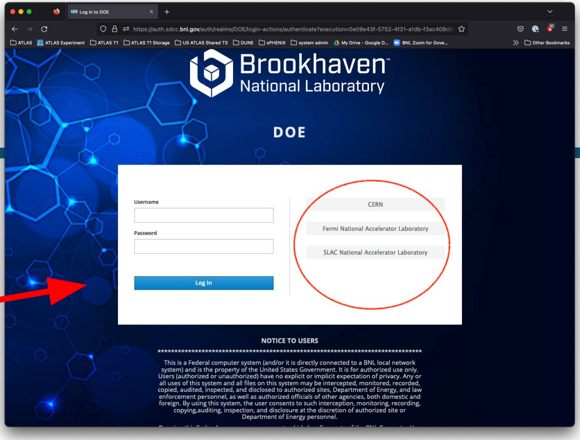


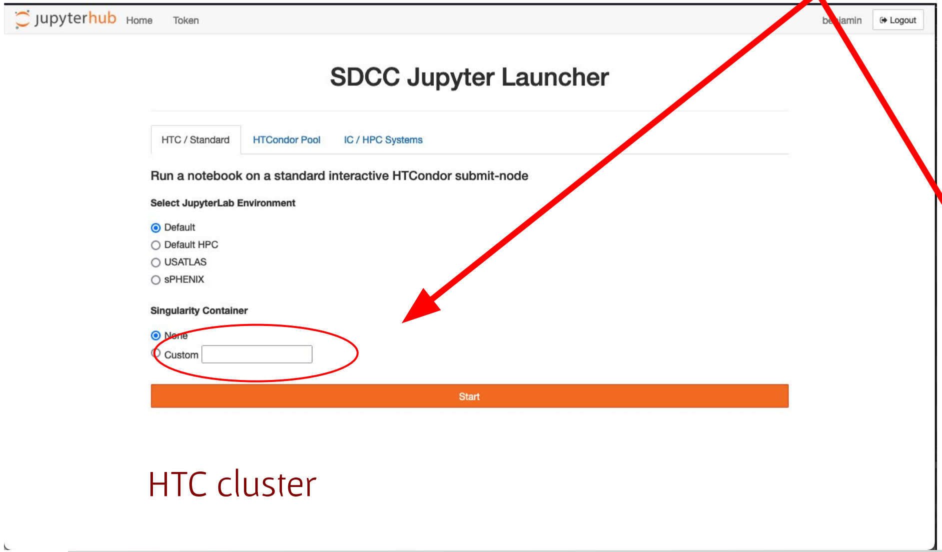
Jupyter web portal based on Open OnDemand

- A pull down menu of Jupyter environments in Singularity or Conda
- Or “bring-your-own-jupyter”
- Jupyter instance run as Slurm batch job
- Use Slurm account to choose between US ATLAS purchased resources or shared/opportunistic resources

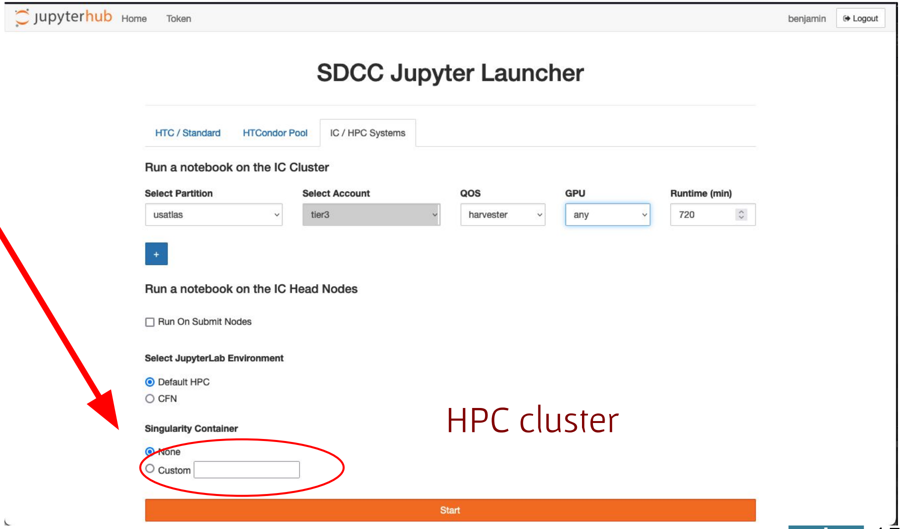
Jupyter Access @BNL

- Federated ID Jupyter Hub at SDCC
  - Allows ATLAS users to use their CERN/FNAL/SLAC credentials as well as local credentials
- Users can use their own custom container





HTC cluster

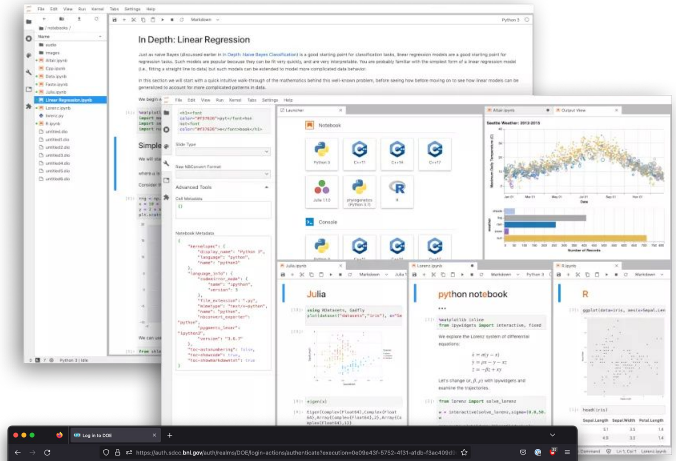


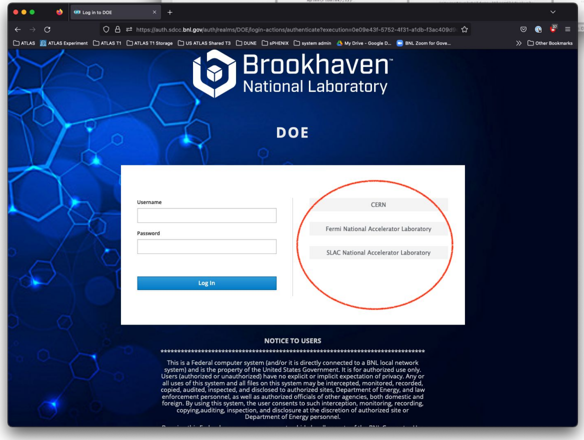
HPC cluster

Evolution of User Analysis Tools

US ATLAS, NP, Belle II, NSLS II…

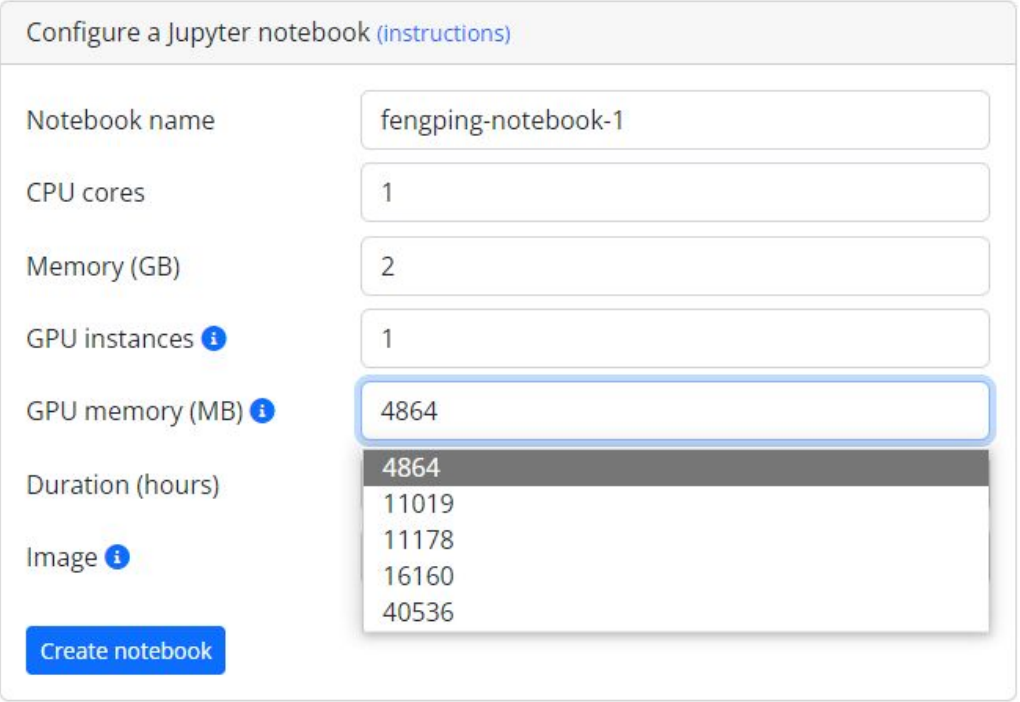
- Pythonic Big Data tools being used increasingly at Data centers
    - *JupyterLab allows users to access compute resources from within a web browser, instead of via traditional ssh command line interface (CLI)*
- Federated ID Jupyter Hub at SDCC
    - *Allows ATLAS users to use their CERN/FNAL/SLAC credentials as well as local credentials*
- Our users can access storage and compute farm through this mechanism.
    - *Leverage tools developed and maintained by a larger community outside of HEP*

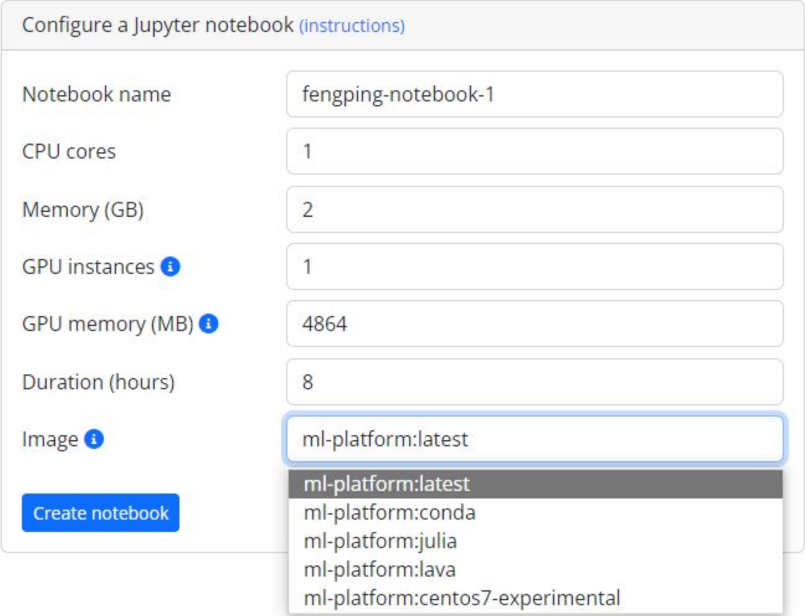




E. Lancon et al., A Coordinated Ecosystem for HL-LHC Computing R&D (7-9 Nov 2022)

Jupyter Access @UChicago





Unique features @SLAC

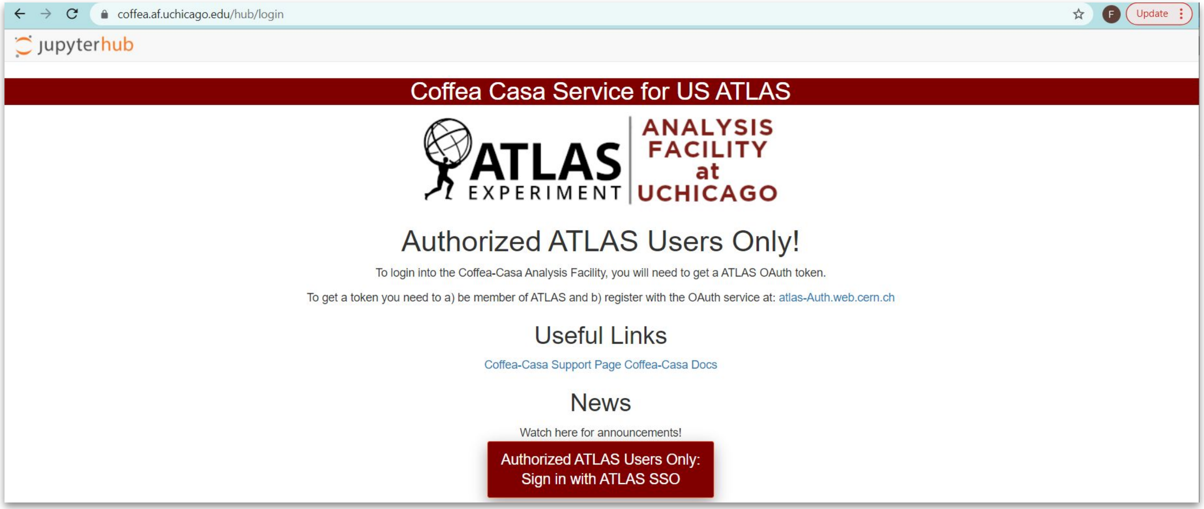
- A large pool of GPU to support opportunistic usage
  - 80x Nvidia A100 (including 4 owned by US ATLAS)
  - 350+ older Nvidia GPU models
- Likely will have a large pool of K8s
  - Vera C. Rubin is k8s on steroids
- Weka Posix storage and large CEPH deployment
  - CEPH is both a Weka posix cold data tier, and
  - A standalone CEPH storage

Unique features @BNL

- Large pool of CPU nodes available to users in shared pool
    - ATLAS users can burst up to 10k cores
- Access to 38.1 PB ATLAS disk storage
- OKD cluster for new services
    - Reana instance
    - ServiceX instance (ATLAS XAOD)
- CVMFS Stratum-0 for publishing software

Unique Features @UChicago – Coffea Casa

- Deployed via Fluxcd
- Docker images served from OSG Harbor
- User authentication via Indico IAM for Atlas
- Dask scale out to htcondor in AF
- Dask scale out to MWT2 to handle bursty interactive workload(in the works)
- Supports multiple data access methods(servicex, local filesystem(/data) etc)

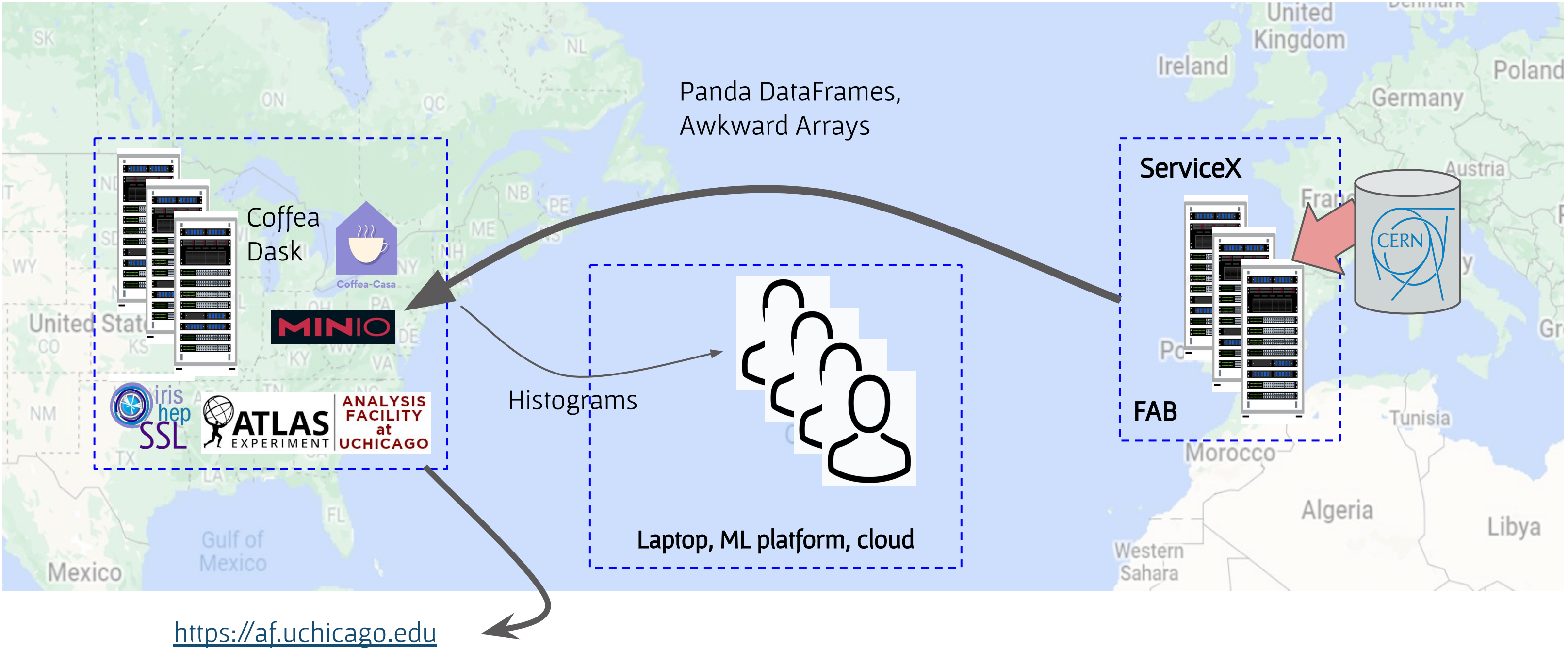


Unique Features @UChicago – ServiceX

- 2 Instances are deployed at AF
  - ATLAS xAOD
  - ATLAS uproot
- Endpoints are publicly accessible
- Authentication via Globus Auth. Account approval via a Slack channel #servicex-signups

R&D Activities @UChicago – ServiceX over FAB

Working with **FAB** (FABRIC Across Borders) to demonstrate ServiceX deployment at CERN, delivery of analysis objects to analysis facilities in the U.S.



https://af.uchicago.edu

Systems integration effort highlights @UChicago

- HTCondor on Kubernetes
  - Pioneered in running a production HTCondor system on Kubernetes
  - Integrated and adapted HPA(Brian's)
- coffea-casa
  - Worked closely with coffea-casa team to support Analysis Grand Challenge
  - Integrated coffea-casa with local account management system: local file system access, fair share.
  - Improved coffea-casa HTCondor integration: created and maintain a HTCondor chart - image prepulling, ephemeral-port-reservation fixes etc.