CS3 2024, CERN

WARNING! KUBERNETES TERMINOLOGY

JupyterHub on Kubernetes as a platform for developing secure shared environment for data analysis at MAX IV

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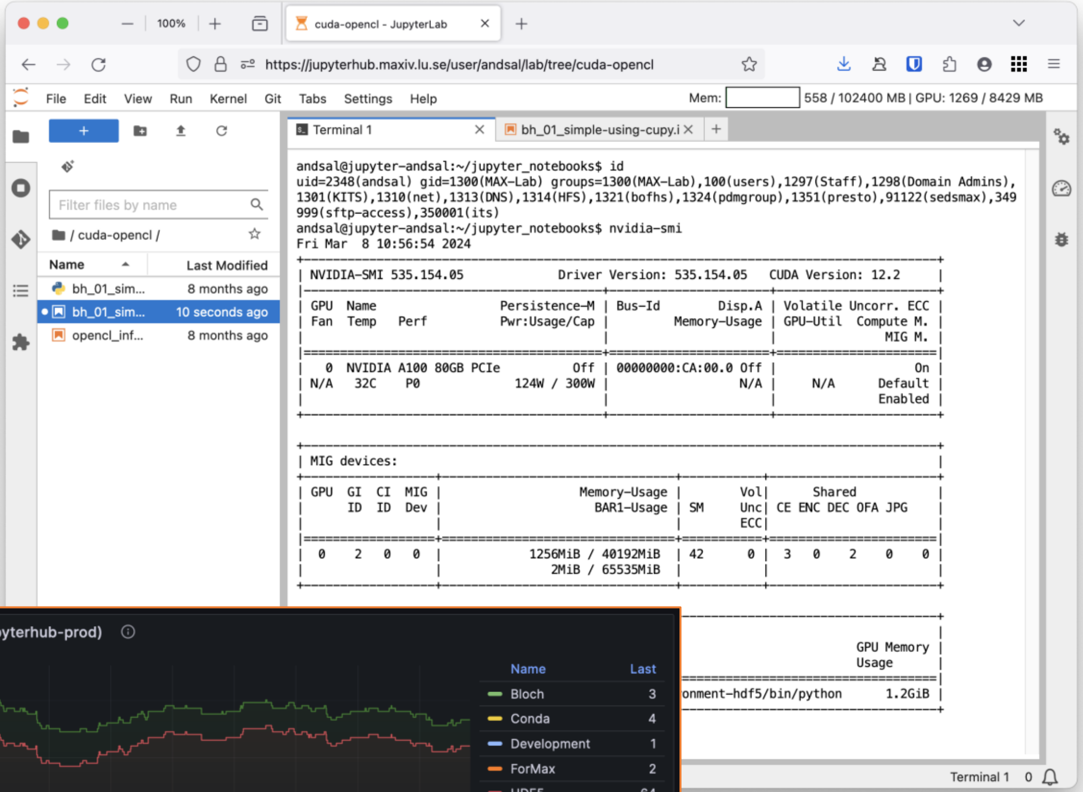
Interactive data analysis environment

- Container images with pre-defined and custom kernels
- Kubernetes cluster
  - as a **resource pool**:
    - Moderate CPU
    - Large RAM
    - V100/A100 GPUs
  - as a **deployment platform:**
    - review/prod/next lifecycle
    - CI testing of notebook images
  - as a **runtime environment**
- Shared service for staff and researchers
  - Remote-desktop style experience
  - Resources overcommit

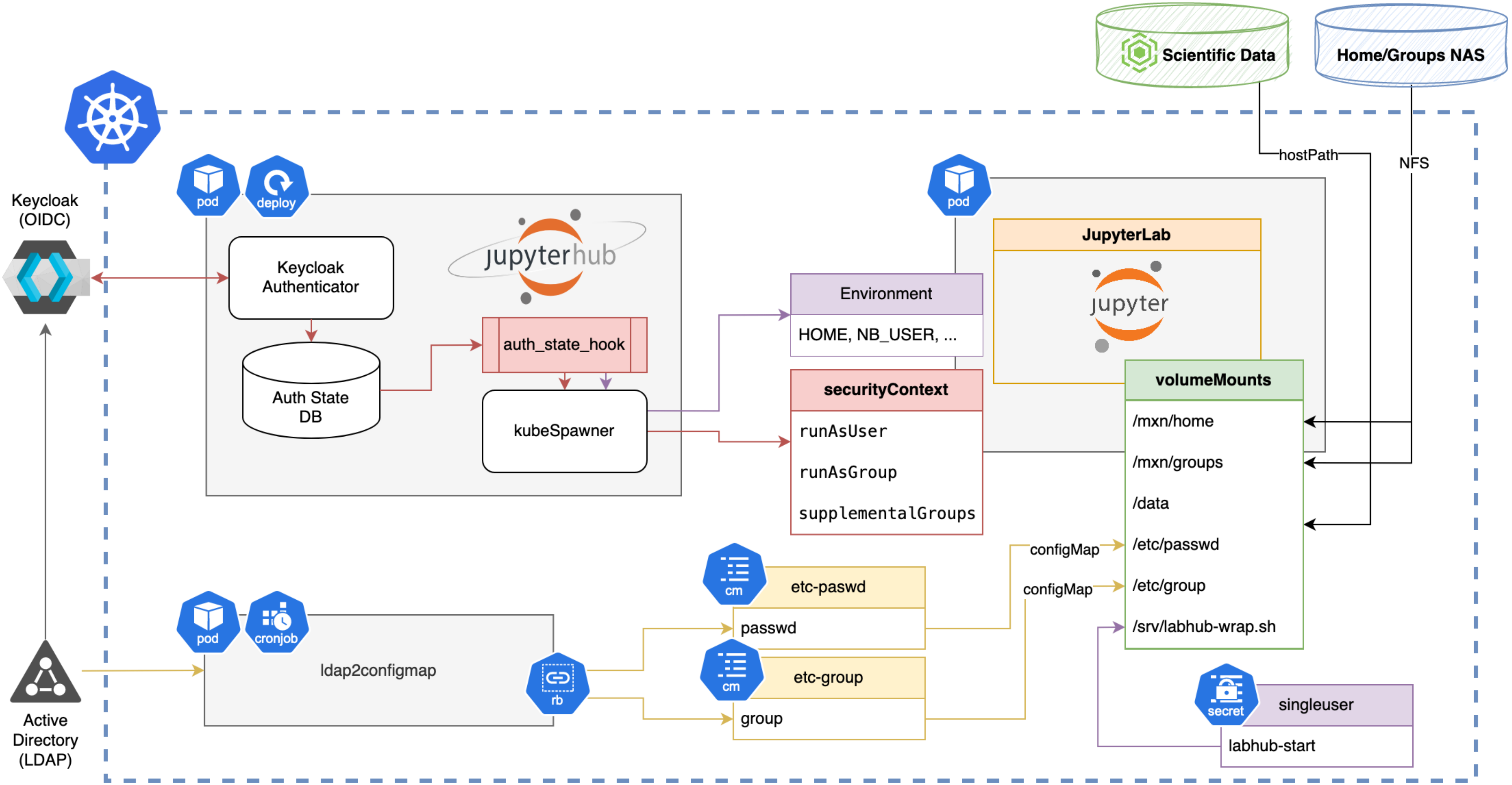


Goals and technical requirements

- **Key objective:** **fully unprivileged** container environment that operates seamlessly **with existing LDAP user credentials**
- **Functional Requirements:**
  - Integration with **MAX IV storage systems** (home, group, data)
  - Run **any notebook images** without modifications
  - Ensure available **resources visibility**
  - Efficient **sharing of available GPU** resources between users
  - Observability of **usage metrics**
- **Operation Requirements:**
  - Zero to JupyterHub with Kubernetes Helm Chart **without** modifications
  - Just custom hooks and proper `values.yaml`

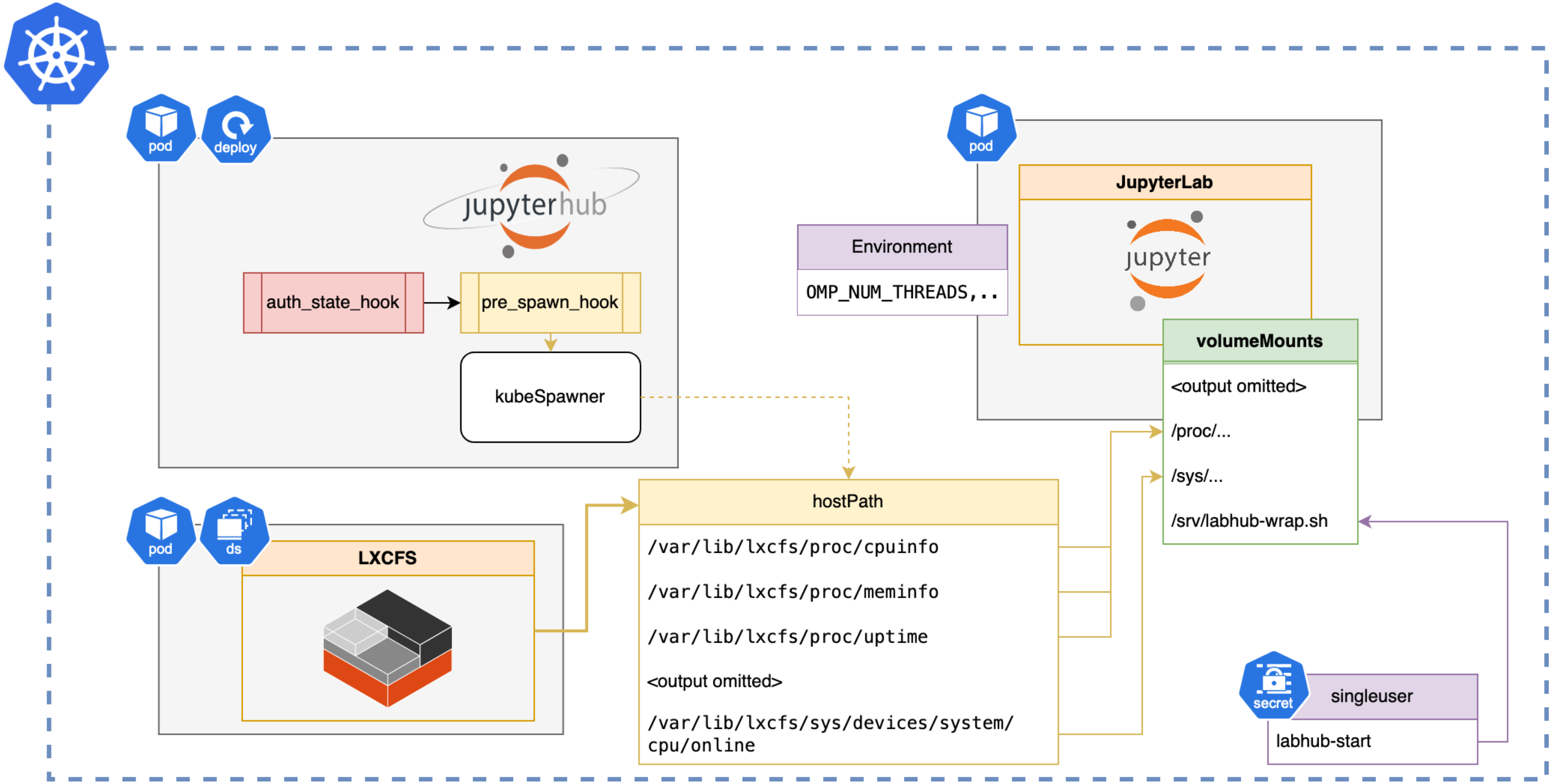
Existing LDAP credentials

- UID/GIDs from Token to `securityContext`
- NSS data sync from LDAP to `configMap` to mount inside container
- Environment variables to define `HOME` directory, etc
- Wrapper startup script to bootstrap environment
- Storage mounts are simply defined in the values.



LXCFS: Resources visibility

- LXCFS is a FUSE filesystem offering overlay files for `cpuinfo`, `meminfo`, `uptime`, etc
- Deployed as DaemonSet on Kubernetes level
- Visible CPU and RAM container limits
- Mounted to `/proc` and `/sys` in `pre_spawn` hook
- Defining additional environment variables in startup scripts



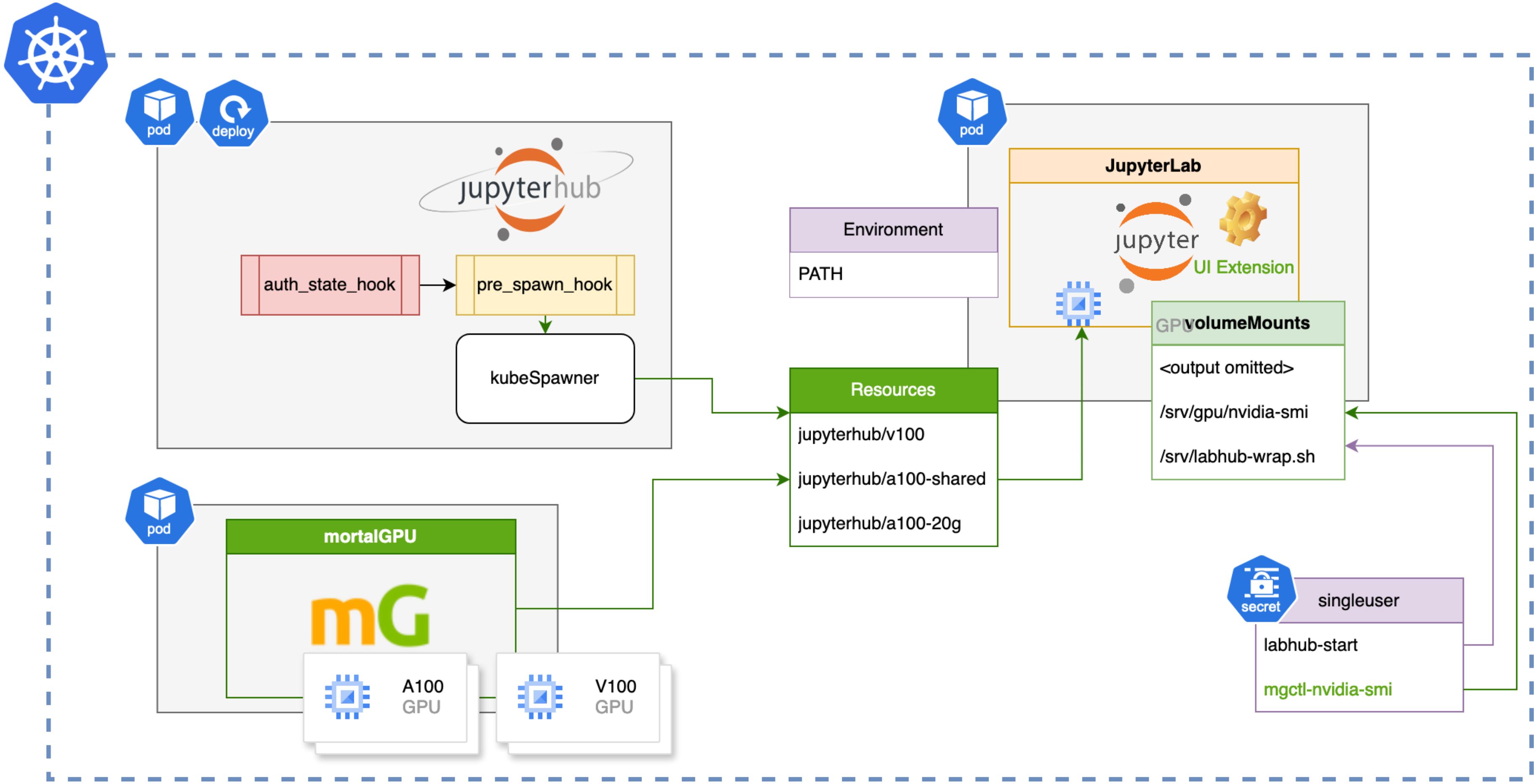
GPU sharing: MortalGPU development

- Kubernetes **device plugin** for GPU **memory overcommit**, while maintaining allocation **l**imit per GPU workload - the approach used for sharing RAM on Kubernetes.
- Fork of MetaGPU with development focus on **interactive workloads** run by mortals (with operations support by mortal admins)
- Provides:
  - Device Plugin: represent GPU (or MIG partition) with configurable number of meta-devices (e.g. `320` of `mortalgpu/v100`)
  - Memory enforcement based on the usage monitoring data
  - Kubernetes-aware observability in general and container-scoped resource usage in particular:
    - `mgctl` tool and Prometheus exporter

Artifact Hub | mortalgpu

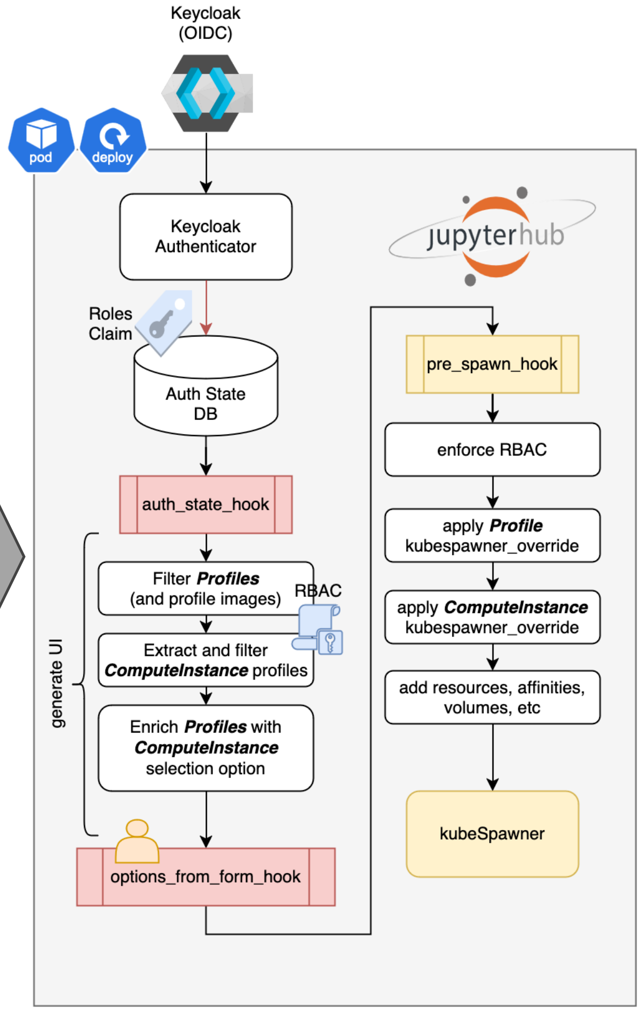
Jupyterhub with MortalGPU

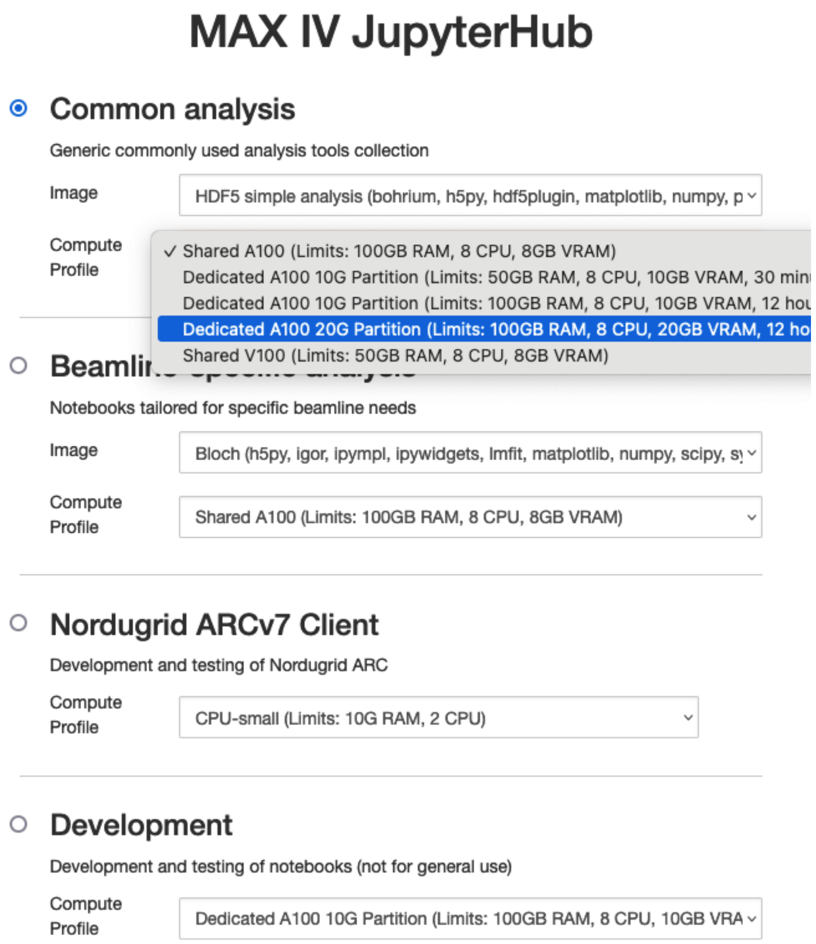
- Kubernetes DaemonSet
- GPU RAM resource requests and limits, **defined the same way as RAM**
- Multiple MortalGPU resources available (different GPUs and partitions)
- Wrapper over `mgctl` to provide `nvidia-smi` output for container processes only



Compute Instance profiles and RBAC

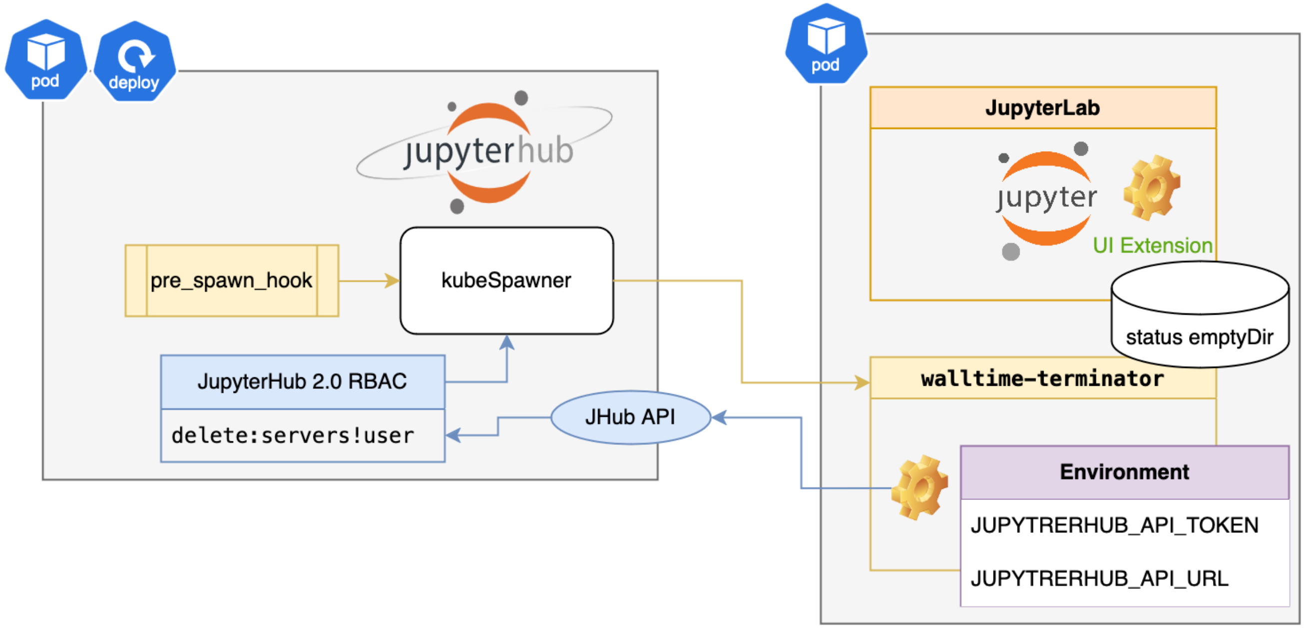
```yaml
profileList:
  # Compute instance resource profiles
  - compute_instances:
      a100_shared:
        display_name: "Shared A100 (Limits: 100GB RAM, 8 CPU, 8GB
        cpu_guarantee: 0.1
        mem_guarantee: 500M
        cpu_limit: 8
        mem_limit: 100G
        gpu_resource_name: jupyterhub/a100-shared
        gpu_guarantee: 4
        gpu_limit: 80
        node_type: a100
      a100_20g:
        display_name: "Dedicated A100 20G Partition (Limits: 100G
        required_role: a100-20g
      # ...
  - display_name: "Beamline-specific analysis"
    description: "Notebooks tailored for specific beamline needs"
    slug: "beamline"
    allowed_compute_instances:
      - a100_shared
      - a100_10g_quick
      - a100_10g
      - a100_20g
      - v100
    profile_options:
      image:
        display_name: Image
        choices:
          bloch:
            display_name: "Bloch (h5py, igor, ipympl, ipywidgets,
            kubespawner_override:
              image: harbor.maxiv.lu.se/jupyterhub/bloch-notebook
```





Extra containers = extra features

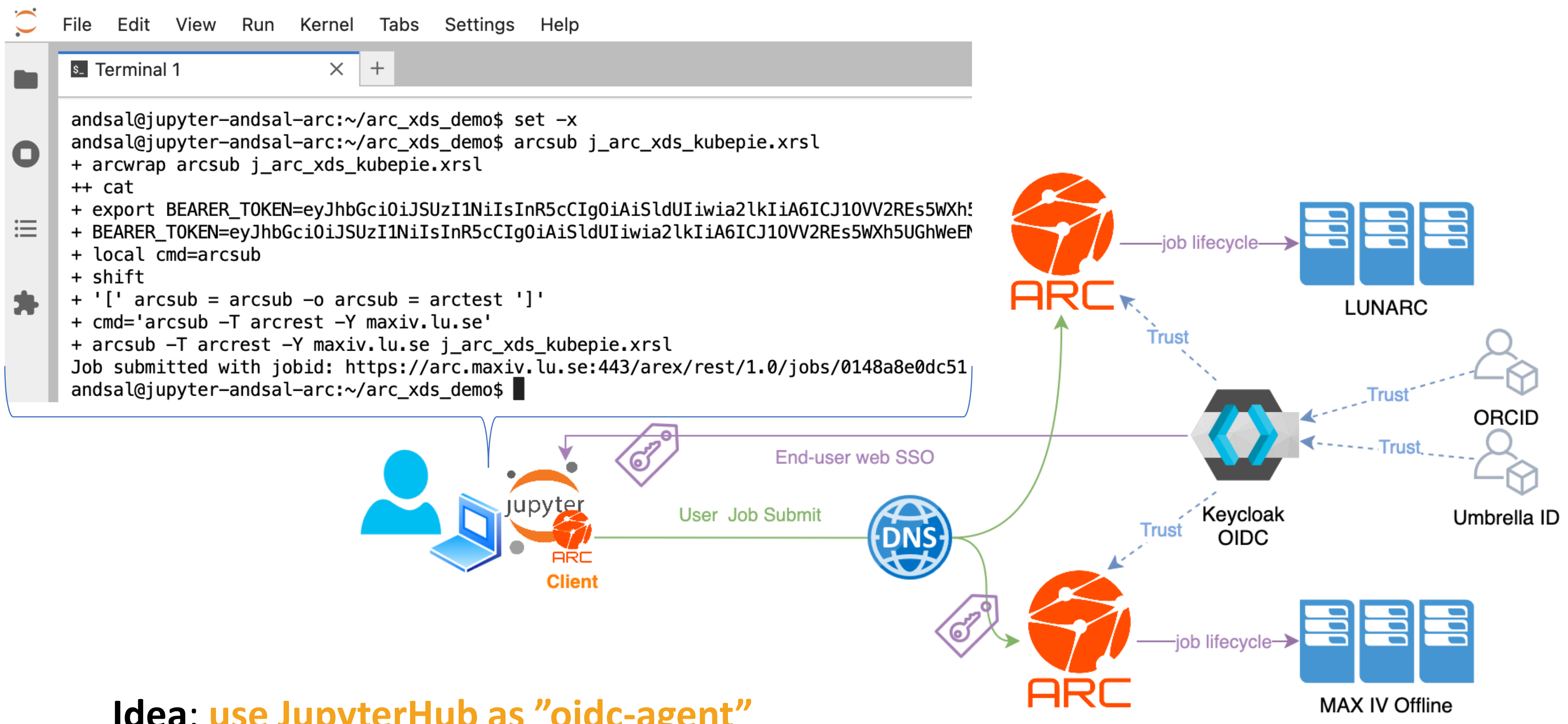
Walltime enforcement



- KubeSpawner is capable of running additional containers in the user Pod
- Isolated walltime countdown container terminating user server via JupyterHub API
  - Using the JupyterHub RBAC feature
- Developed UI extension to show values to end-user

Use-case: Nordugrid ARC Client

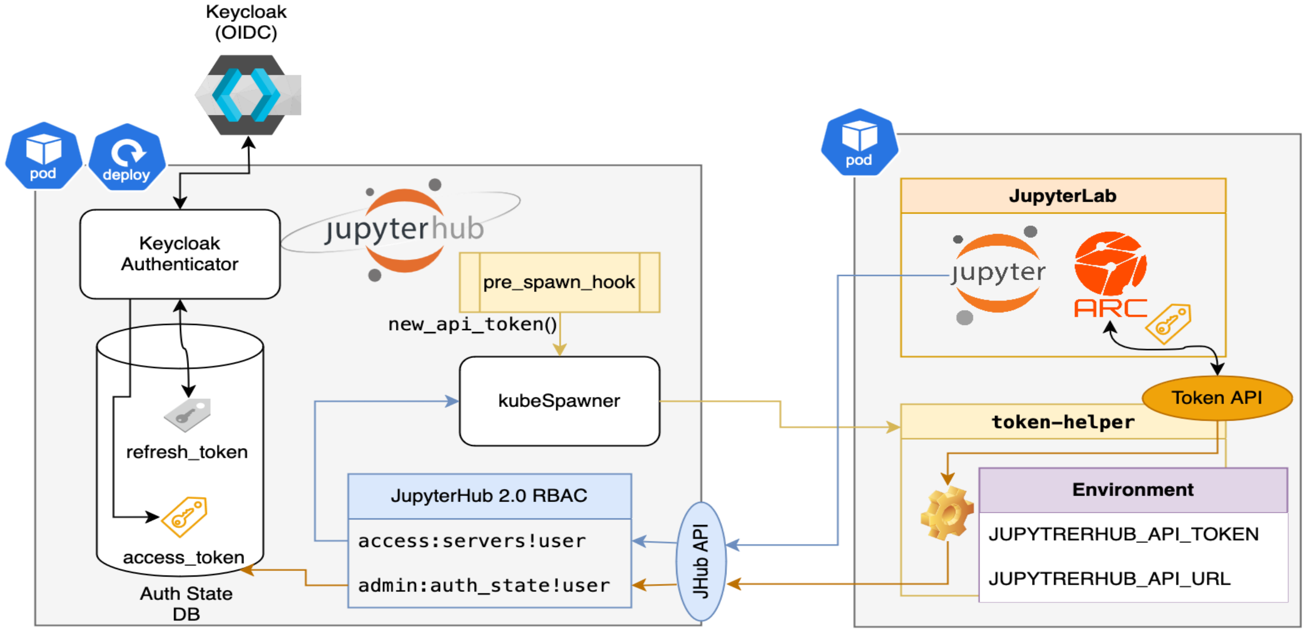
- PoC: Small grid for transparent HPC usage
- ARC with OAuth2 JWT tokens auth:
  - Map to self at MAX IV resources
  - Map to pool on external resources
- Additional challenge: existing data sharing to external sites with JWT auth, following user permissions



Idea: use JupyterHub as "oidc-agent"

Extra containers = extra features

"OIDC-agent" for ARC



- KeyCloak Authenticator to refresh access tokens
- Isolated token-helper container with privileges to read `auth_state`
  - Using the Jupyterhub RBAC feature
- API to provide only Access Tokens to JupyterLab container
  - wrapper to use in ARC CLI transparently

KubePie: sharing existing data over https

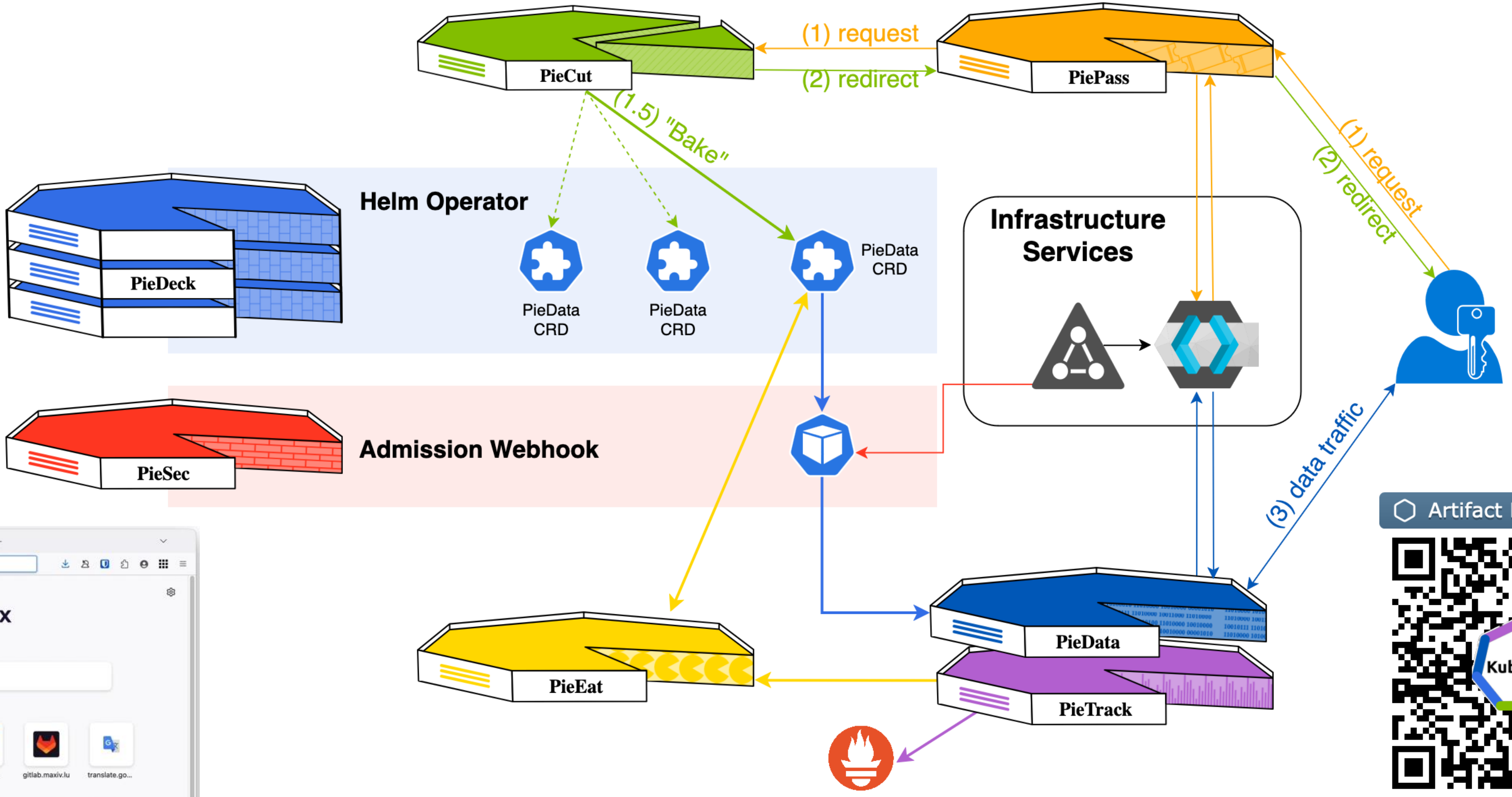
- **Idea**: *”own”* web server for each user with the correct UID/GIDs
  - *Sounds crazy? But we do run such Pods for each user in JupyterHub!*

CHALLENGE ACCEPTED

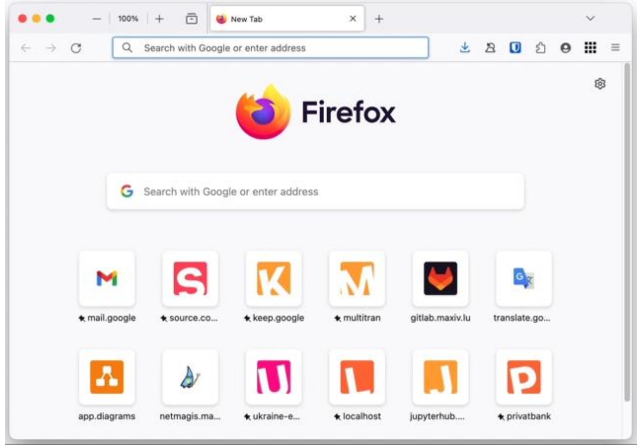
- **KubePie** is harnessing Kubernetes' scalability and deployment capabilities by running, managing and securing web servers for every user
- **KubePie** is strictly relying on *OpenID Connect* flow or *OAuth2 bearer tokens* when it comes to the user identification
  - OAuth2 used in ARC PoC for data transfers
  - Claims-based user-mapping during Pod instantiation (admission)
  - Other auth credentials accessible via OIDC:
    - WebDAV with S3-like credentials is implemented as an example

Artifact Hub kubepie

KubePie: Baking process



KubePie@MAX IV is running on the Data Acquisition Kubernetes Cluster



Artifact Hub kubepie

KubePie

Conclusions

- Extensibility of both JupyterHub and Kubernetes *allows* to build data analysis platforms, matching organization needs in functionality and security.
- LXCFS on the Kubernetes *brings* allocated resources visibility to both interactive and batch containerized workloads.
- Flexible and observable GPUs sharing with MortalGPU *enriches* the interactive shared environments with CUDA capabilities.
- Compute Instance profiles and RBAC *extends* the usage patterns of the shared platform, improving the end-user experience.
- Additional containers in the running Pod *open a way* to securely add features beyond the usual JupyteHub capabilities.

Thank you for attention!

Ask me about:

Source code and deployment configuration can be found on gitlab.com

EUROPEAN OPEN SCIENCE CLOUD

We are working towards establishing similar deployment for providing EOSC service as Open Data analysis platform

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