Data Lake as a Service for Open Science

Riccardo Di Maria (CERN)

June 2nd, 2022 - HSF Analysis Facilities Forum

ESCAPE - The European Science Cluster of Astronomy & Particle Physics ESFRI Research Infrastructures has received funding from the European Union's Horizon 2020 research and innovation programme under the Grant Agreement n° 824064.

ESCAPE
European Science Cluster of Astronomy & Particle physics ESFRI research Infrastructures

Science Projects

HiLumi HL-LHC PROJECT
SKA SQUARE KILOMETRE ARRAY
VIRGO
FAIR
KM3NeT
JIVE Joint Institute for VLBI ERIC
cta cherenkov telescope array
LSST
EST european solar telescope
ESO
CERN

ESCAPE

European Science Cluster of Astronomy & Particle physics ESFRI research Infrastructures

EUROPEAN OPEN SCIENCE CLOUD

Horizon2020
European Union Funding
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Partners

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INFN
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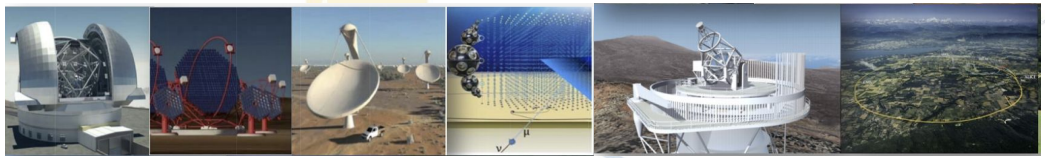
rijksuniversiteit groningen
CCIN2P3
cnrs
PIC port d'informació científica
LAPP Laboratoire d'Annecy de Physique des Particules
INAF ISTITUTO NAZIONALE DI ASTROFISICA NATIONAL INSTITUTE FOR ASTROPHYSICS

Project Goals

- Prototype an infrastructure adapted to exabyte-scale **future needs** of large science projects
- Ensure sciences drive the development of EOSC
- Address FAIR data management principles



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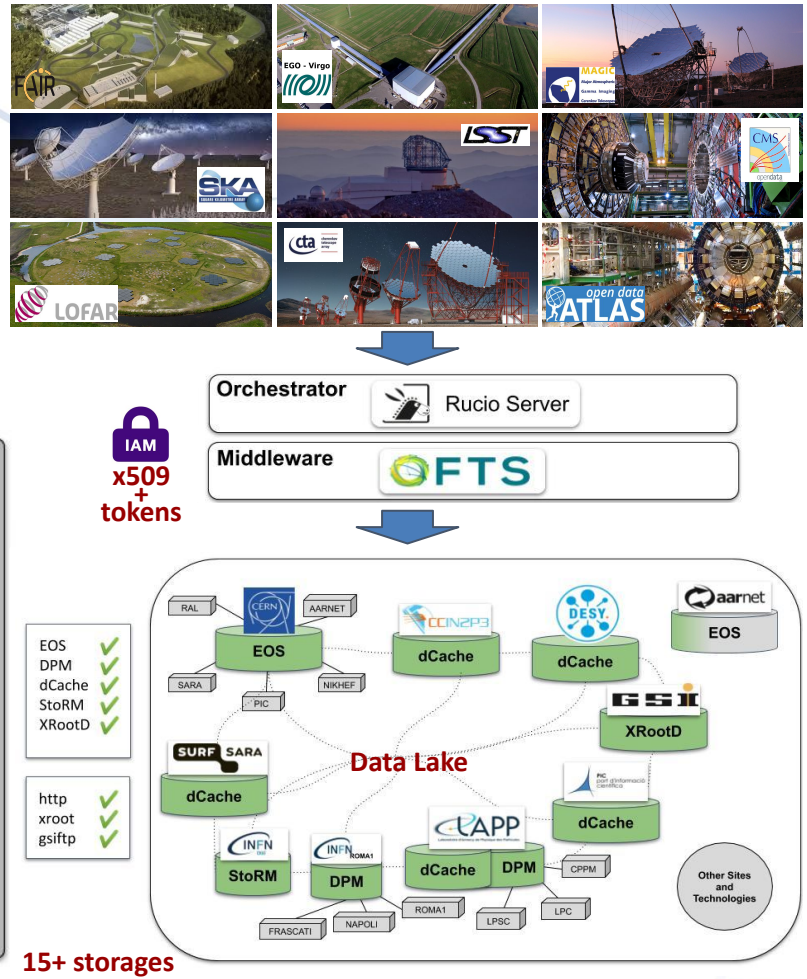
The Data Lake

- Data Lake as modular ecosystem of services and tools shaped around the ESCAPE scientific communities
  - federated data management and access solution
  - heterogeneous resources
    - e.g. integration of HPC and **commercial Clouds**
- Hiding complexity and providing transparent access to data
  - layer for orchestration of resources as entry point for sciences
    - define data policies and rules
  - content delivery and caching layer
    - HTTP data access and Tokens awareness for future sustainability
    - latency hiding and file re-usability
    - facilitate ingress/egress with Clouds and HPC
- Storage and compute resources not necessarily colocated



Further info: https://wiki.escape2020.de/index.php/WP2_-_DIOS#Datalake_Status

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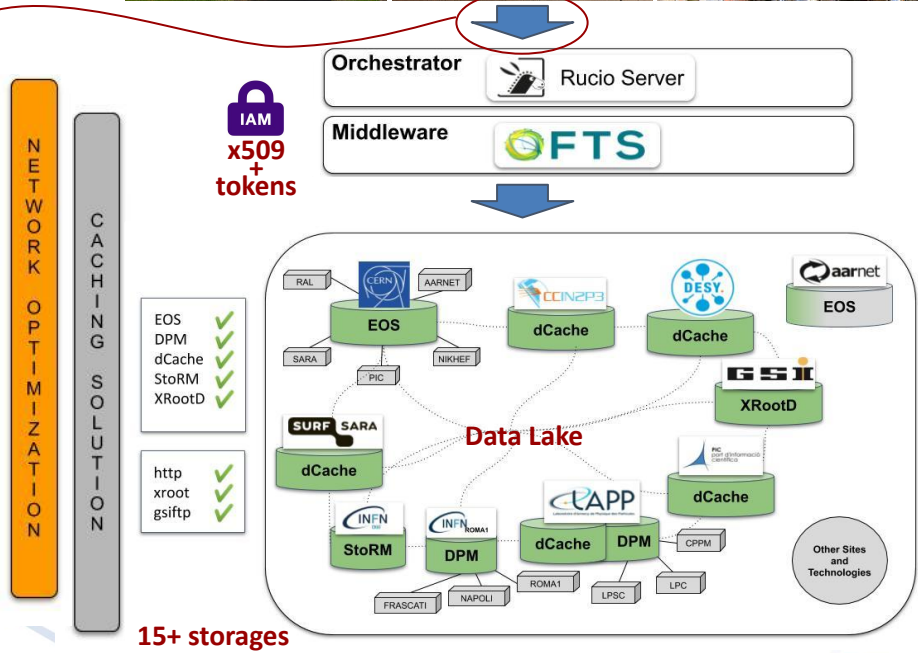
DLaaS for Open Science

- Goal: make **end-user comfortable** in embarking on a Data Lake experience
  - abstract the complexities of the Data Lake from the scientists
    → focus on doing science instead of data procurement
- An ever-increasing number of experiments are looking at Rucio Data Management system
  - **DLaaS** potentially interesting for both **aficionados** and **newcomers**



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As It All Started

- An idea presented at CS3 2020 by the Rucio team [1]
- Development of a “Rucio JupyterLab Extension” as part of GSoC 2020 [2,3]
- A long time has passed, many things have happened…
  - CERN OpenLab Summer Student to concretise the effort in 2021
    - deployment, docker-images, documentation
  - DataLake-as-a-Service (DLaaS) in production-like phase
    - extensively exploited during ESCAPE “Data and Analysis Challenge” in November 2021 by SKA, MAGIC, CTA, ATLAS, KM3NET, LOFAR, FAIR
      → 3rd ESCAPE DIOS Workshop
    - EU projects e.g. EOSC-Future and CS3Mesh4EOSC/ScienceMesh
    - other communities e.g. EGI

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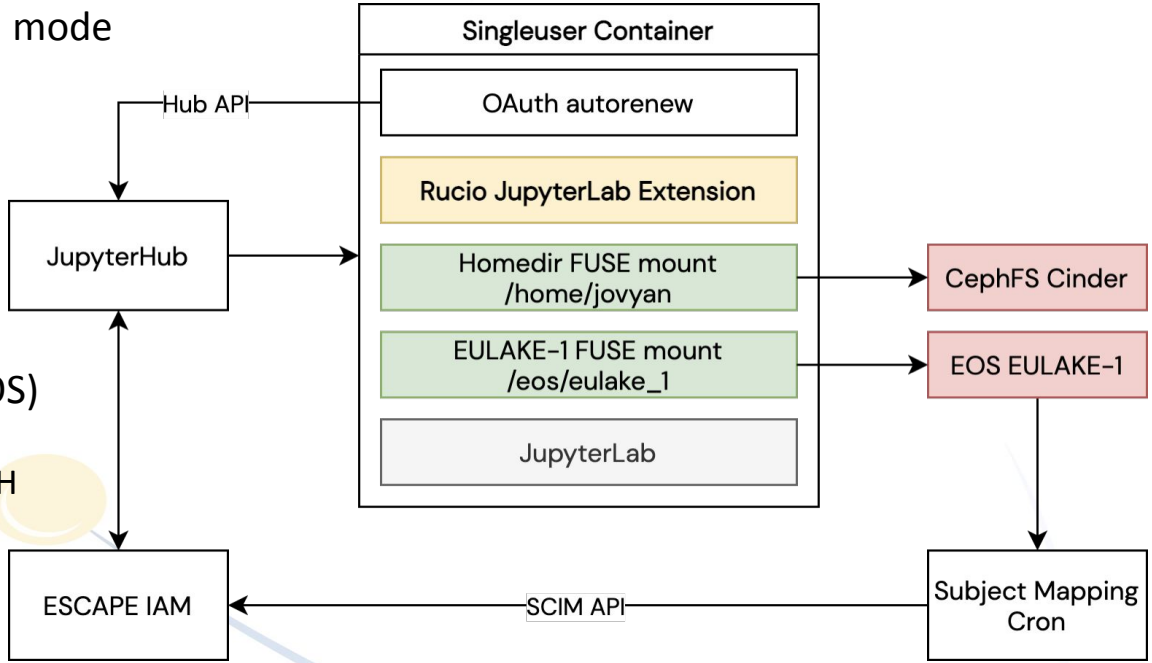
DLaaS Implementation

RSE = Rucio Storage Element

- Deployed in Kubernetes, using Zero-to-JupyterHub Helm chart → https://escape-notebook.cern.ch
- OAuth authentication using ESCAPE IAM (X509 still supported)
- Rucio JupyterLab Extension in Replica mode (i.e. TPC to local storage) used
  - download mode still possible (if configured)
  - connected to ESCAPE Data Lake
  - automatically pre-configured to use OpenID Connect
  - 2 FUSE mounts to EULAKE-1 (EOS)
    - ESCAPE RSE in r-only
    - additional RSE in r/w: SCRATCH
  - making files available *aka* creating a replication rule to move files to EULAKE-1



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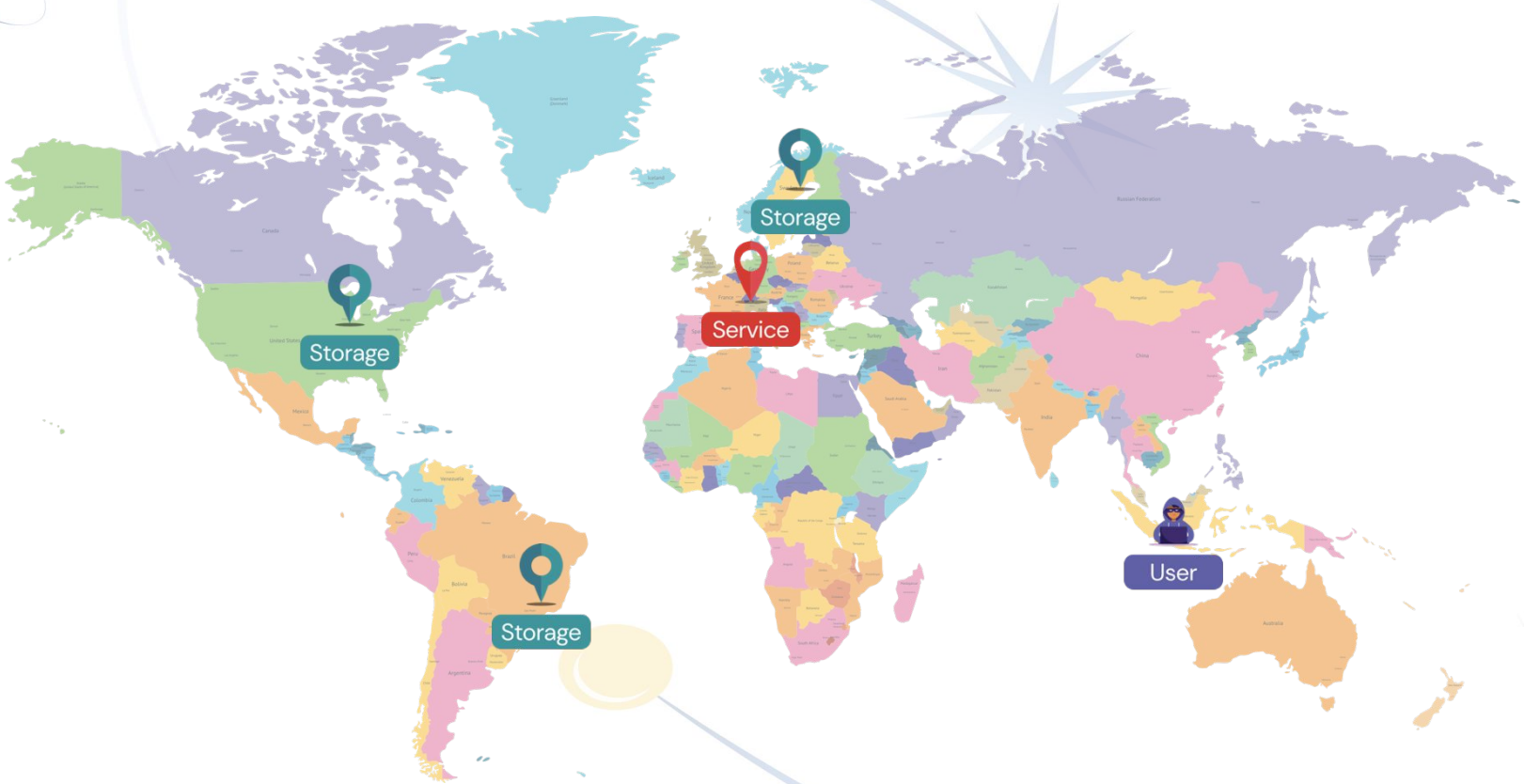
DataLake-as-a-Service for Open Science



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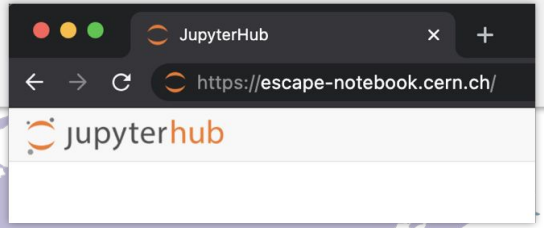
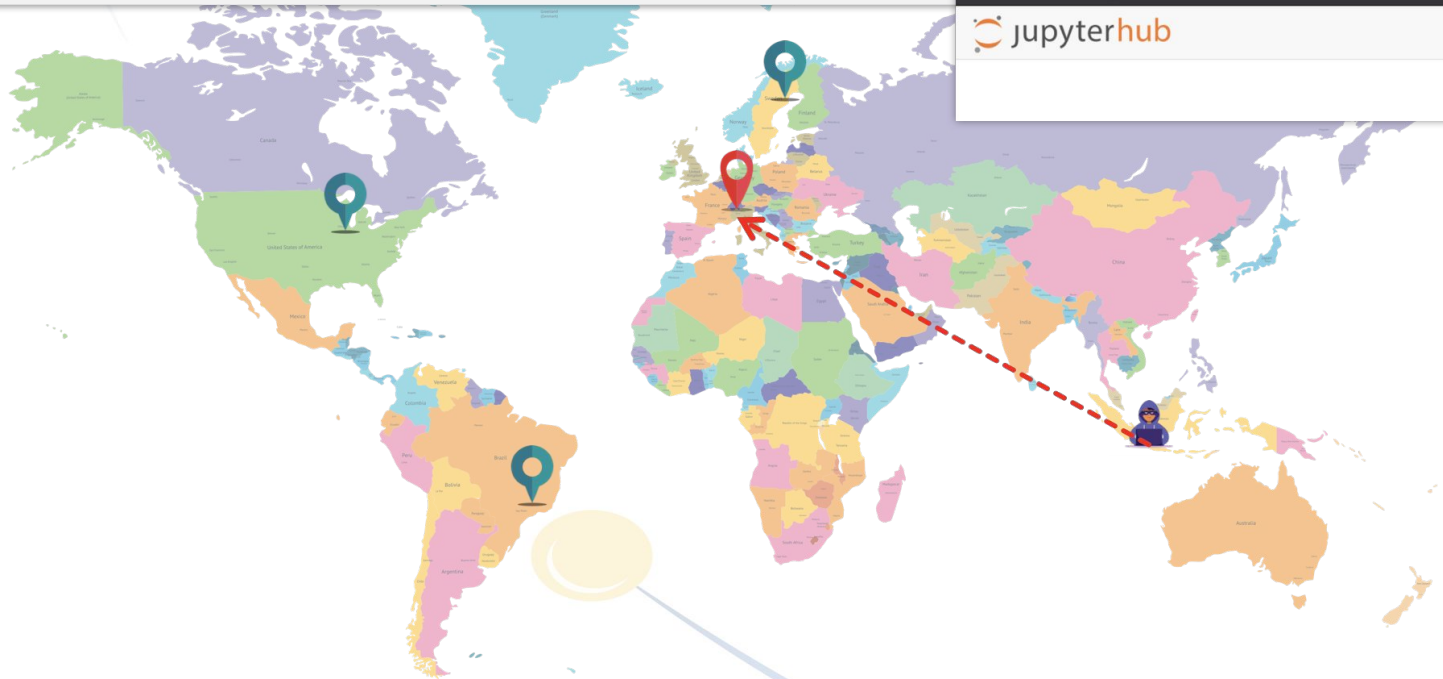
Contact DLaaS

→ Scientists Contact DataLake-as-a-Service

Requests are handled by Jupyter servers at CERN, Geneva





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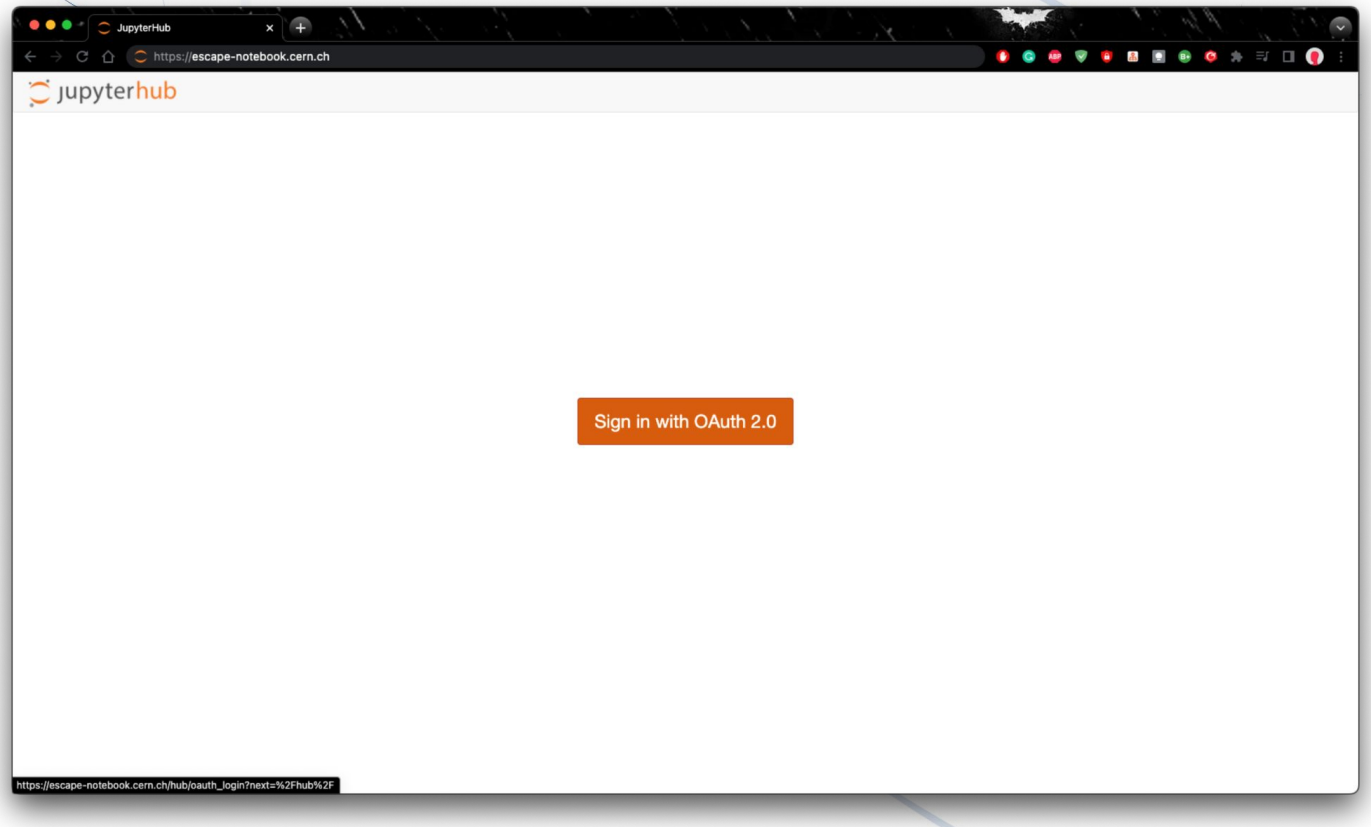
Sign in with OAuth 2.0



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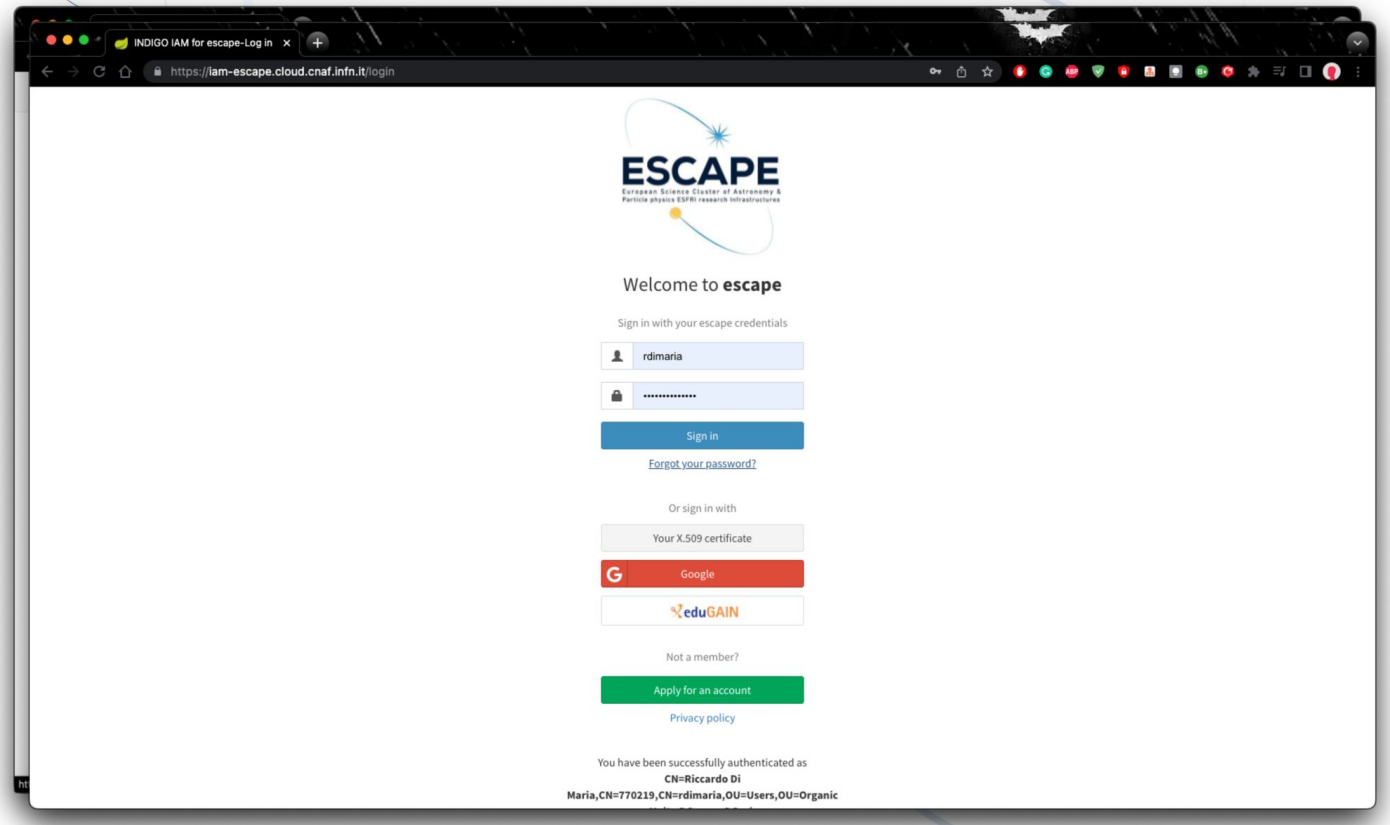
ESCAPE Indigo IAM for Auth



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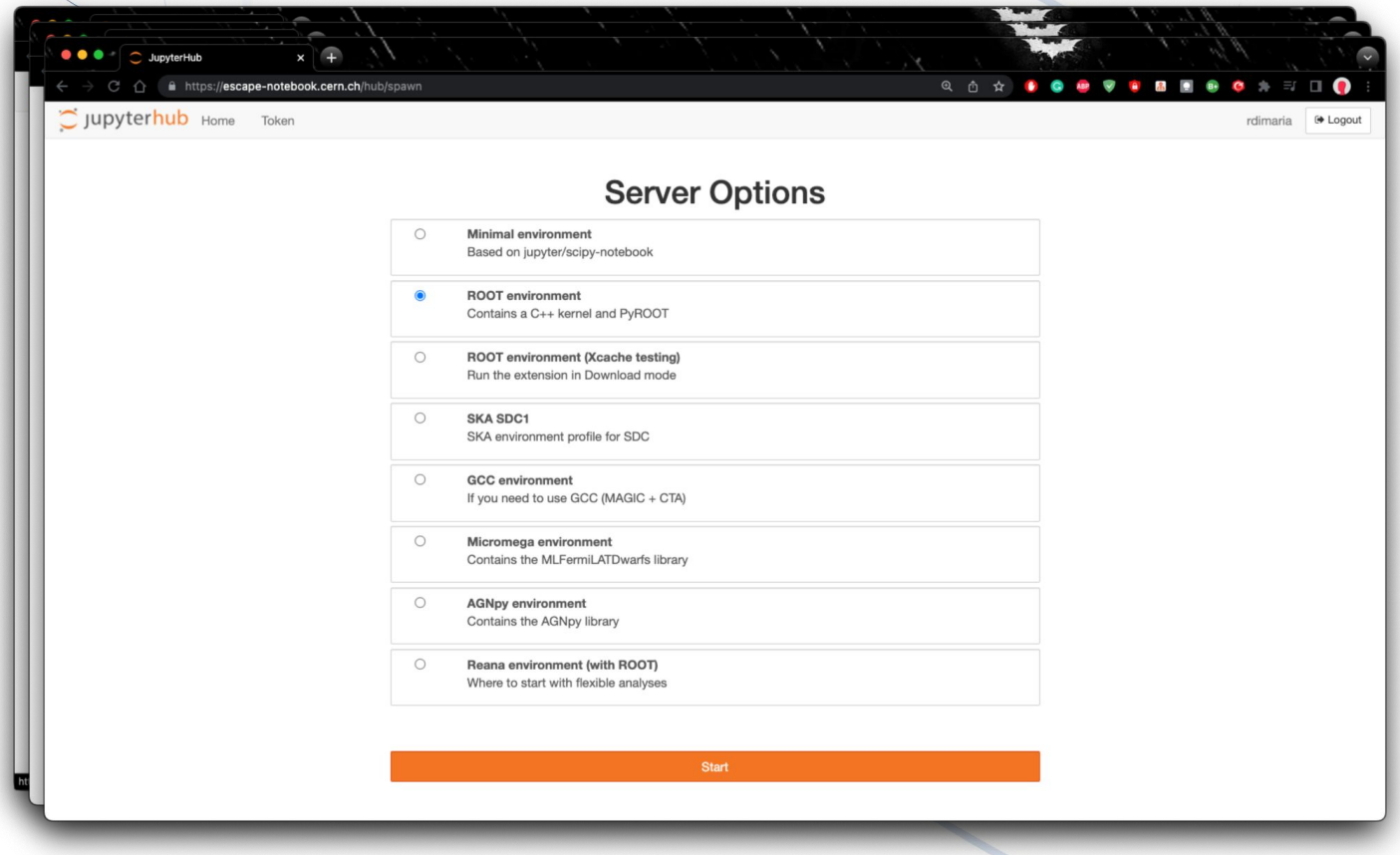
Multiple Server Options for Sciences



Each experiment builds and manage the image, which is available to be selected before starting the user session through the **Server Options** page.

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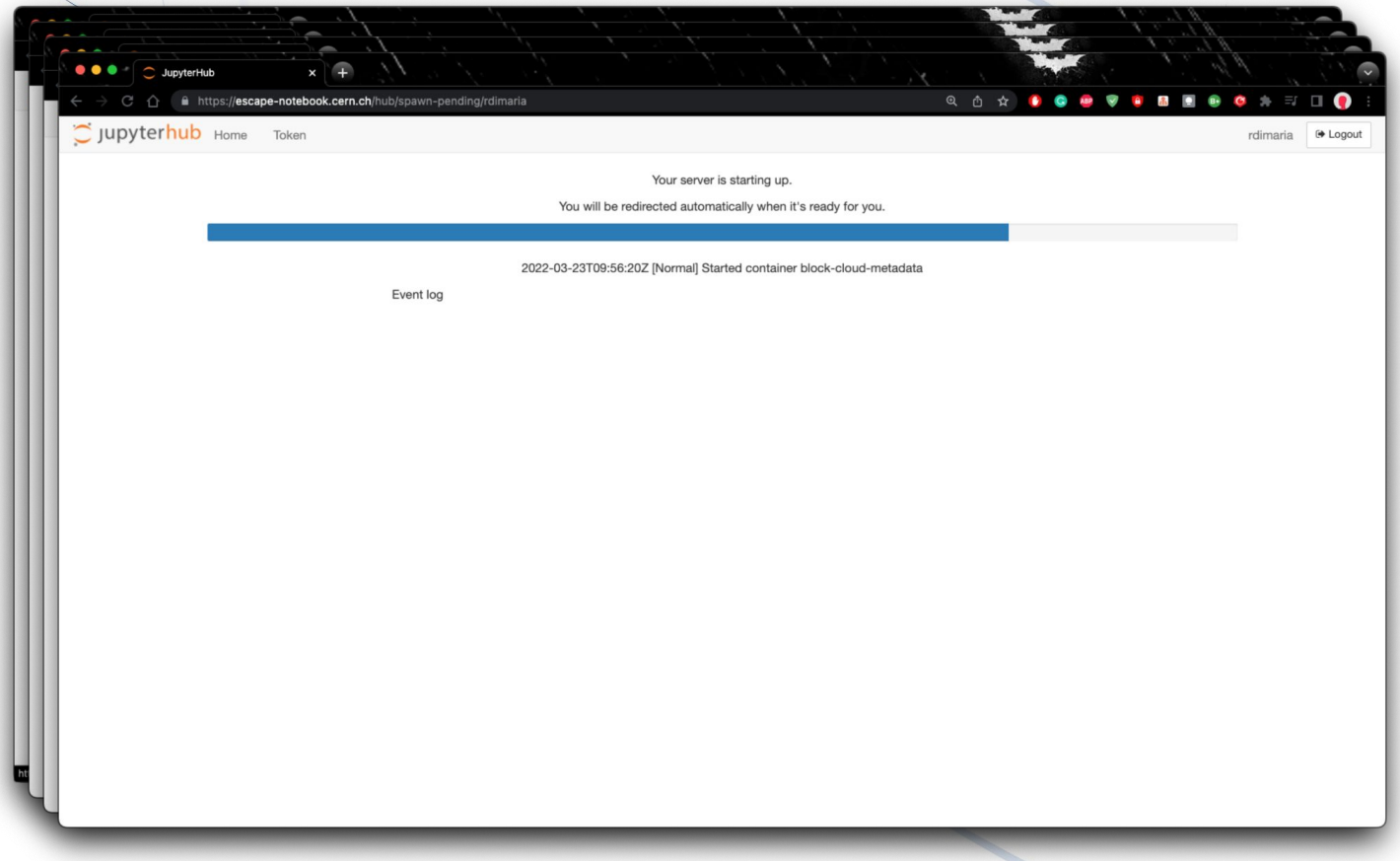
K8s-Pod per User



The user session is realised spawning a dedicated k8s-Pod.

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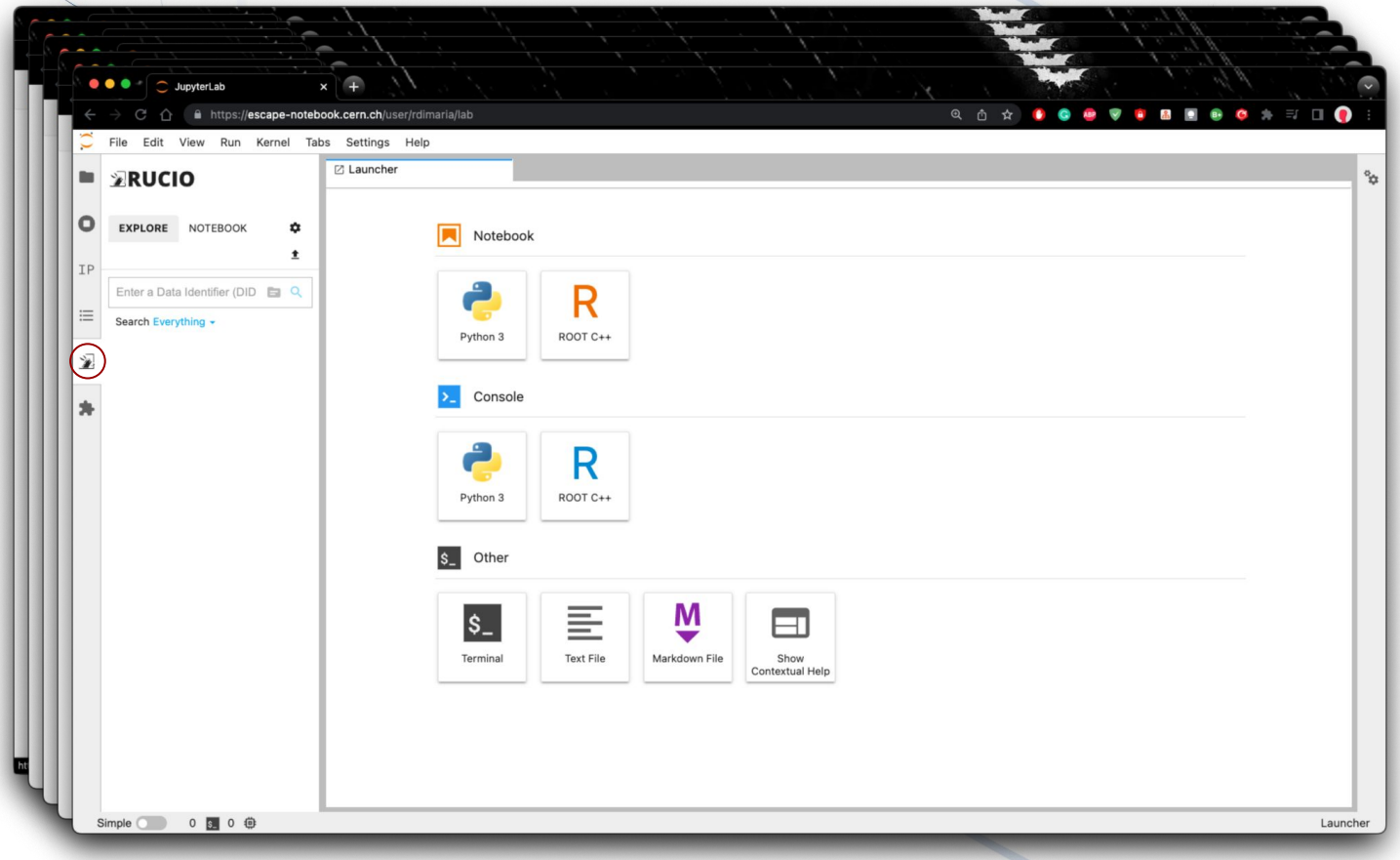
Jupyter Notebook with Rucio Extension



The [Rucio JupyterLab extension] is the core of DLaaS.

The relegated repo is hosted by Rucio, and jointly maintained with ESCAPE and EOSC-Future, and whoever is interested in improving it.

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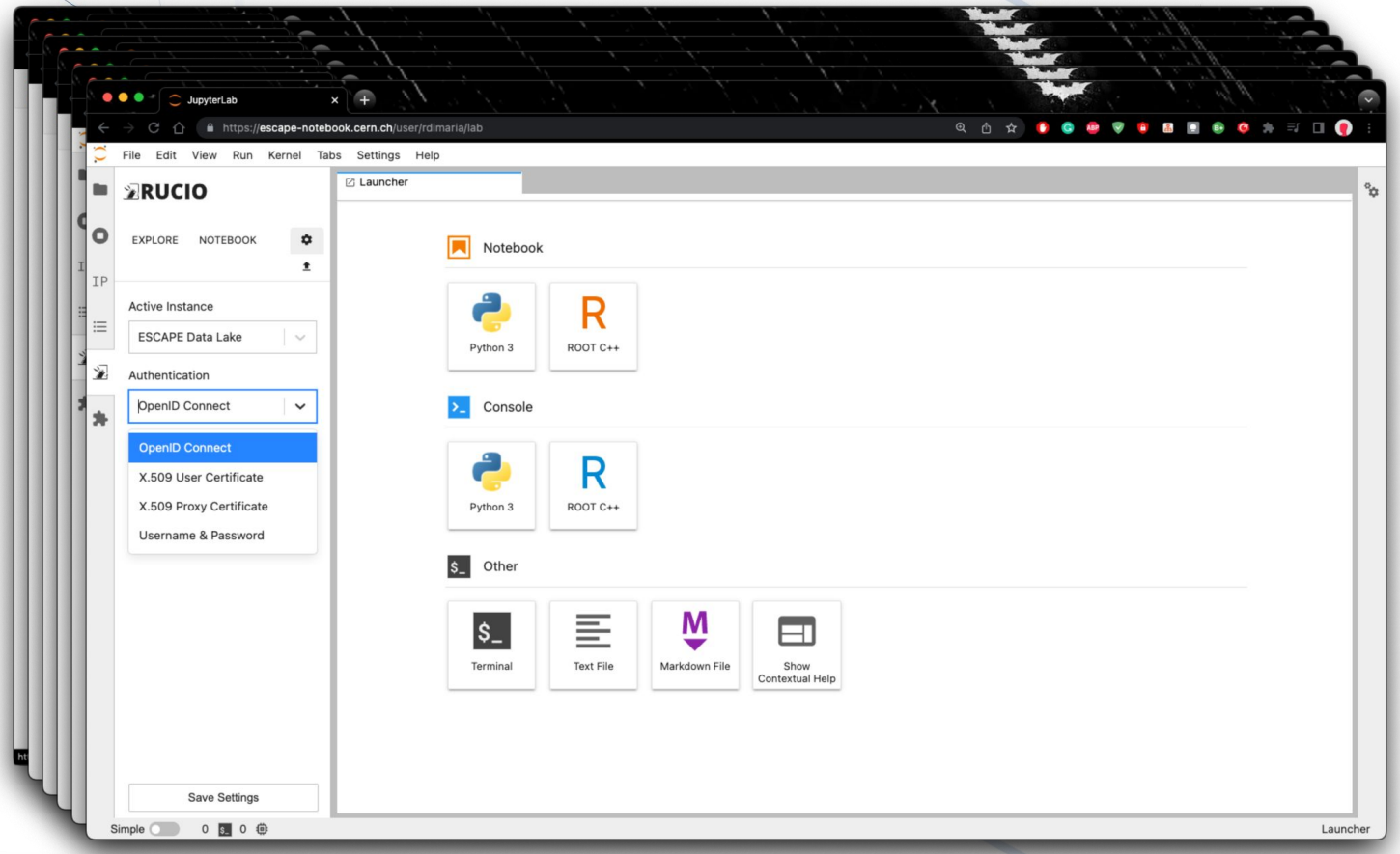
ESCAPE Rucio Instance and OpenID Connect



OpenID Connect Auth is by default. Changing it to X509 cert or proxy results in a manual action needed from the user (rucio.cfg to be changed accordingly). Dev work is needed in this respect.

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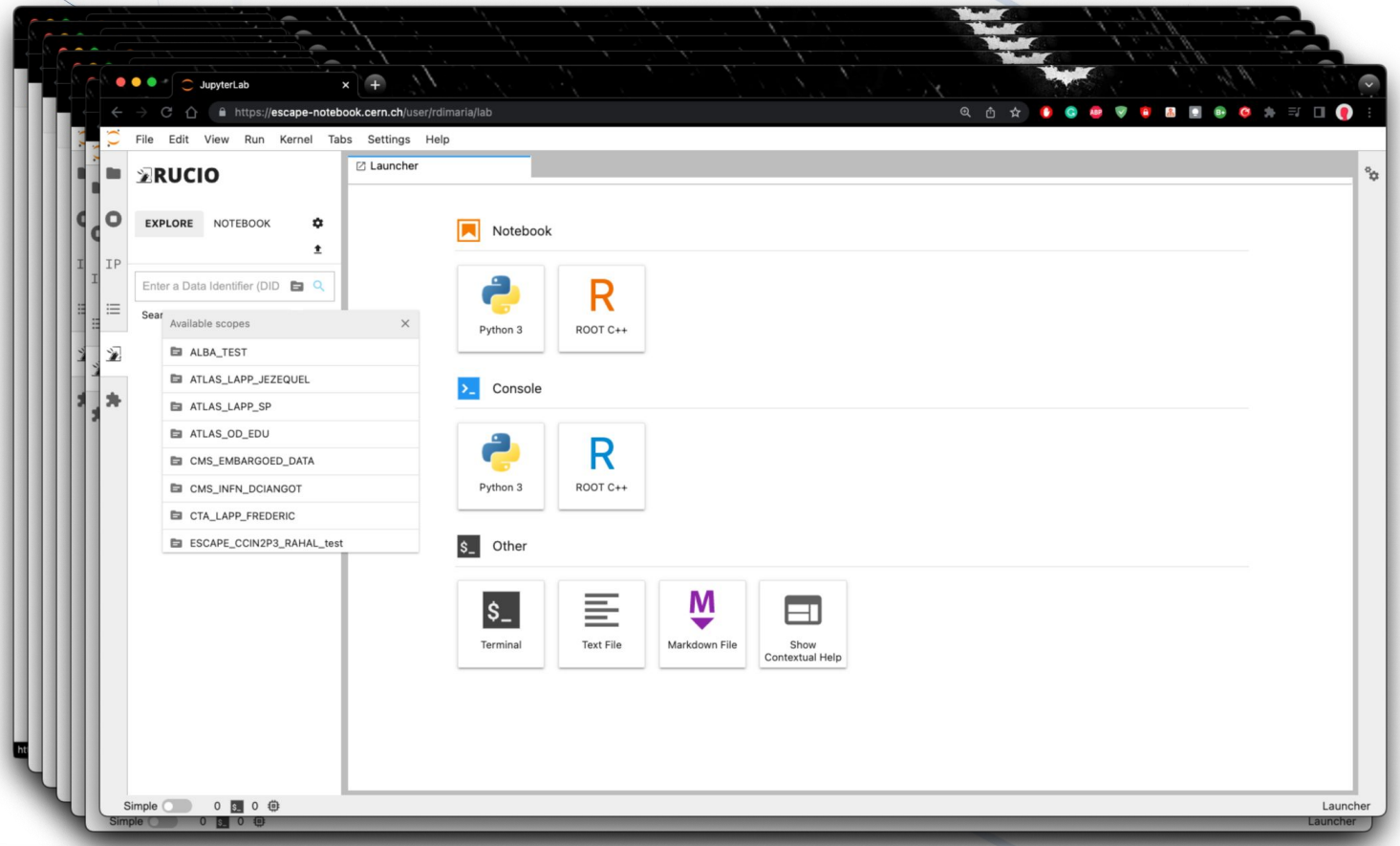
Data Browsing



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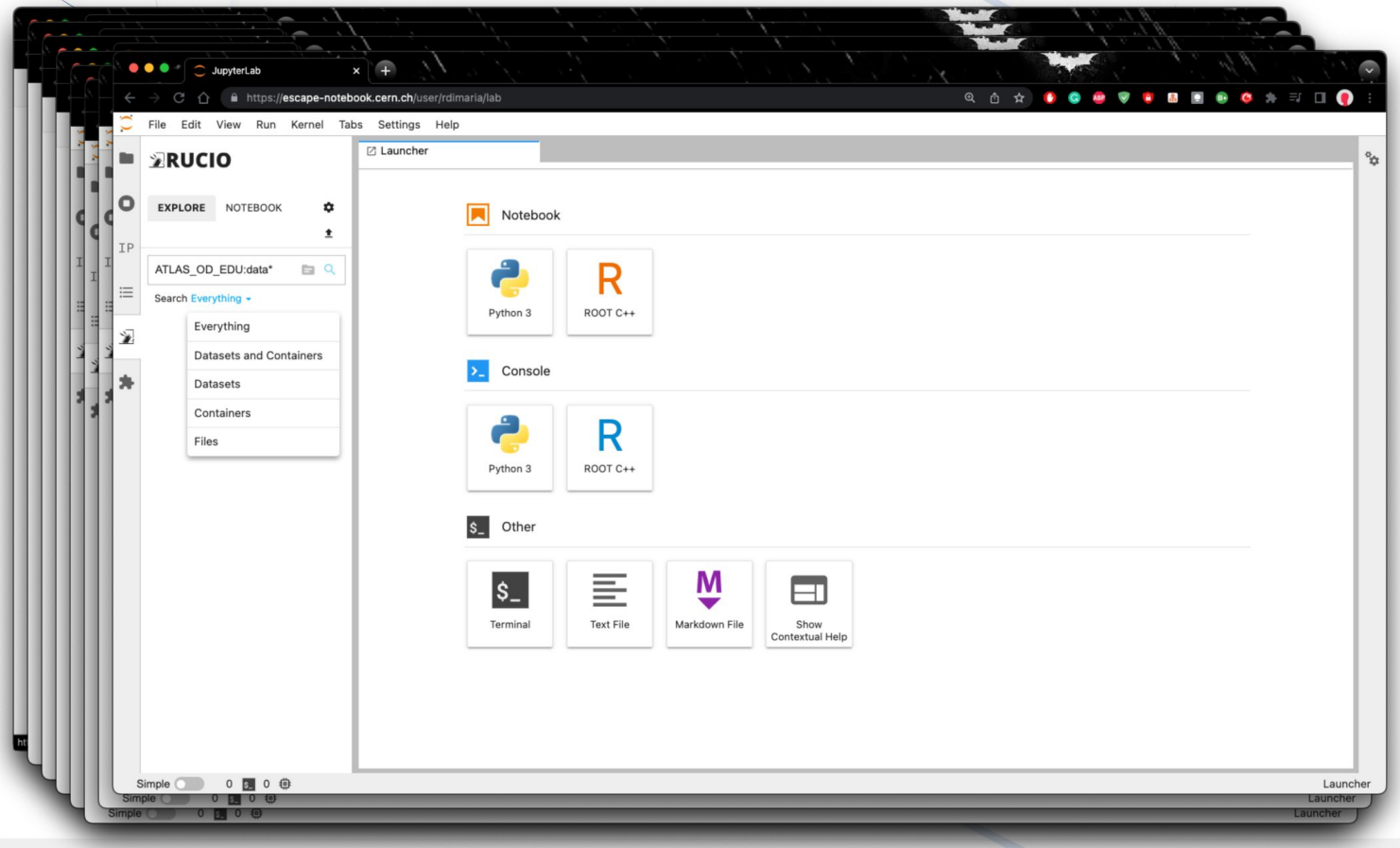
Data Browsing



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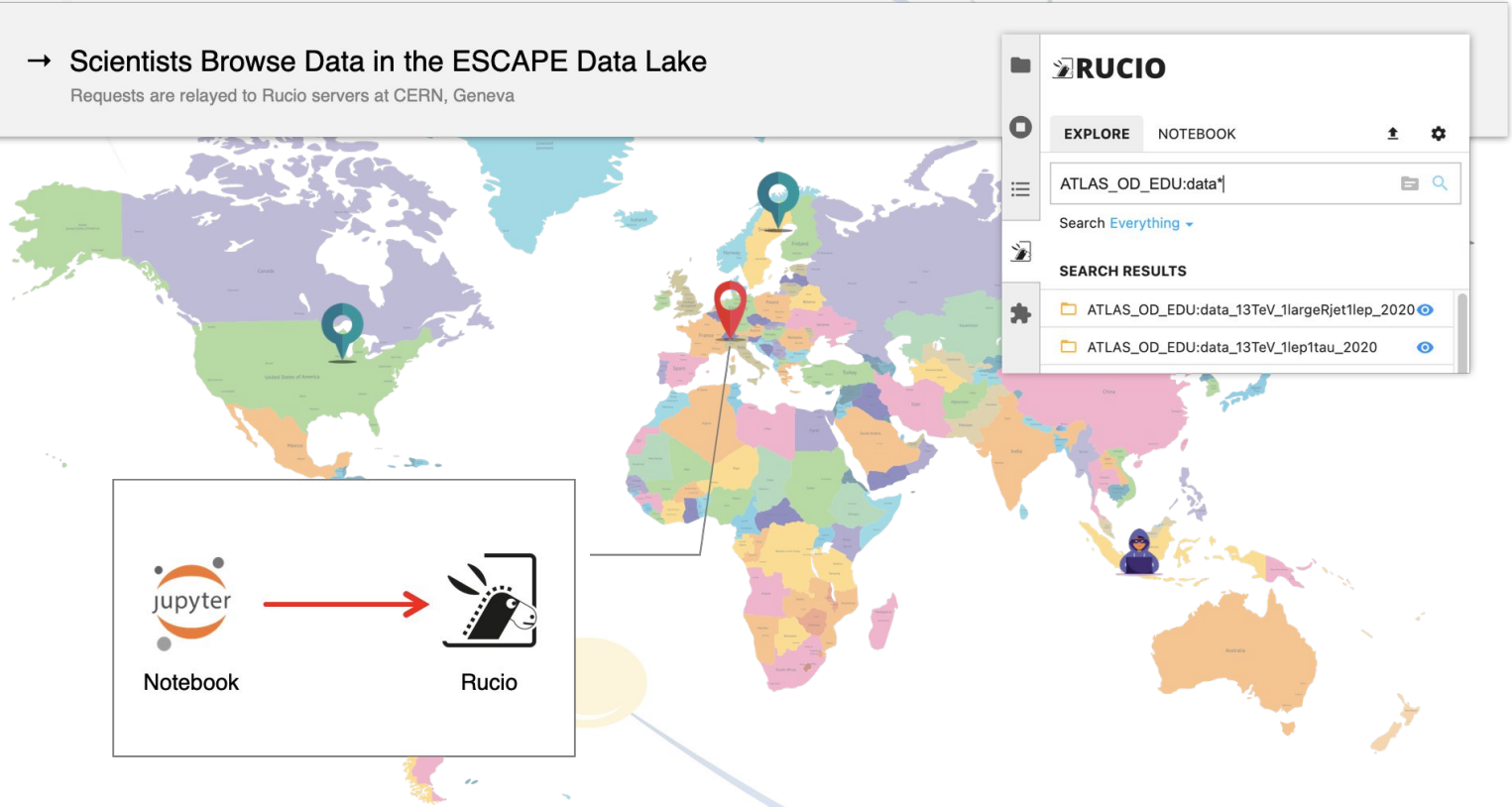
Data Browsing

→ Scientists Browse Data in the ESCAPE Data Lake

Requests are relayed to Rucio servers at CERN, Geneva



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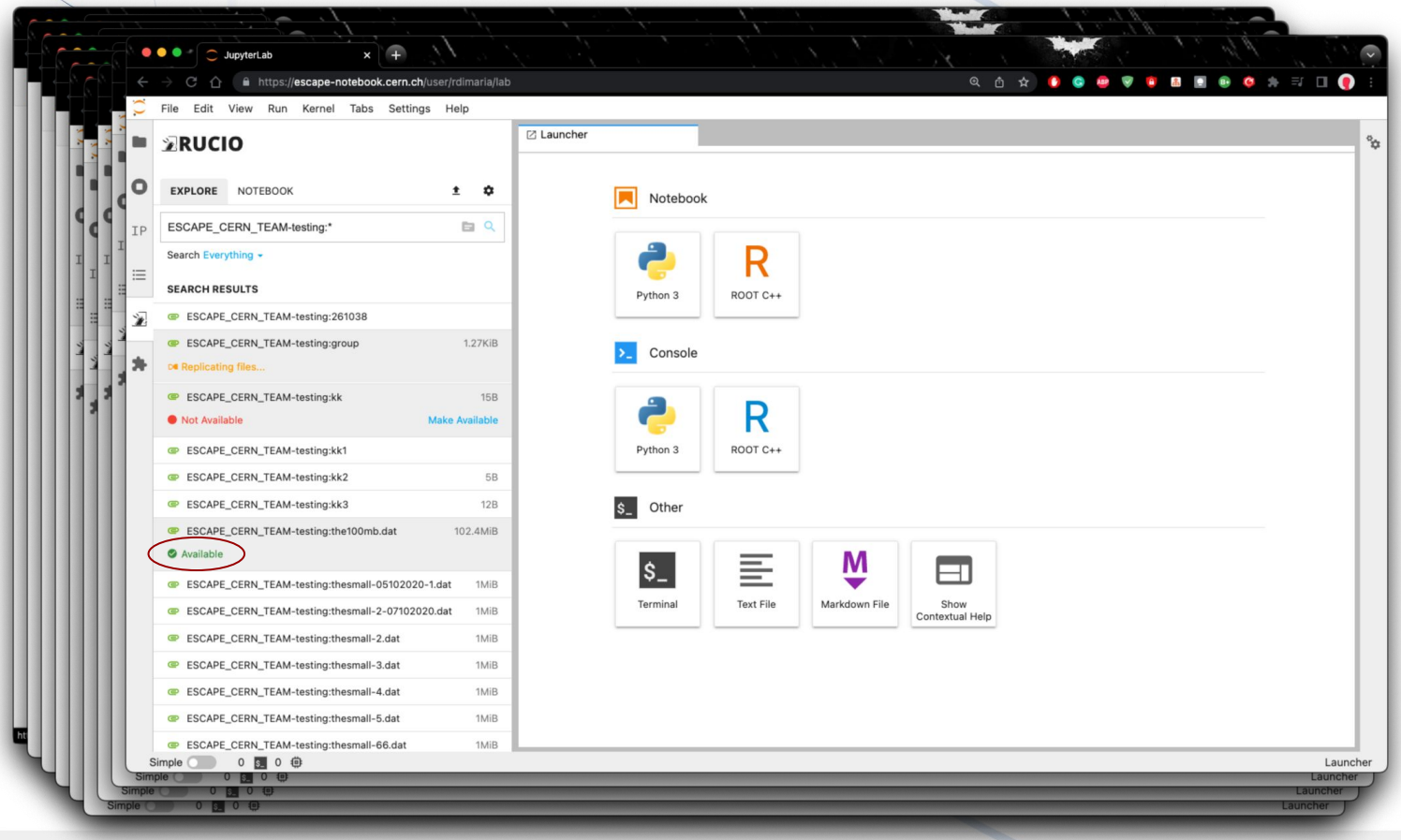
Data Browsing



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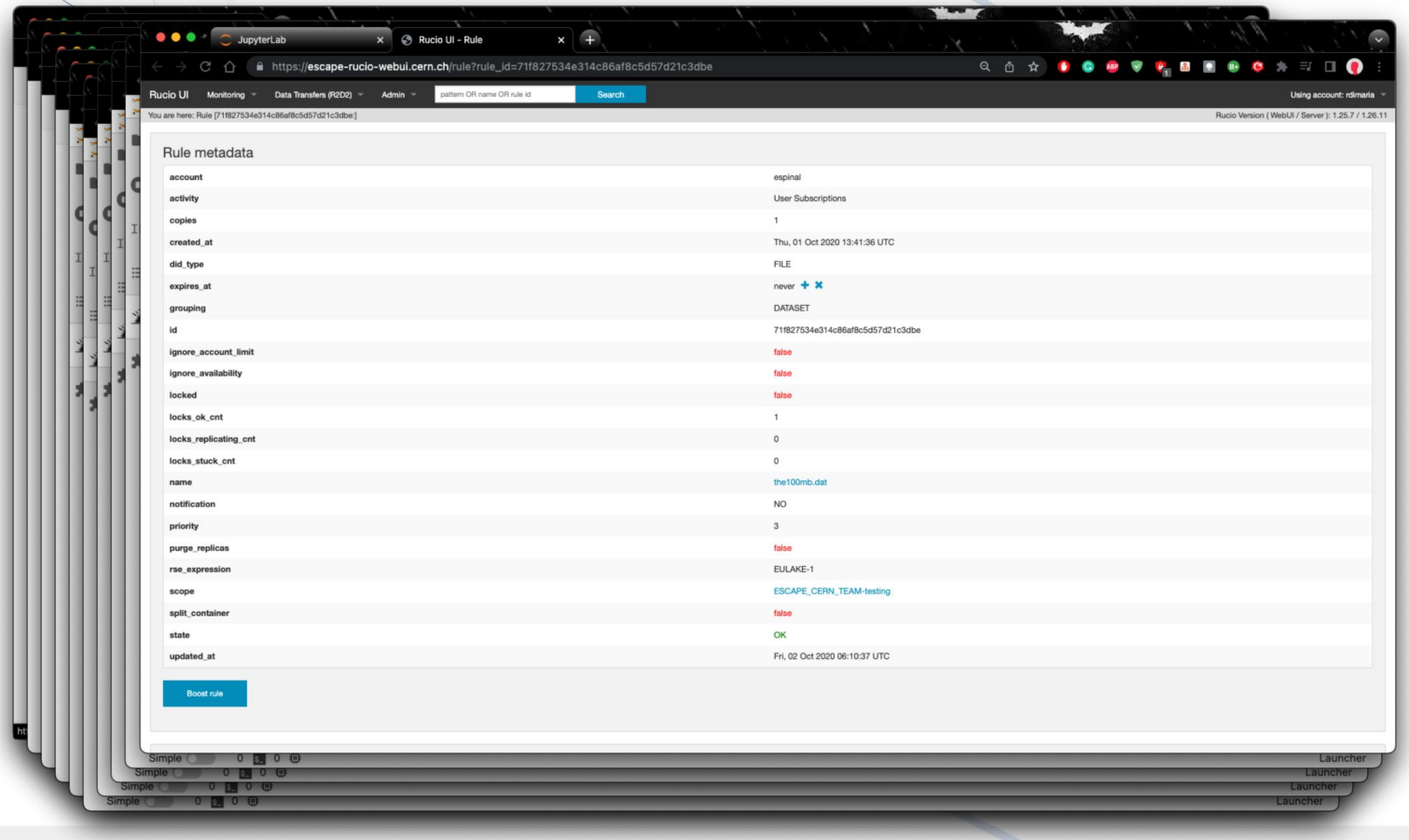
Redirection to ESCAPE Rucio WebUI



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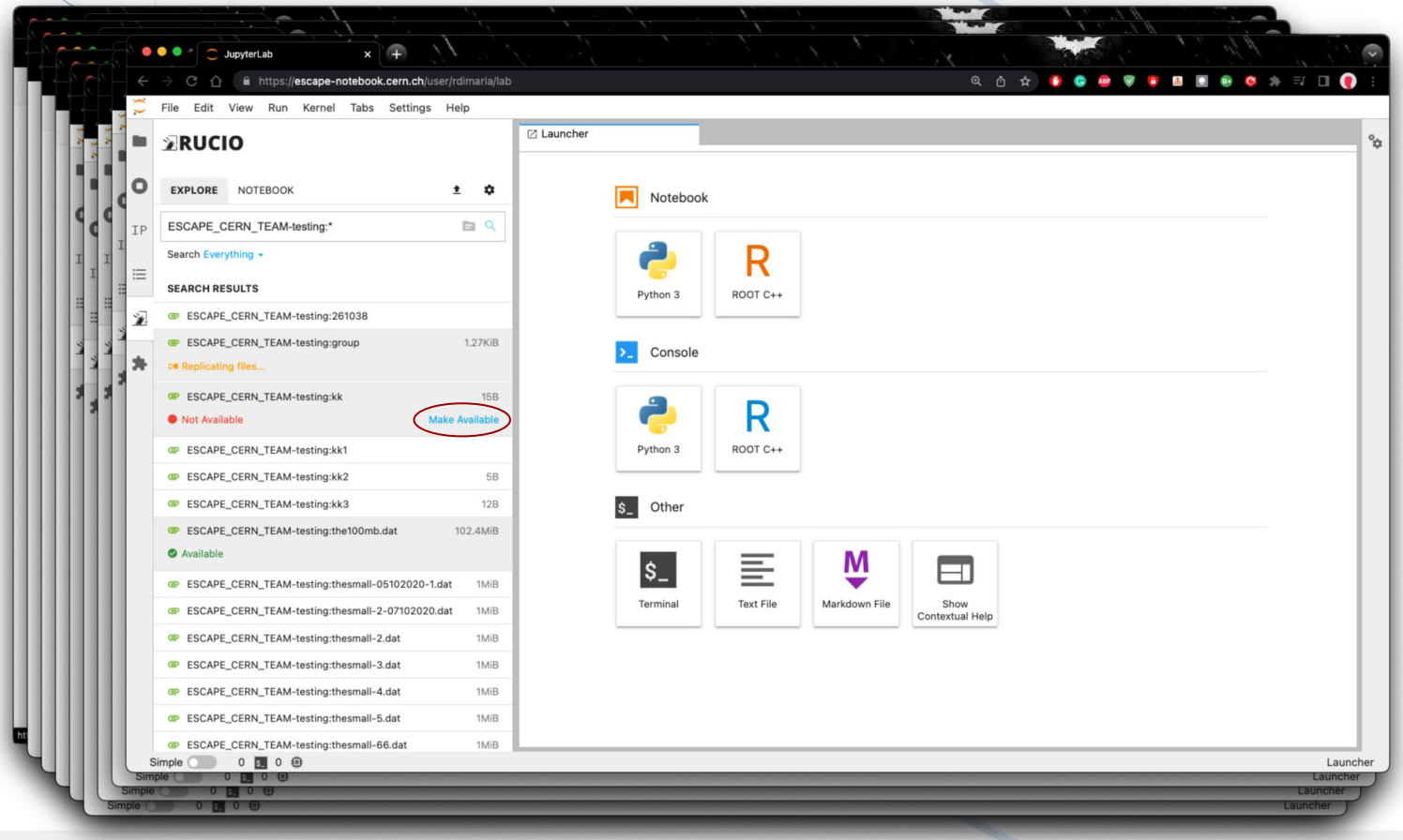
Make Data Available “Locally”



Extension used in Replica Mode, i.e. TPC.

Make Available *aka* creating a replication rule (lifetime configurable - 7d) to move files to EULAKE-1 (read-only).

Once replication status is OK, extension translates PFN into local path.

EULAKE-1 is a design choice as RSE and server are co-located → FUSE mount. Files accessible as if they were local.

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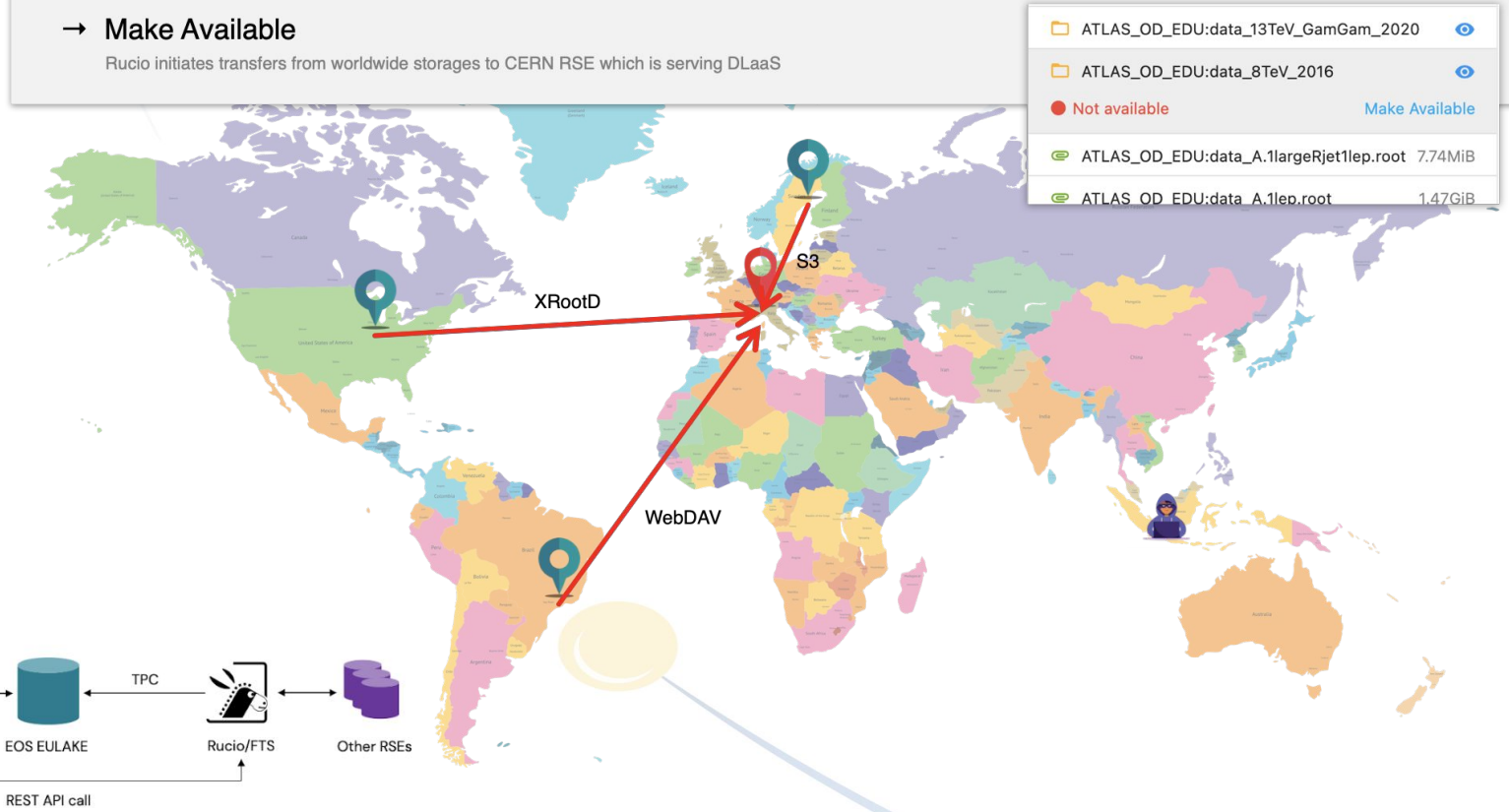
Make Data Available “Locally”

→ **Make Available**

Rucio initiates transfers from worldwide storages to CERN RSE which is serving DLaaS



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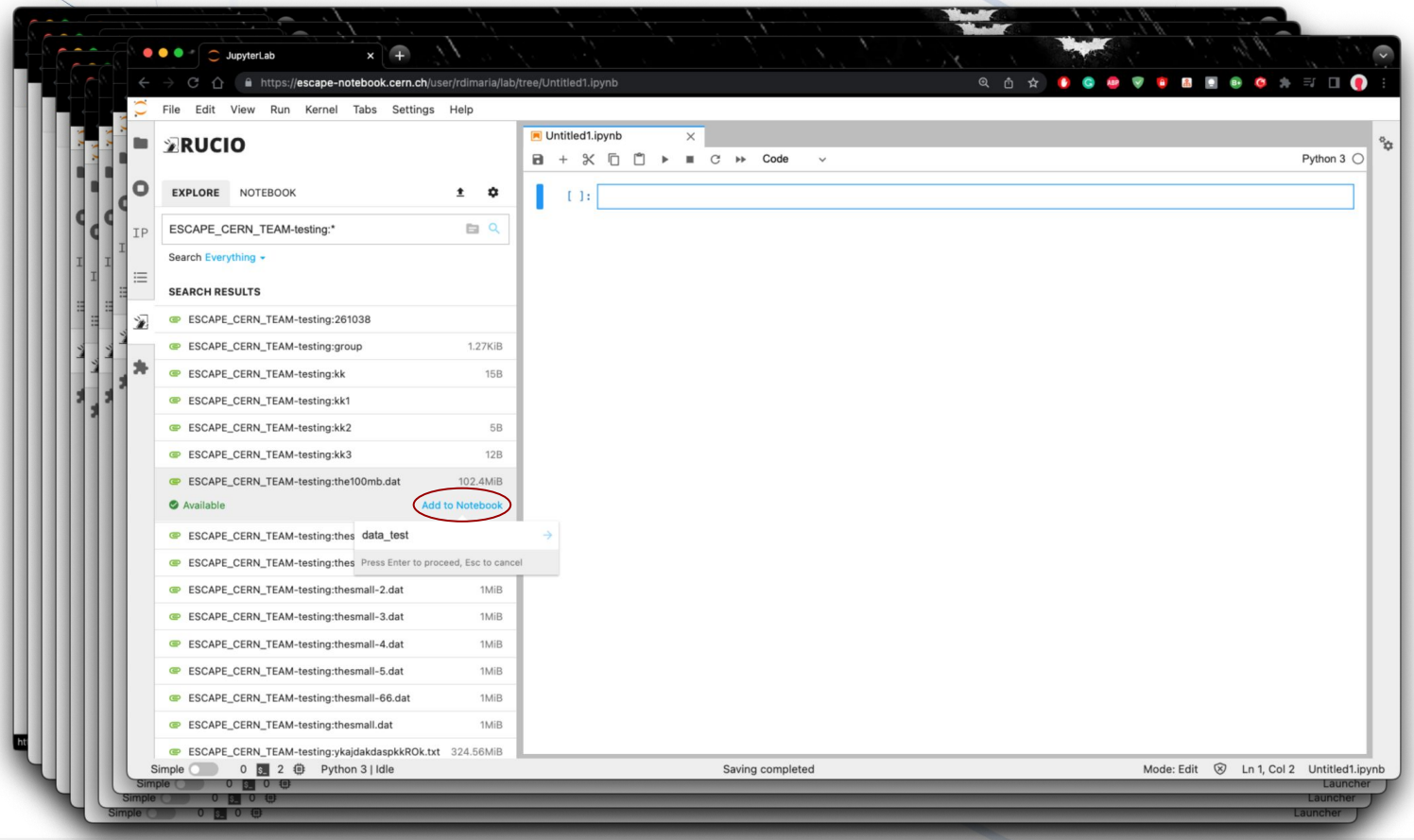
Add Data to Notebook



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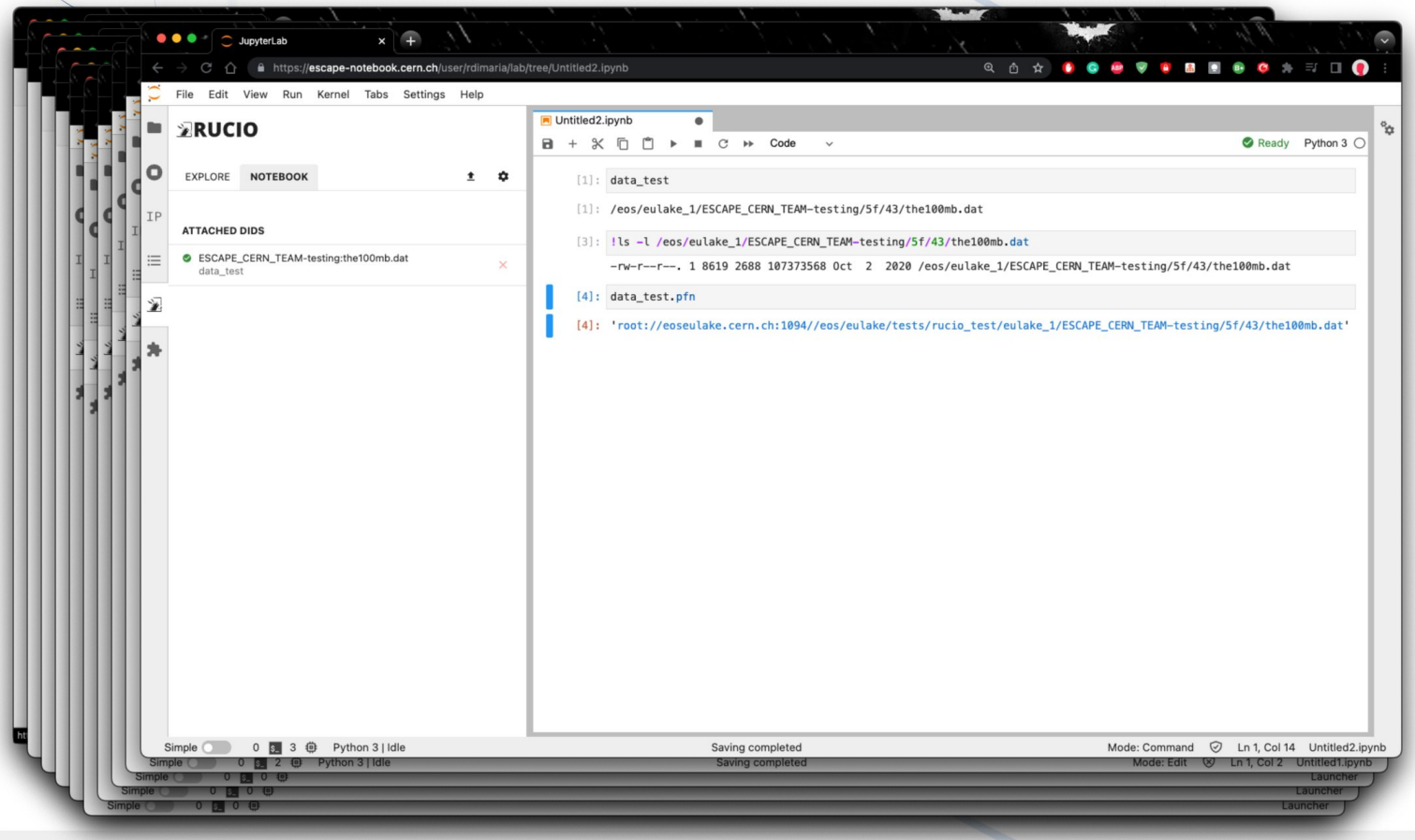
Use Data for Analysis



.pfn feature allows distributed analysis, retrieving the file location from within the Notebook session.

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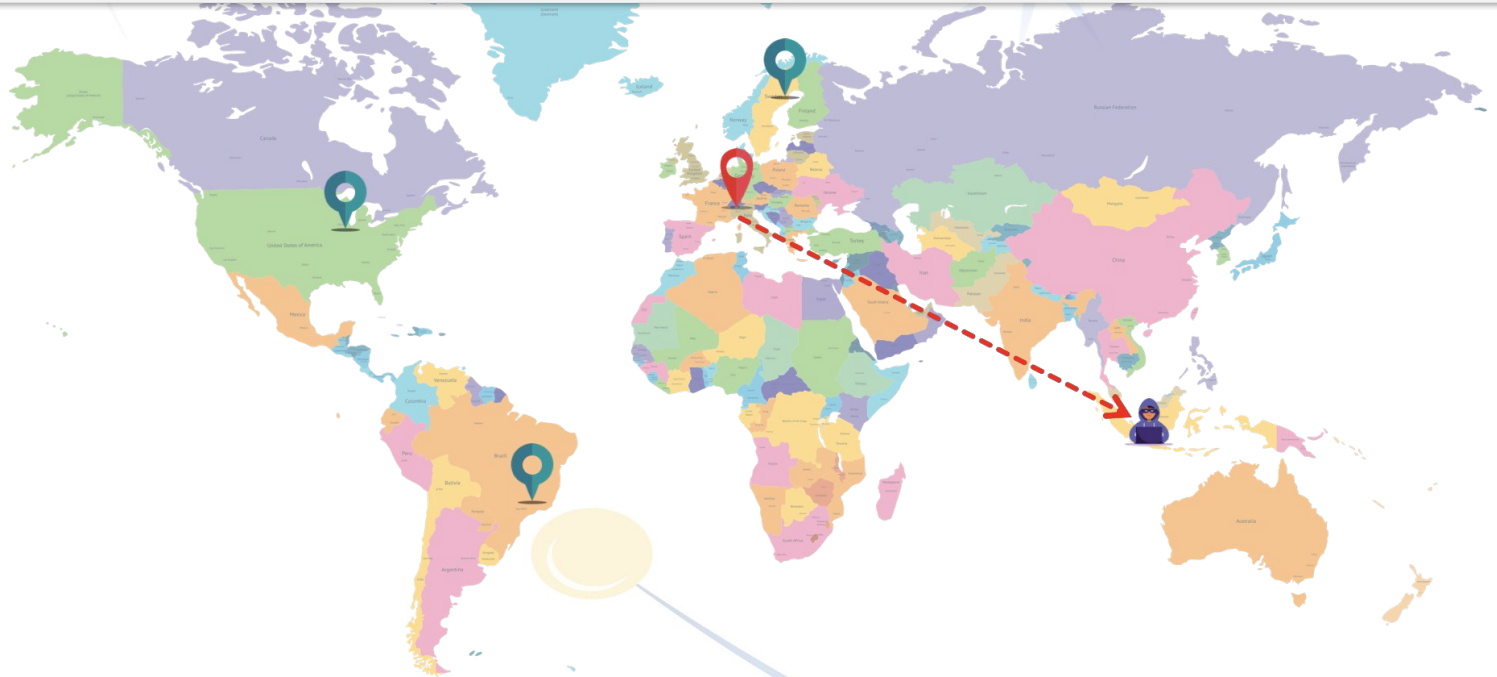
DataLake-as-a-Service for Open Science

→ **Scientists' Analysis Workflows Read Data**

The code runs on the Notebook server at CERN, and the output is shown to the user



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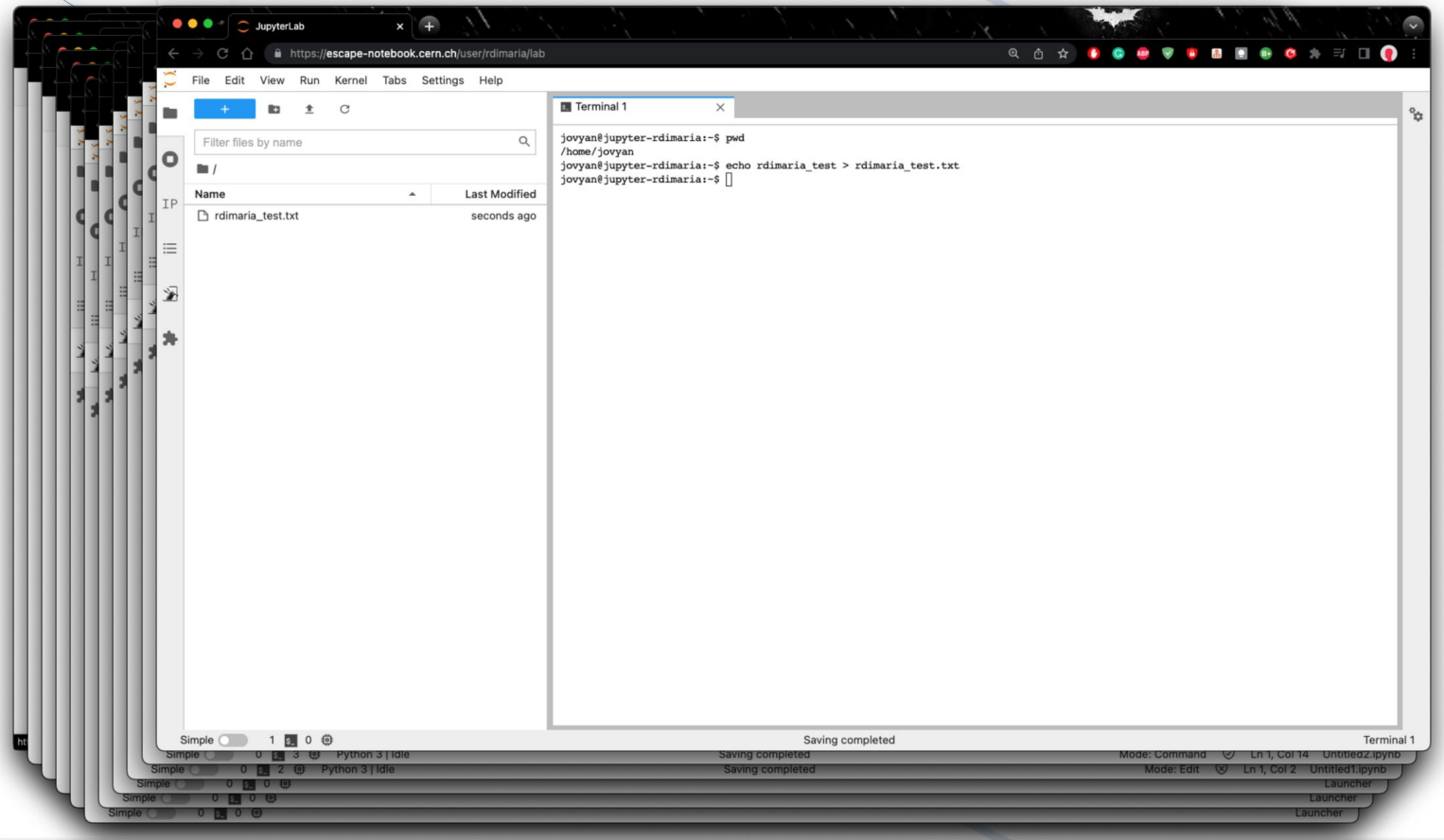
Output of Analysis (Small-Sized Files)



Small-sized files are automatically stored in the common volume (homedir decoupled, space shared).

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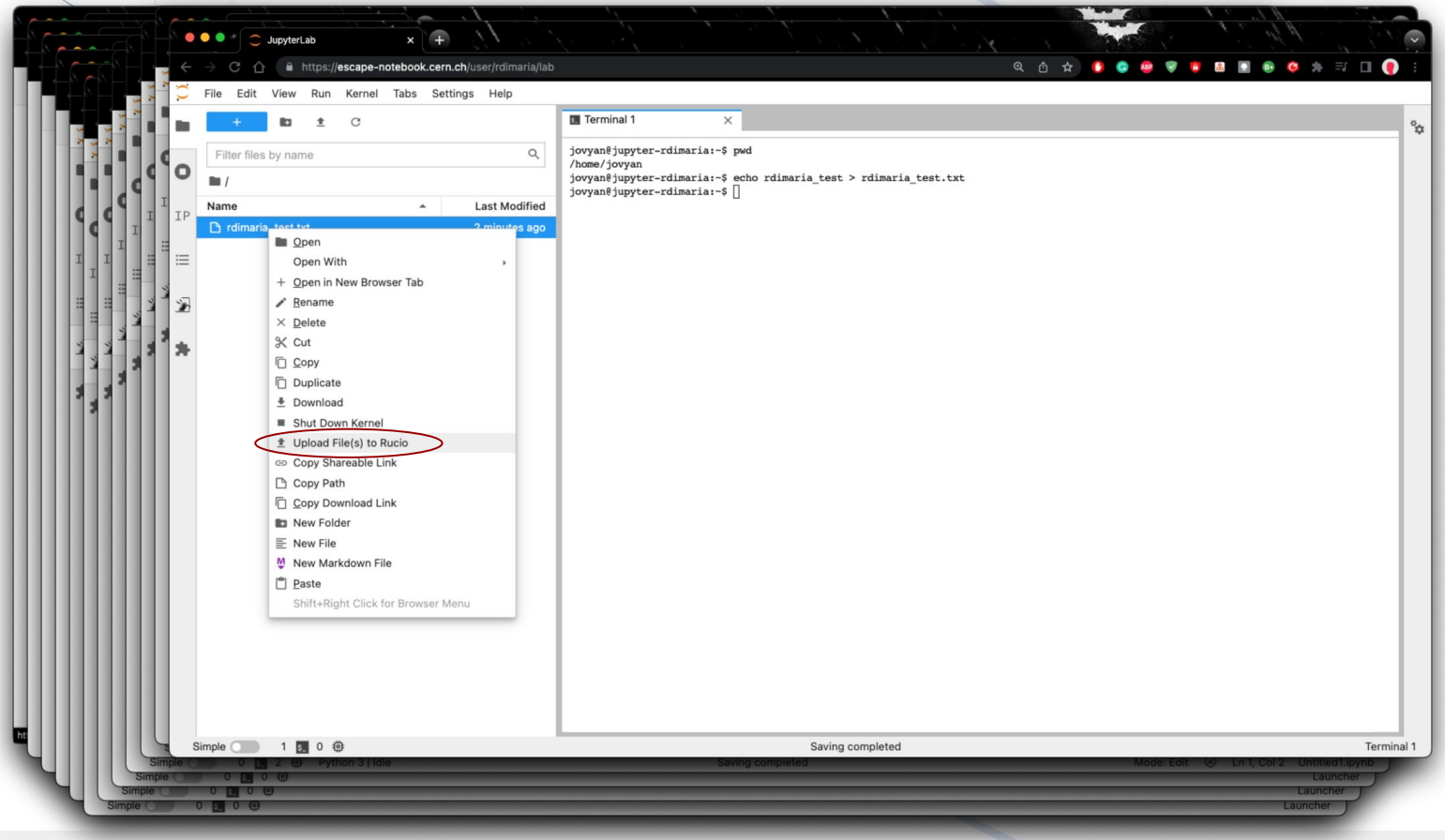
Data Preservation Use Case



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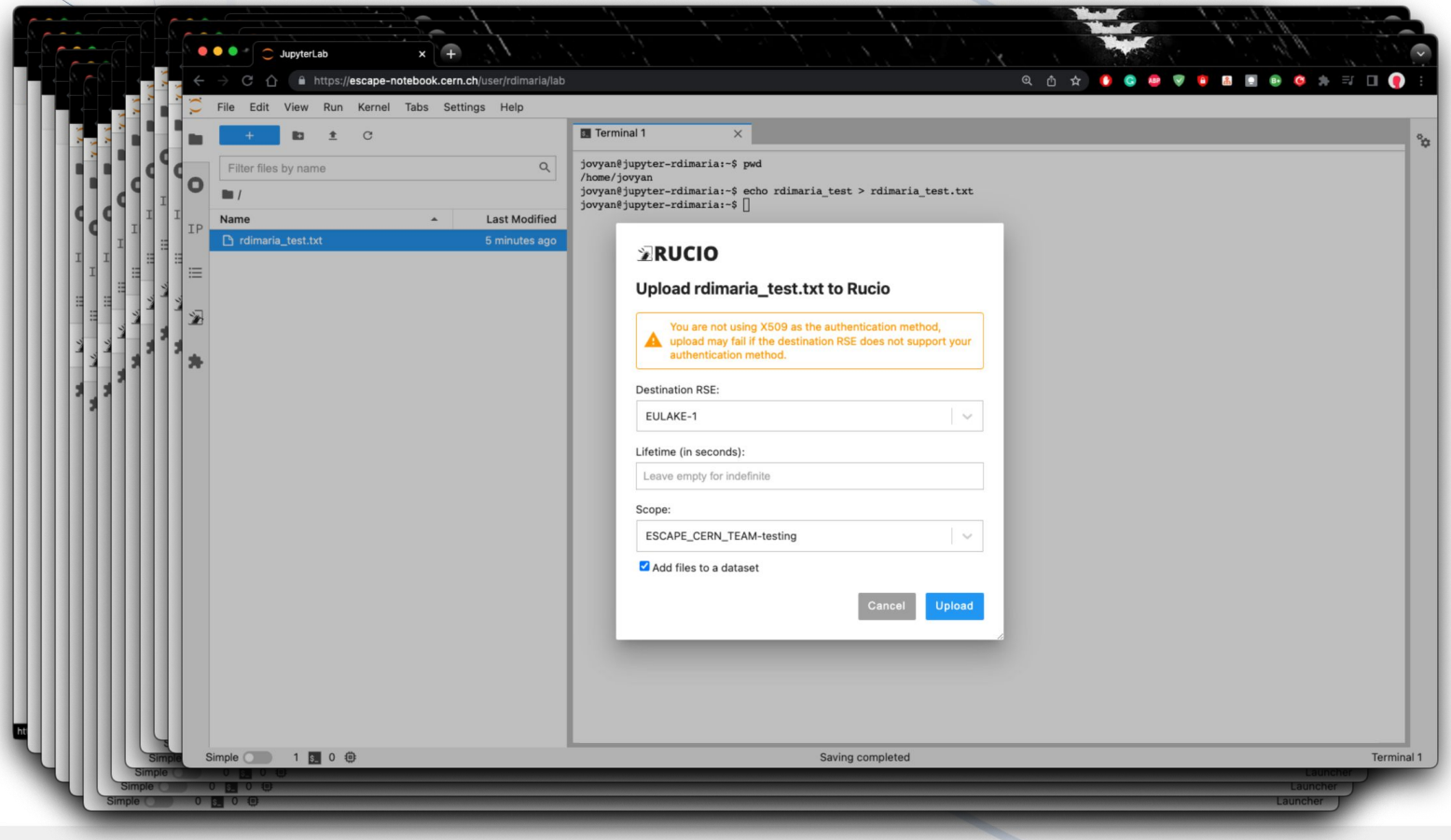
Data Preservation Use Case



RSE should be compliant with the provided token, and end2end token flow should be properly tested.

For direct upload/download, X509 is the solution till dev work is performed in this respect.

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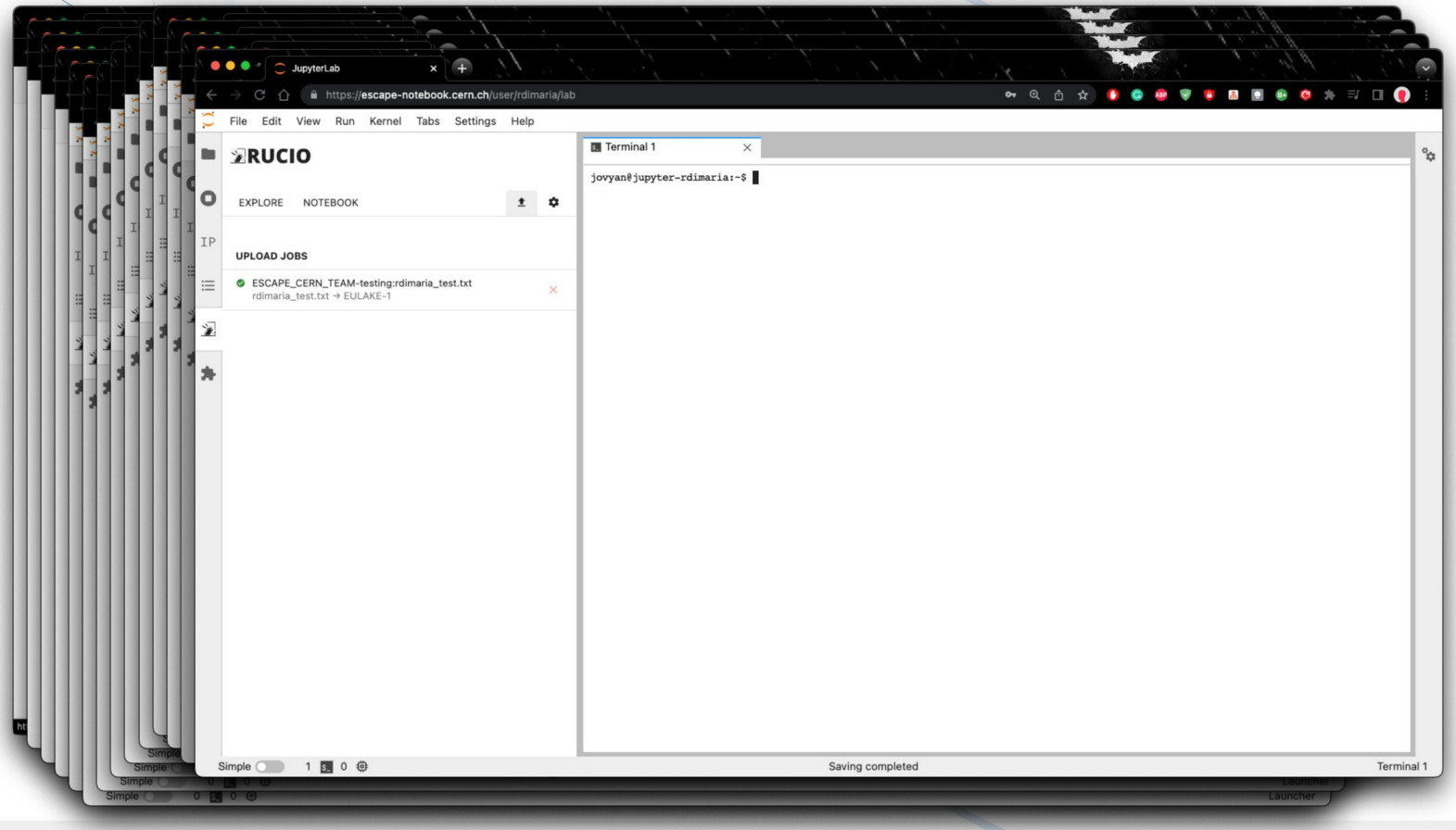
Data Preservation Use Case



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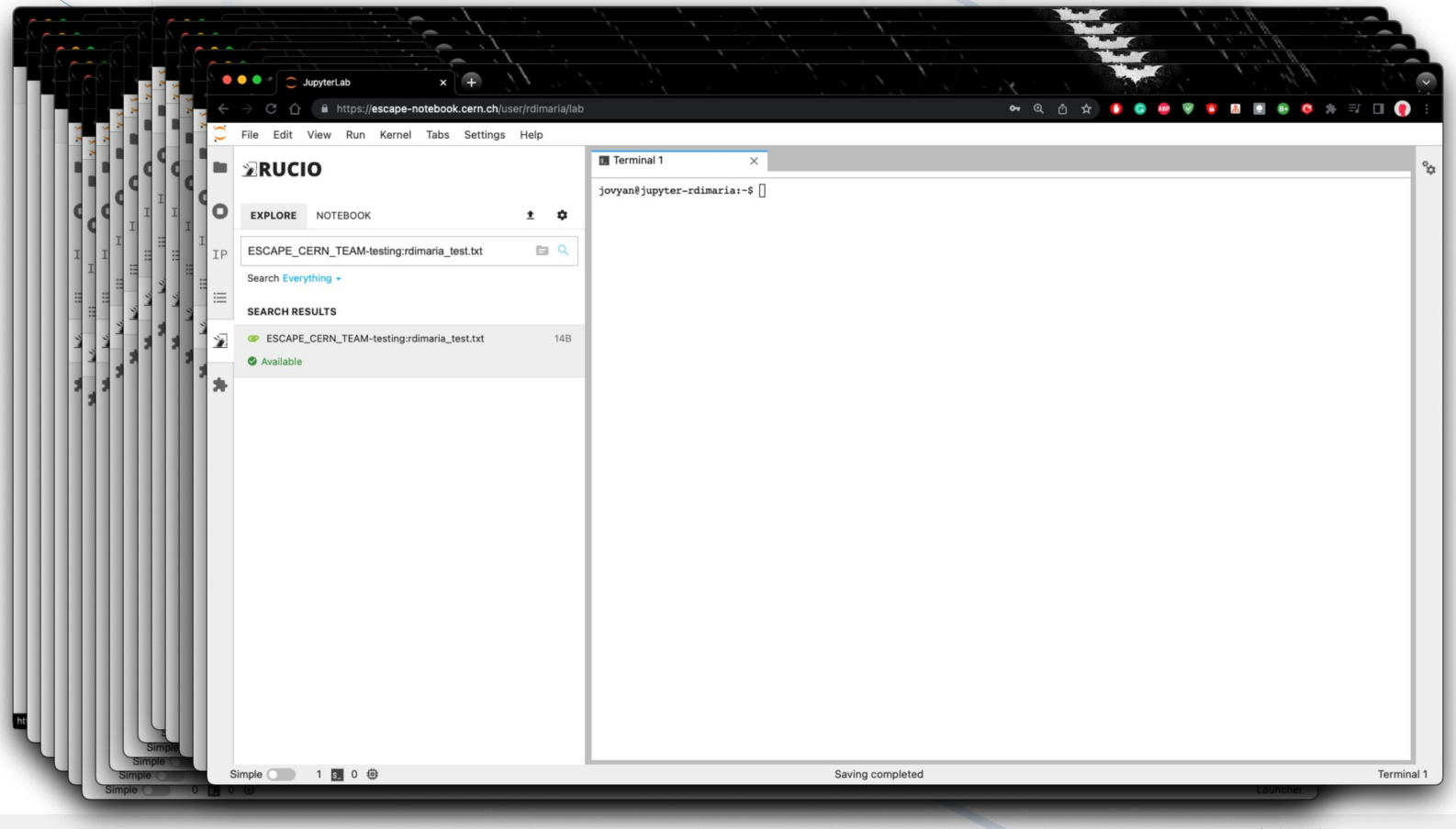
Data Preservation Use Case



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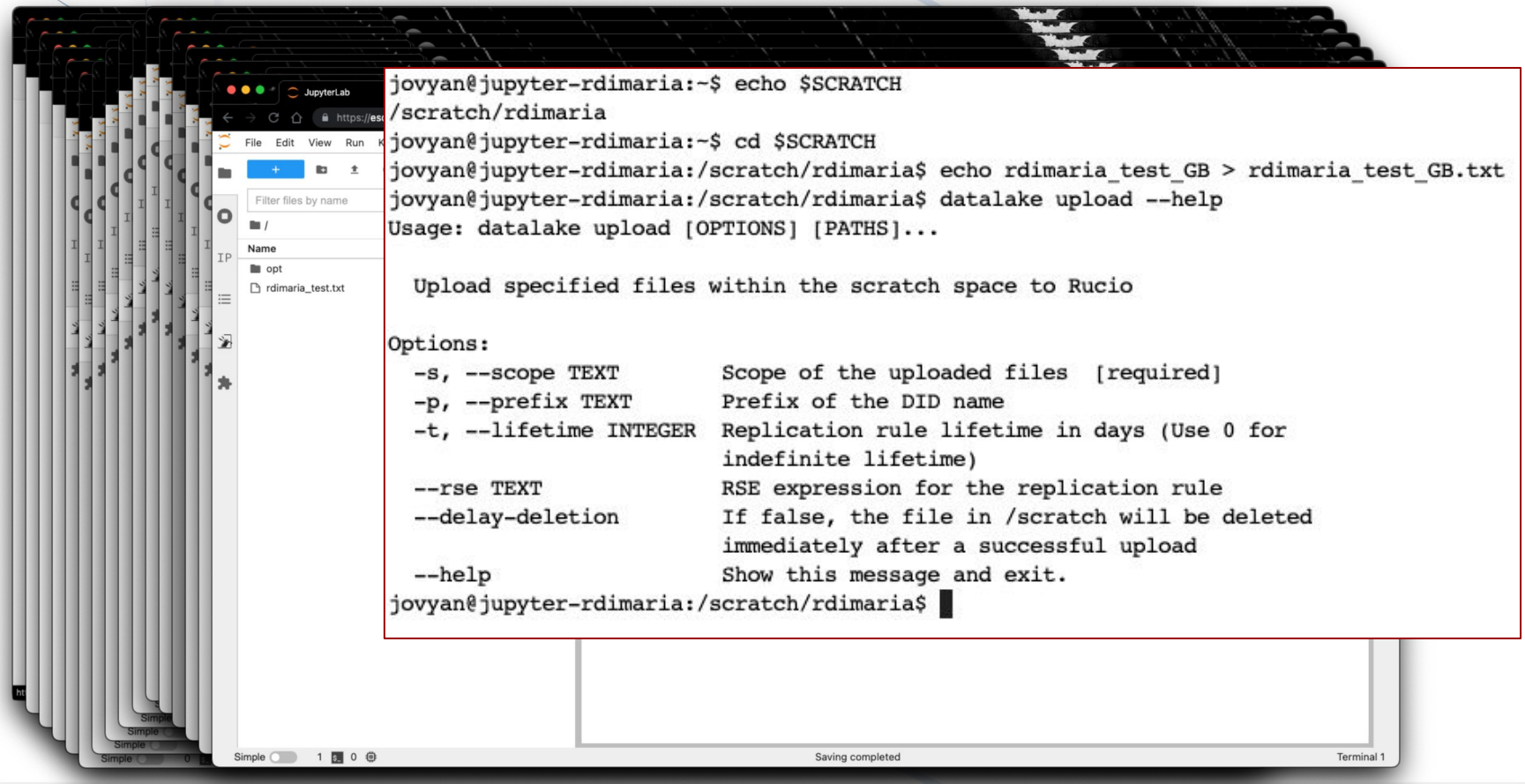
Output of Workflow or Analysis (Large-Sized Files)




```
jovyan@jupyter-rdimaria:~$ echo $SCRATCH
/scratch/rdimaria
jovyan@jupyter-rdimaria:~$ cd $SCRATCH
jovyan@jupyter-rdimaria:/scratch/rdimaria$ echo rdimaria_test_GB > rdimaria_test_GB.txt
jovyan@jupyter-rdimaria:/scratch/rdimaria$ datalake upload --help
Usage: datalake upload [OPTIONS] [PATHS]...

  Upload specified files within the scratch space to Rucio

Options:
  -s, --scope TEXT        Scope of the uploaded files  [required]
  -p, --prefix TEXT       Prefix of the DID name
  -t, --lifetime INTEGER  Replication rule lifetime in days (Use 0 for
                          indefinite lifetime)
  --rse TEXT              RSE expression for the replication rule
  --delay-deletion        If false, the file in /scratch will be deleted
                          immediately after a successful upload
  --help                  Show this message and exit.
jovyan@jupyter-rdimaria:/scratch/rdimaria$
```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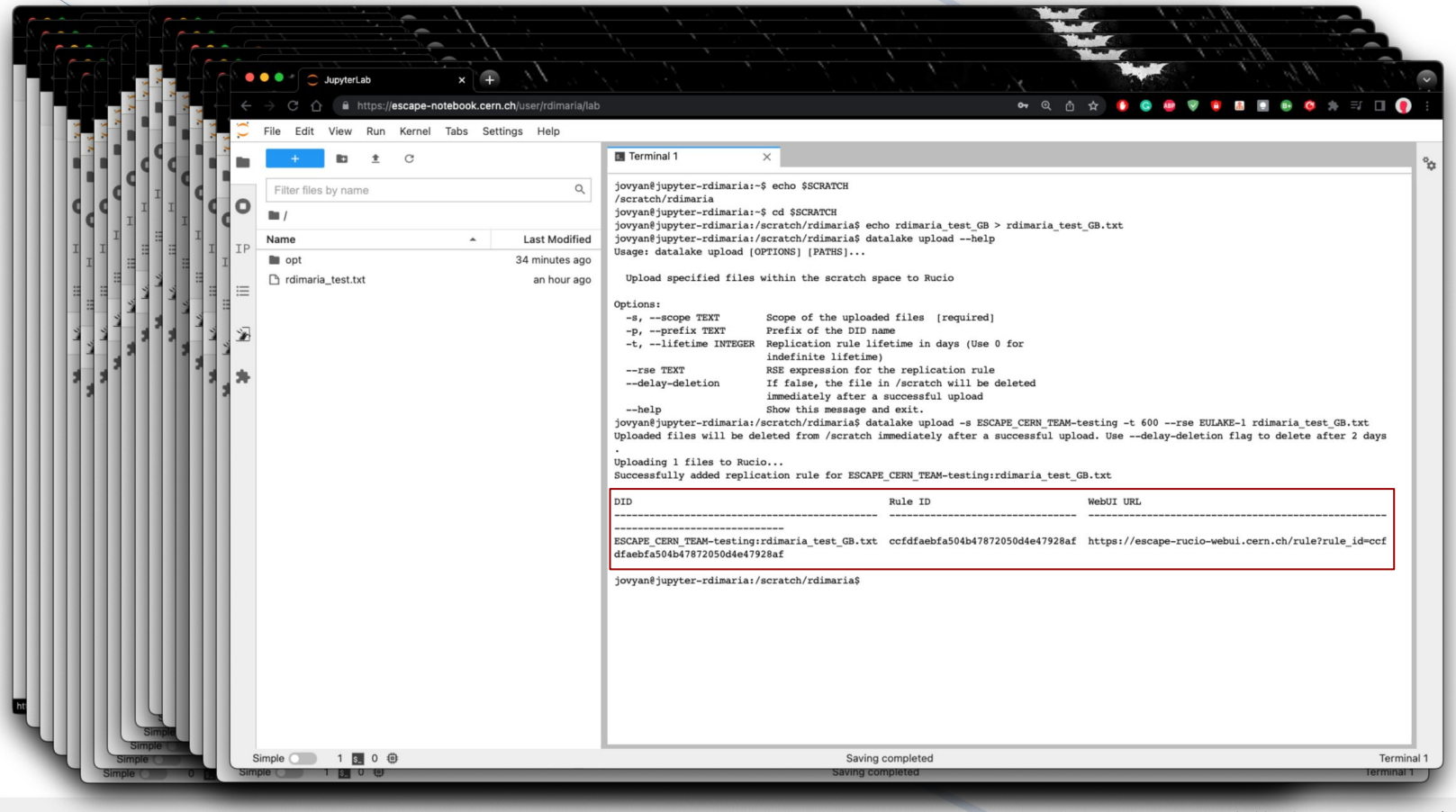
Data Preparation and Processing Use Case



datalake upload translates local path to PFN, the file is added to Rucio replica catalogue, and a replication rule is created.

When the replication status is OK, Rucio deletes files from SCRATCH.

Cron job cleans old files and folders that might not be in the Rucio catalogue.

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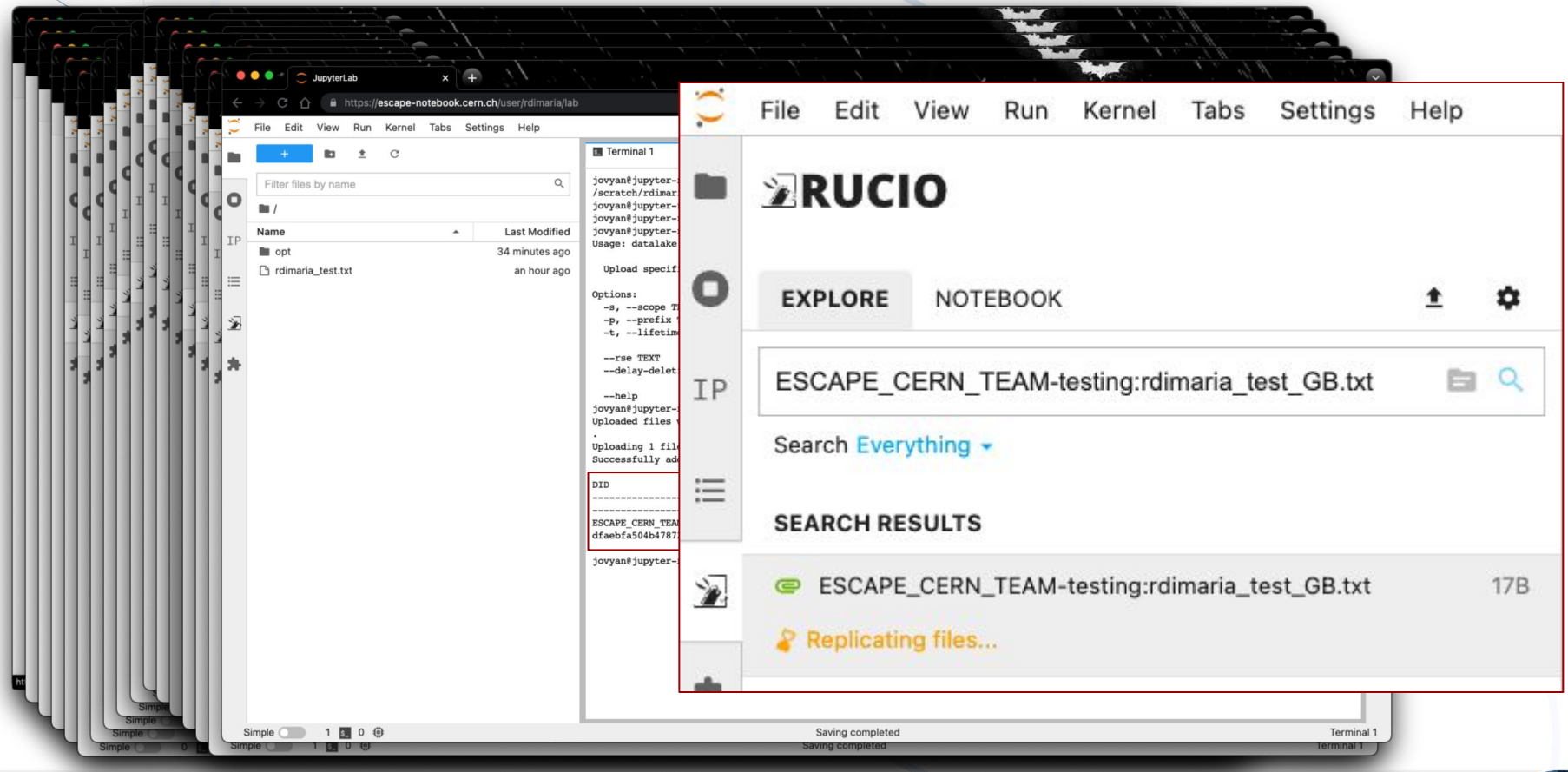
Data Preparation and Processing Use Case



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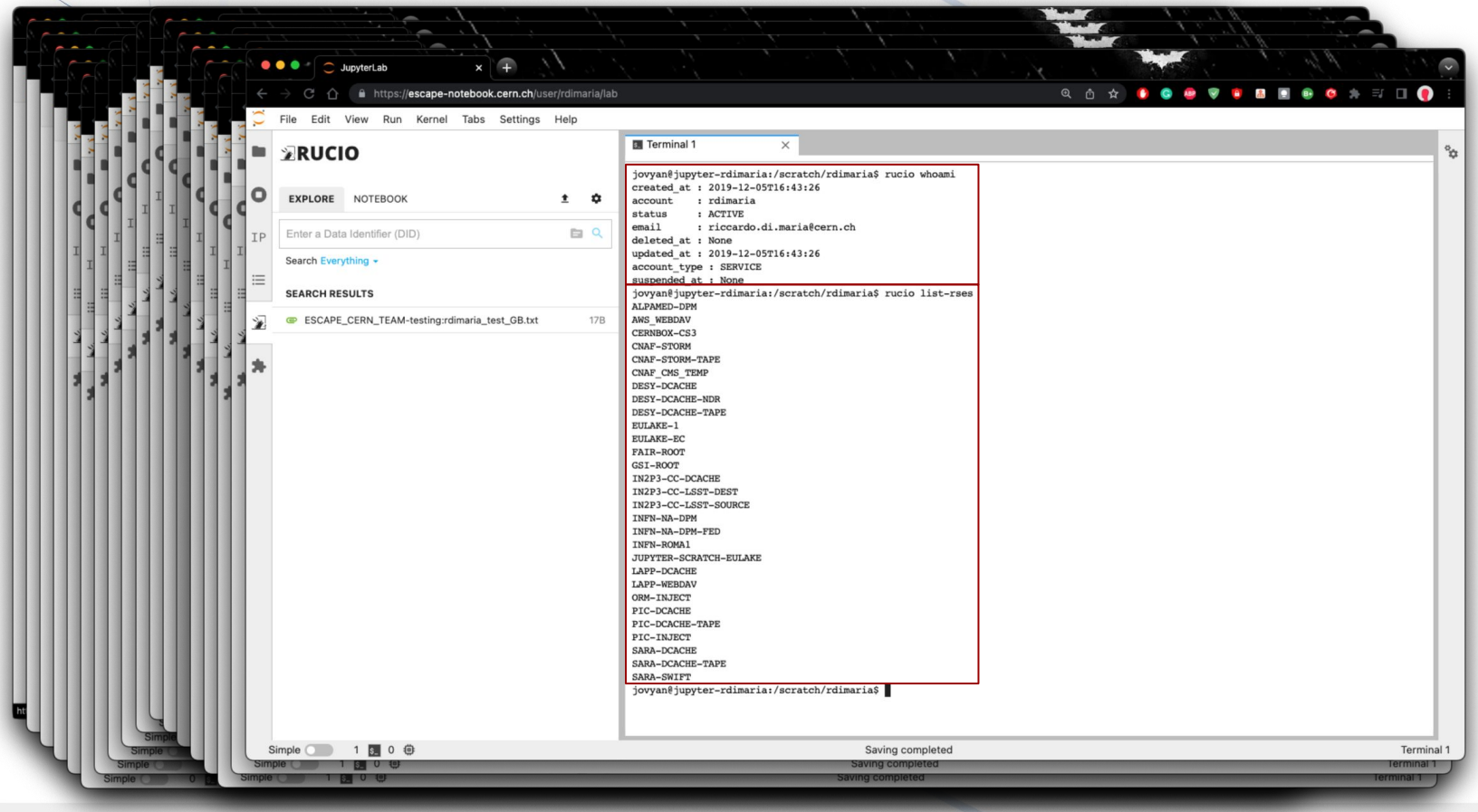
Rucio CLI Available



Rucio CLI available from Notebook terminal and already configured to connect to the ESCAPE Data Lake.

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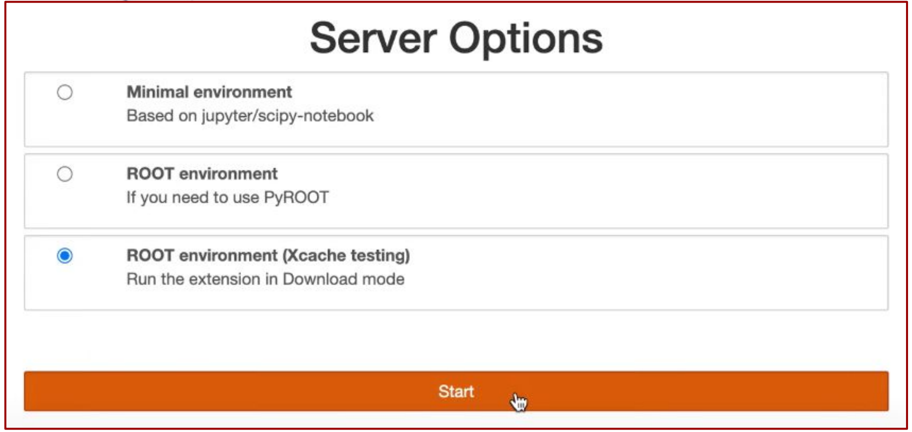
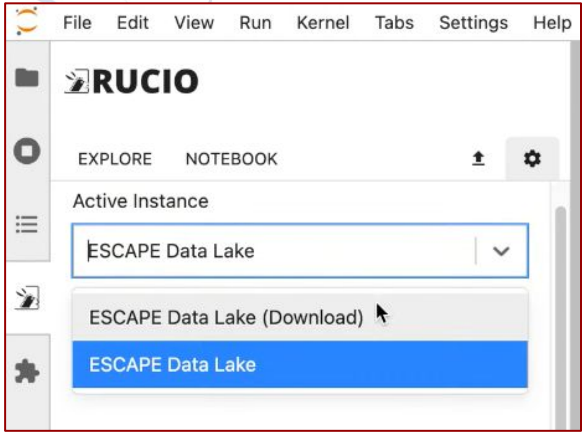
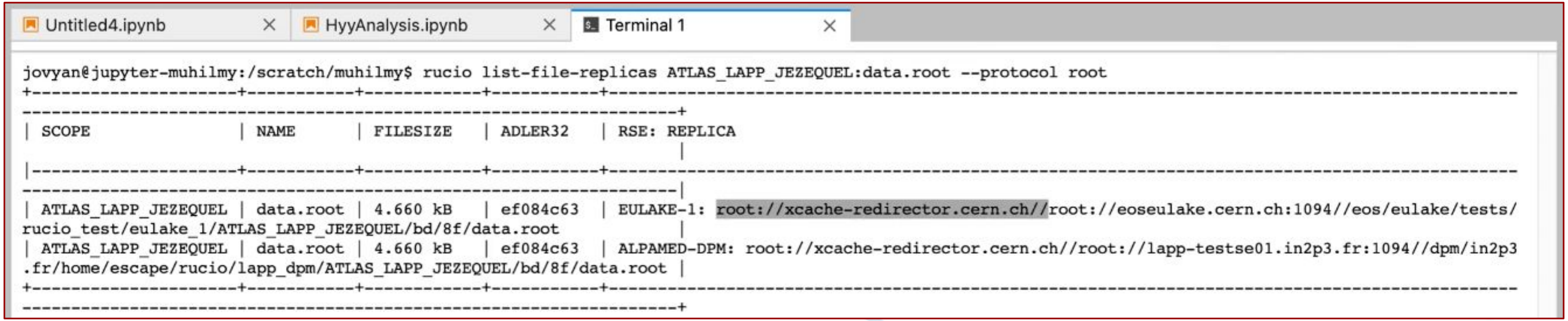
XCache Integration







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DLaaS Use Cases

- Data discovery and access
- Submitting jobs to external services (remote computing)
  - conveniently browse data in Rucio through the extension
  - access file PFN directly from the Notebook
- Data preparation and processing
  - prepare/process data and upload back to the Data Lake
- Data preservation
  - produce data and upload to the Data Lake

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Future Developments

- Additional kernel compatibility (currently, only Python supported)
- Token-support for direct download and upload → OIDC integration ongoing at storage level
- Integration with content delivery and caching layer (successfully tested only at small scale)
  - XCache can be integrated to allow faster file download → transparent for the end-user
- Multi-VO or off-site (CERN) deployment, and distribution model for sciences
- **DLaaS** interesting for both **aficionados** and **newcomers** of **Rucio**
  - community-driven “development and operation”
    - needs and requirements of different experiments and sciences
  - addressing long term sustainability beyond ESCAPE mandate
    - ongoing proposal to establish a **Special Interest Group**

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Conclusion and Next Steps

- **DLaaS** hides the complexities of the Data Lake from the end users (so that they are happy and productive!)
  - interesting for both **aficionados** and **newcomers** of **Rucio**
  - community-driven development, hence driven by the needs of different experiments and sciences
- ESCAPE managed to pilot and prototype a Data Lake infrastructure fulfilling functional data management needs of flagship ESFRIs from several scientific disciplines
  - sensible technologies choice from WLCG environment and LHC experiments
  - successful assessments of the Data Lake in 2020 and 2021
    - pivotal to test model and concepts for several communities:
      Astro-particle Physics, Electromagnetic and Gravitational-Wave Astronomy, Particle Physics, and Nuclear Physics **pursuing together** FAIR and open-access data principles
    - exploring non-HEP-standard scenarios and collaboration with other communities, e.g. PaNOSC, ExPaNDS, CS3MESH4EOSC
- ESCAPE end in 2022 → addressing long term sustainability

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Backup Slides

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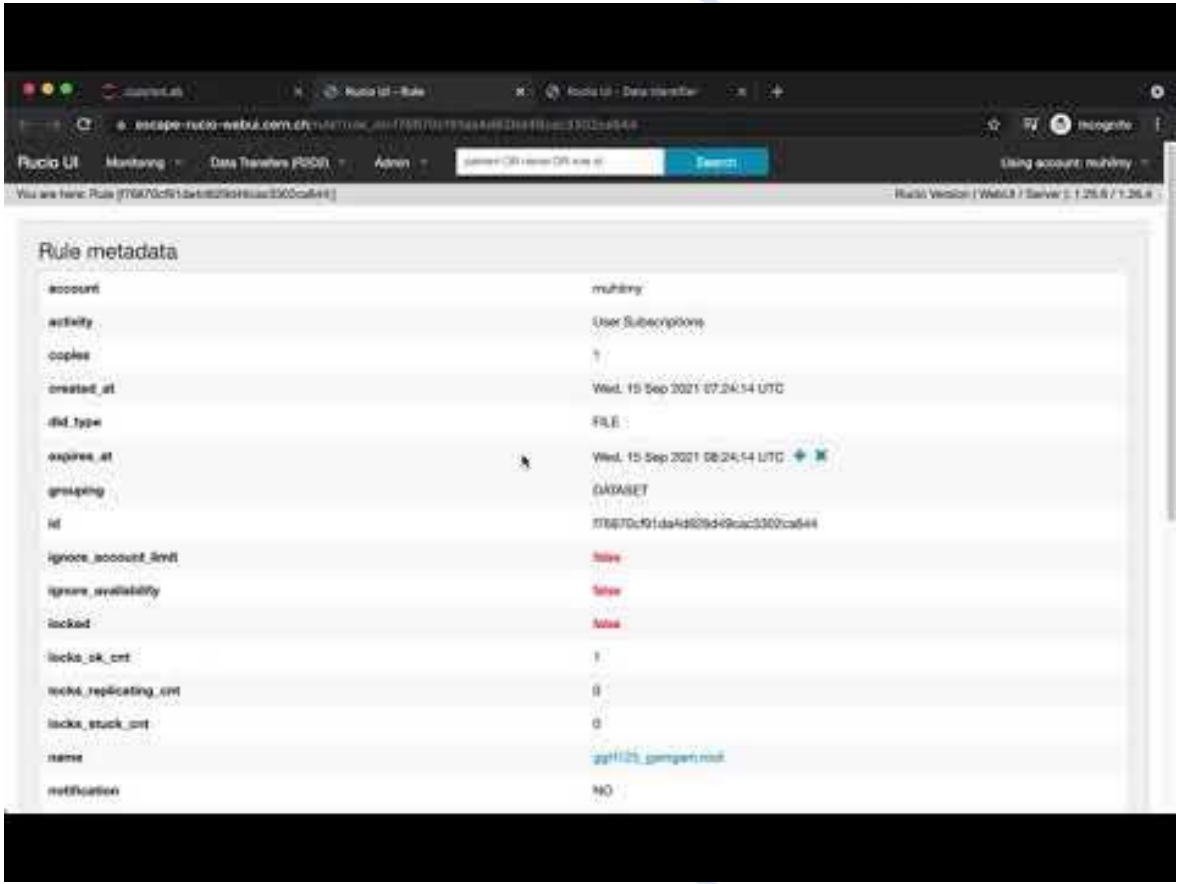
DataLake-as-a-Service for Open Science



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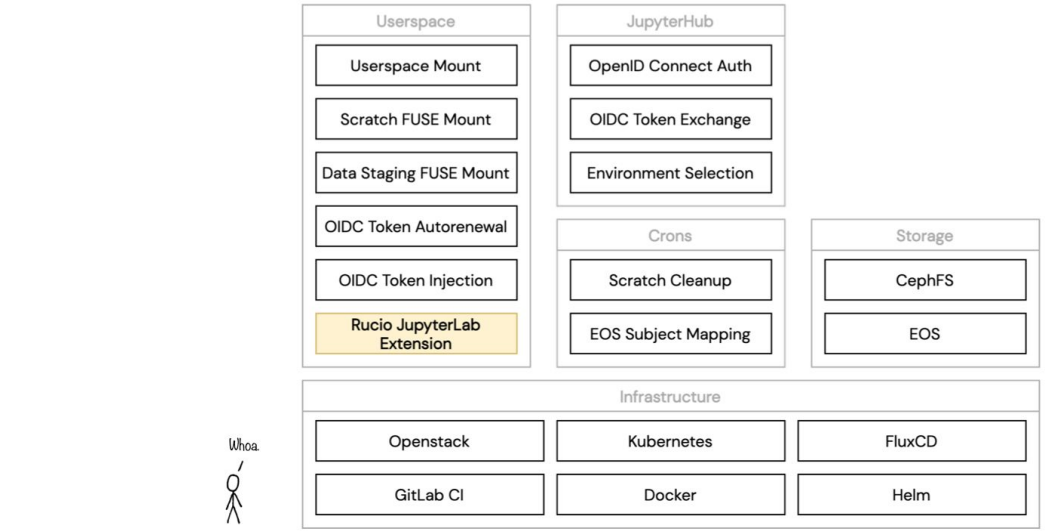
Backup Slides

The DataLake as a Service



CERN openlab

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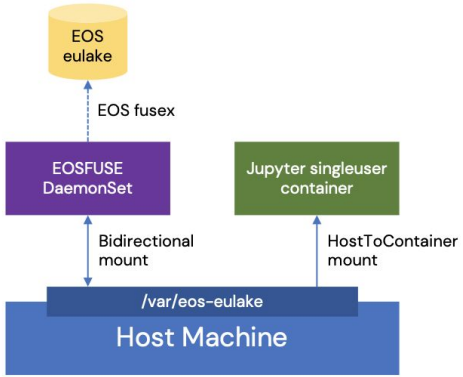
Backup Slides

FUSE mount to EOS eulake

- There are two FUSE mounts to the same EOS instance:
  - /eos/eulake_1 → /eos/eulake/tests/rucio_test/eulake_1
  - /scratch → /eos/eulake/tests/jupyter-scratch
- FUSE mount is implemented using k8s DaemonSet, mounting to a folder in the host, with Bidirectional mount propagation
- Singleuser containers bind to the mount folder, with HostToContainer mount propagation
- Uses OAuth2 authentication
  - ESCAPE IAM user is mapped to EOS user using crons



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OAuth2 in EOS FUSE mount

- In the singleuser container:
  - JWT is stored in a file in the following format:
    - `oauth2:<jwt>:<token-introspection-endpoint>`
    - Example: `oauth2:eyJ...:iam-escape.cloud.cnaf.infn.it/userinfo`
    - Note: token introspection endpoint doesn't have the "https://" part
    - The token file must have at most 0600 permission
  - An environment variable needs to be set:
    - `OAUTH2_TOKEN=FILE:/path/to/token/file`
- In the EOSFUSE DaemonSet container:
  - EOS FUSEx daemon (eosxd) needs to be configured for SSS authentication
  - SSS keytab needs to be present

Docs: https://eos-docs.web.cern.ch/using/oauth2.html

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Backup Slides

Singleuser container setup

Some things need to happen:

- OAuth token exchange (eos-eulake and rucio)
  - Uses a modified version of SWAN's KeyCloakAuthenticator
- Enable token autorenewal
  - Uses swanoauthrenew
- Write token files to /tmp
- Set OAUTH2_TOKEN env for EOS authentication
- Write rucio.cfg file

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