

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.



Science Projects















EUROPEAN OPEN SCIENCE CLOUD Horizon2020

for Research & Innovation

Partners



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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ESCAPE 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

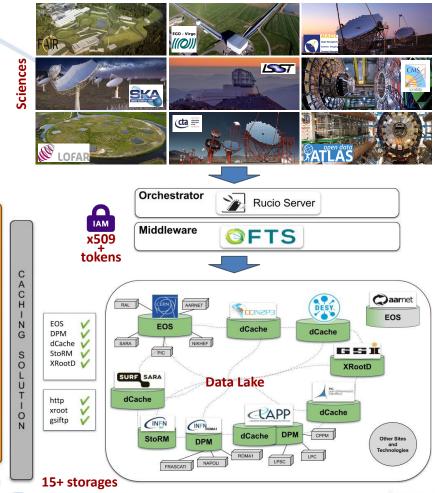
OR

K

- 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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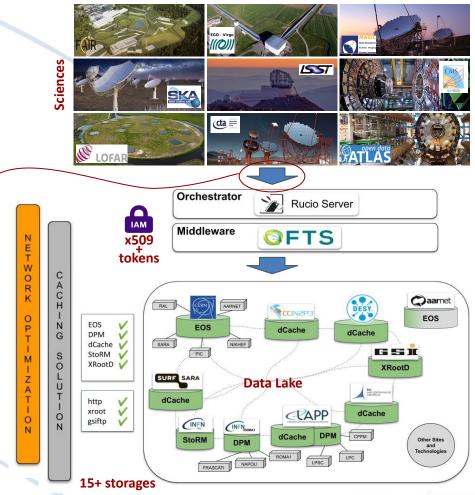
ESCAPE DLaaS for Open Science

- <u>Goal</u>: 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







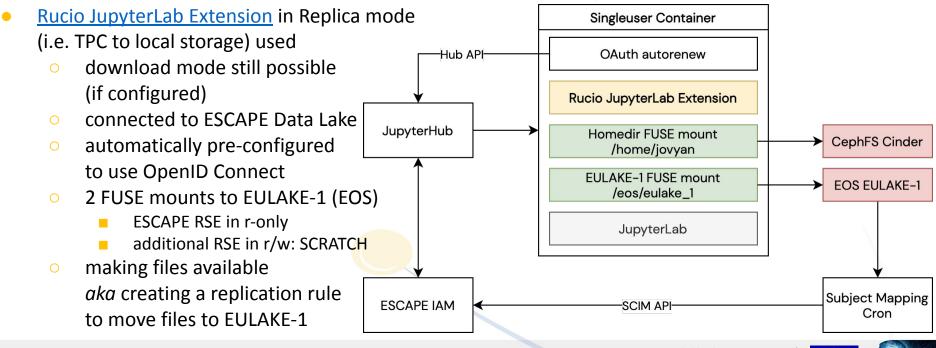
- An idea presented at CS3 2020 by the Rucio team [1]
- Development of a "Rucio JupyterLab Extension" as part of GSoC 2020 [2,3]
- A long time has passed, many things have happened...
 - CERN OpenLab Summer Student to concretise the effort in 2021
 - <u>deployment</u>, <u>docker-images</u>, <u>documentation</u>
 - 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





ESCAPE DLaaS Implementation

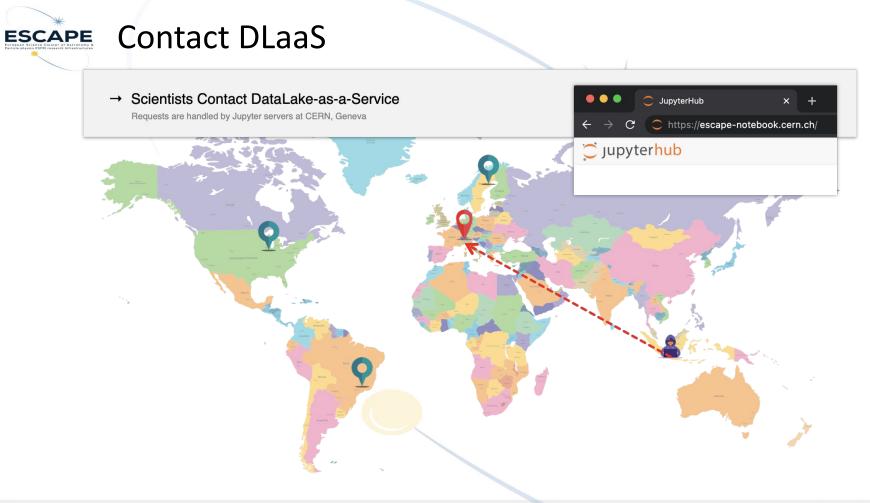
- Deployed in Kubernetes, using Zero-to-JupyterHub Helm chart
 <u>https://escape-notebook.cern.ch</u>
- OAuth authentication using ESCAPE IAM (X509 still supported)



ESCAPE DataLake-as-a-Service for Open Science









ESCAPE Sign in with OAuth 2.0

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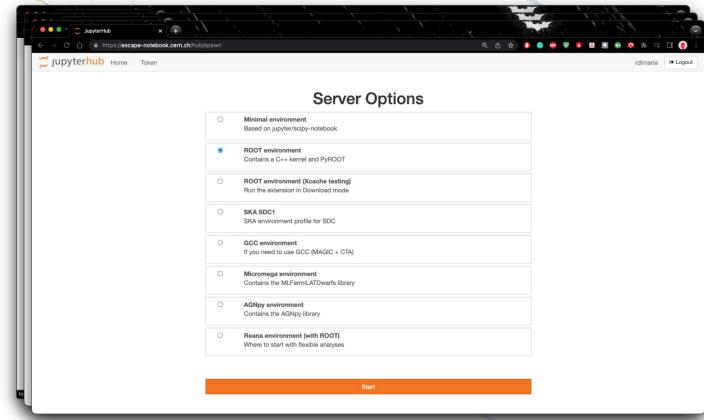
ESCAPE Indigo IAM for Auth

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	Apply for an account
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ESCAPE Multiple Server Options for Sciences



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



ESCAPE K8s-Pod per User

	aria	
Event log	Your server is starting up. You will be redirected automatically when it's ready for you.	rdimaria

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



ESCAPE Jupyter Notebook with Rucio Extension

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The <u>Rucio</u> <u>JupyterLab</u> <u>extension</u> 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.



ESCAPE ESCAPE Rucio Instance and OpenID Connect

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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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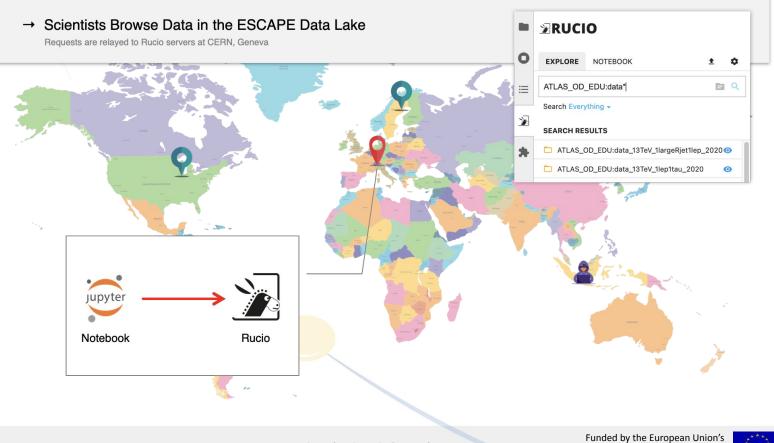
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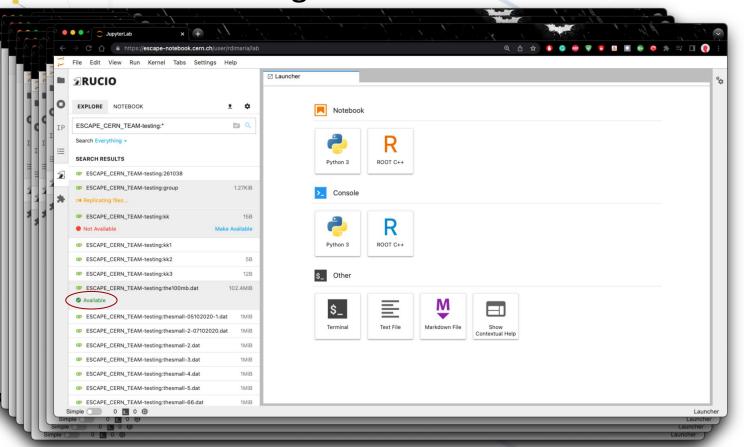
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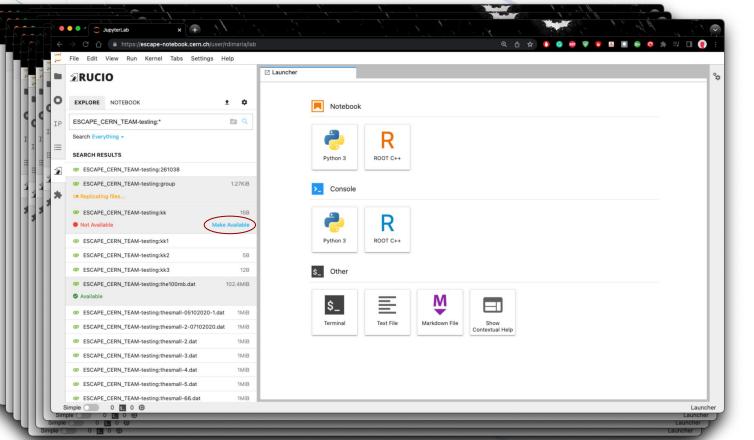


ESCAPE Redirection to ESCAPE Rucio WebUI

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	ignore_account_limit	false
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	locks_replicating_cnt	0
	locks_stuck_cnt	0
	name	the100mb.dat
	notification	NO
	priority	3
	purge_replicas	false
	rse_expression	EULAKE-1
	scope	ESCAPE_CERN_TEAM-testing
	split_container	false
	state	ОК
	updated_at	Fri, 02 Oct 2020 06:10:37 UTC
	Boost rule	



ESCAPE 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).

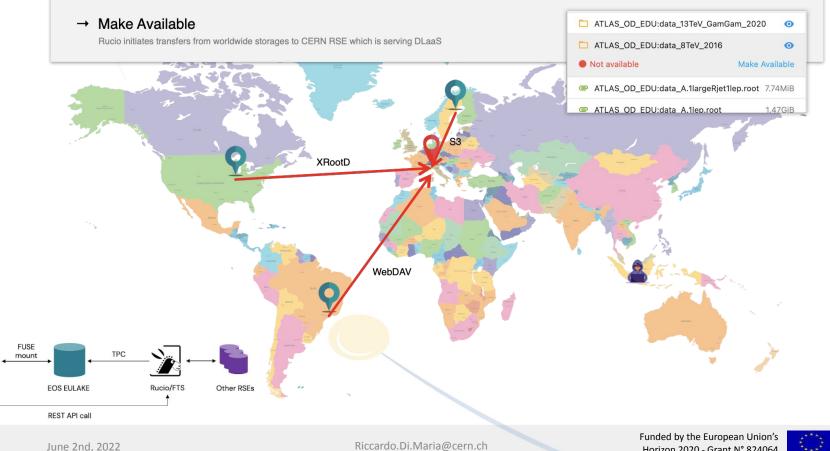
Once replication status is OK, extension translates PFN into local path.

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"

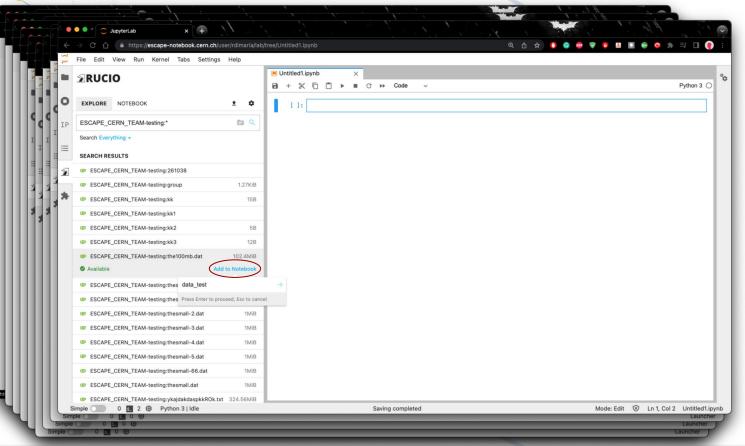


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ESCAPE Add Data to Notebook



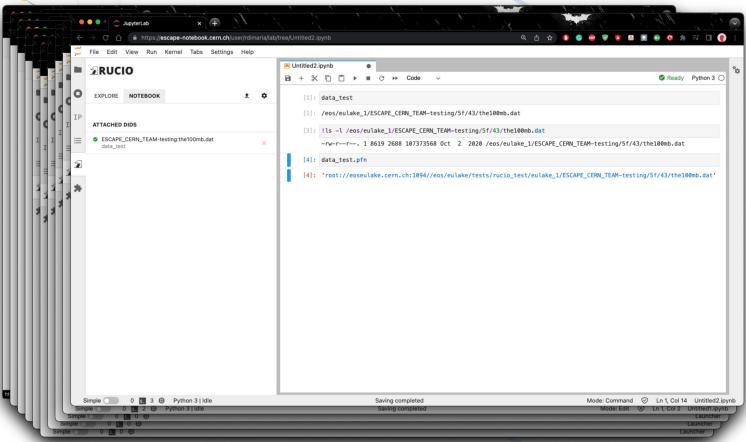
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ESCAPE Use Data for Analysis



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

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ESCAPE DataLake-as-a-Service for Open Science

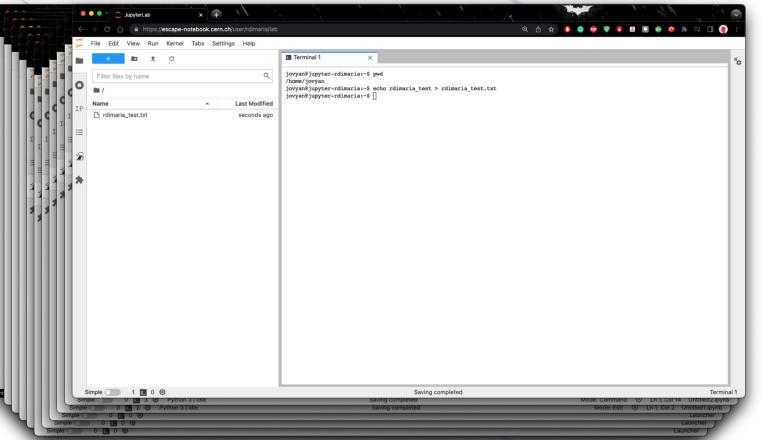
→ Scientists' Analysis Workflows Read Data

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





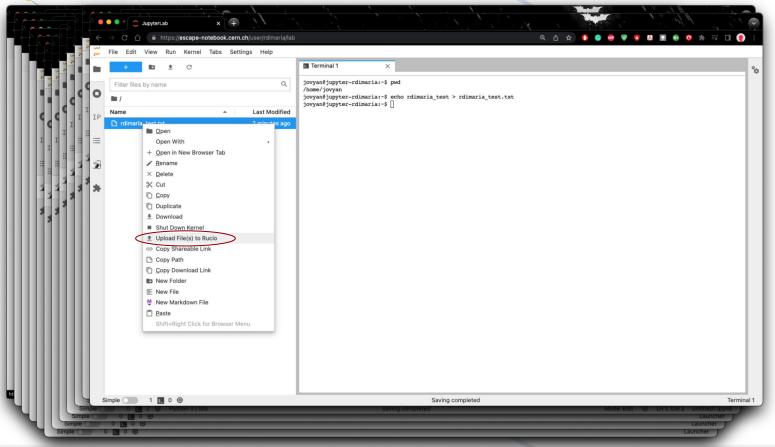
ESCAPE Output of Analysis (Small-Sized Files)



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

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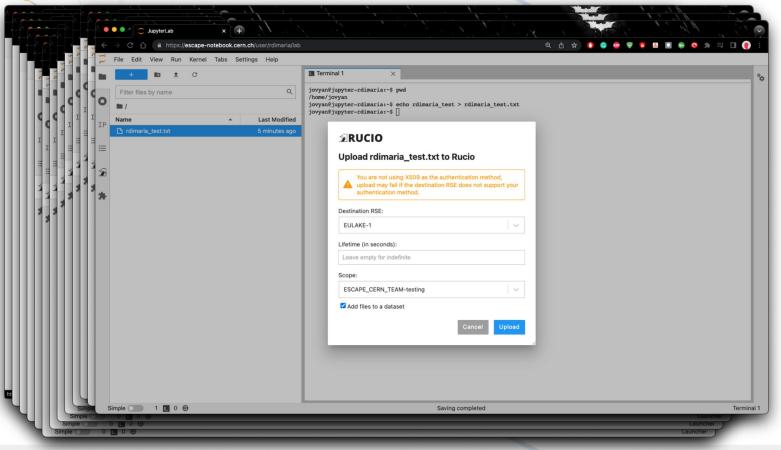


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RSE should be compliant with the provided token, and end2end token flow should be properly tested.

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



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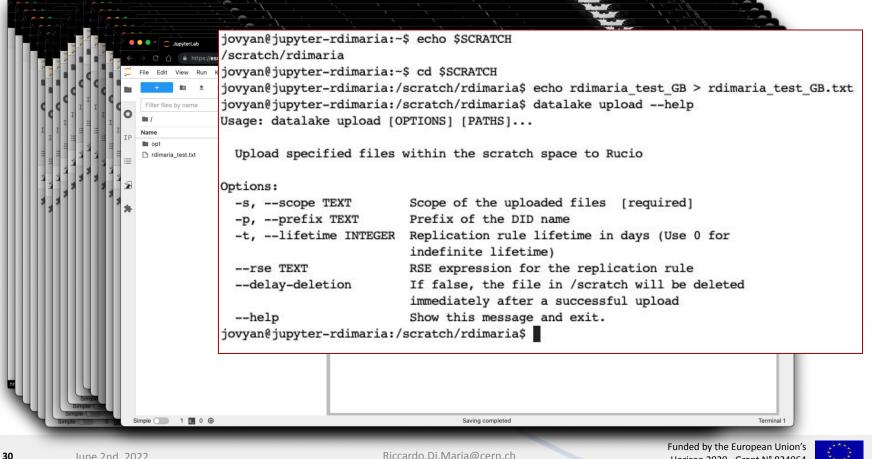


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Output of Workflow or Analysis (Large-Sized Files) ESCAPE





ESCAPE Data Preparation and Processing Use Case

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	Usage: datalake upload [OPTIONS] [PATHS]	

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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ESCAPE Data Preparation and Processing Use Case

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ESCAPE Rucio CLI Available

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

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ESCAPE XCache Integration	
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Minimal environment Based on jupyter/scipy-notebook ROOT environment If you need to use PyROOT ROOT environment (Xcache testing) Run the extension in Download mode	 EXPLORE NOTEBOOK EXPLORE NOTEBOOK Active Instance ESCAPE Data Lake ESCAPE Data Lake (Download) ESCAPE Data Lake
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- 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

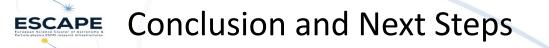




ESCAPE Future Developments

- Additional kernel compatibility (currently, only Python supported)
- Token-support for direct download and upload \rightarrow 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 \rightarrow 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





- **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**
 - o 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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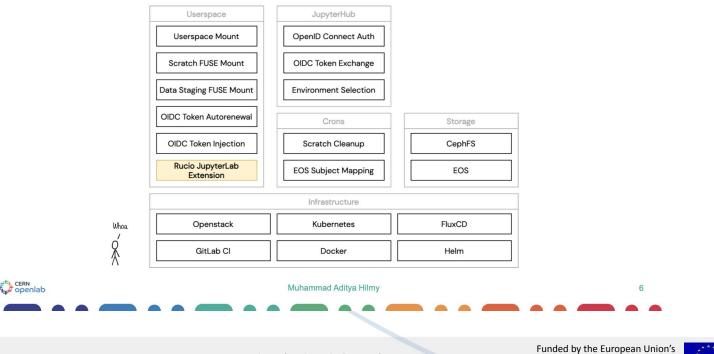
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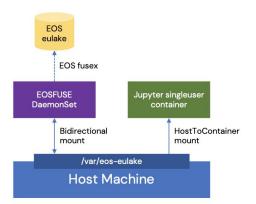
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FUSE mount to EOS eulake

- 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

Backup Slides

ESCAPE IAM user is mapped to EOS user using crons





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Backup Slides

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

ESCAPE





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 <u>swanoauthrenew</u>
- Write token files to /tmp
- Set OAUTH2_TOKEN env for EOS authentication
- Write rucio.cfg file

