

# 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



ISTITUTO NAZIONALE **DI ASTROFISICA** NATIONAL INSTITUTE FOR ASTROPHYSICS





Riccardo.Di.Maria@cern.ch

June 2nd, 2022

Funded by the European Union's Horizon 2020 - Grant N° 824064



## 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

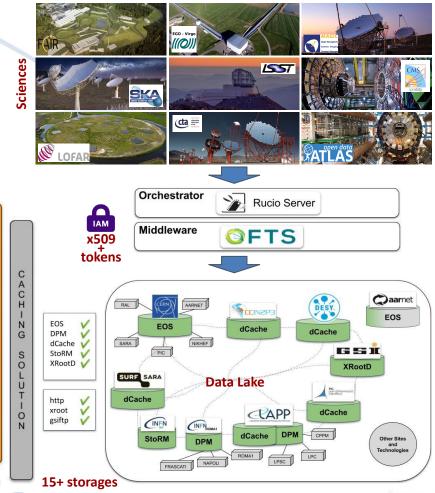
OR

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

 3
 June 2nd, 2022
 Riccardo.Di.Maria@cern.ch



Funded by the European Union's Horizon 2020 - Grant N° 824064



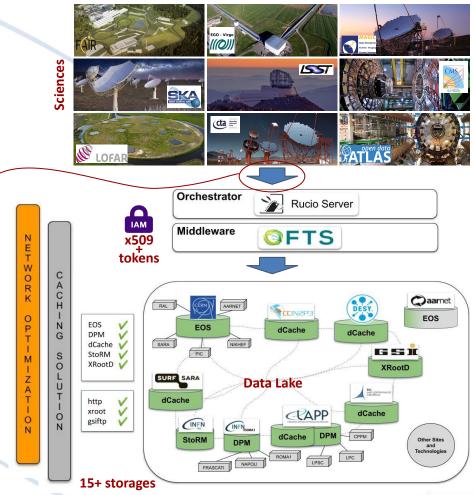
## **ESCAPE** DLaaS for Open Science

- <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







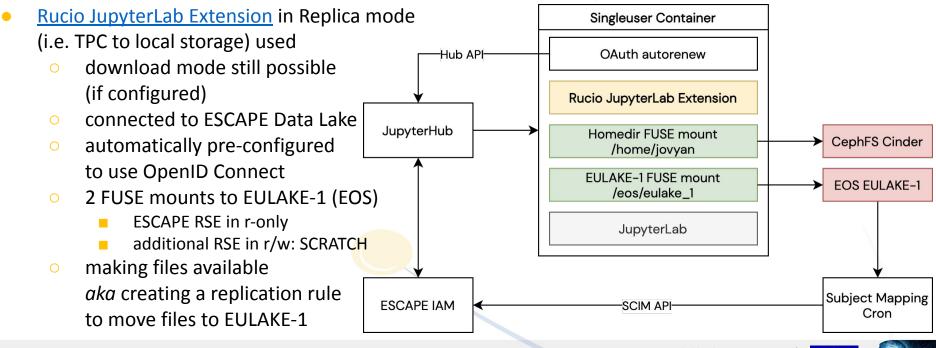
- An idea presented at CS3 2020 by the Rucio team [1]
- Development of a "Rucio JupyterLab Extension" as part of GSoC 2020 [2,3]
- A long time has passed, many things have happened...
  - CERN OpenLab Summer Student to concretise the effort in 2021
    - <u>deployment</u>, <u>docker-images</u>, <u>documentation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

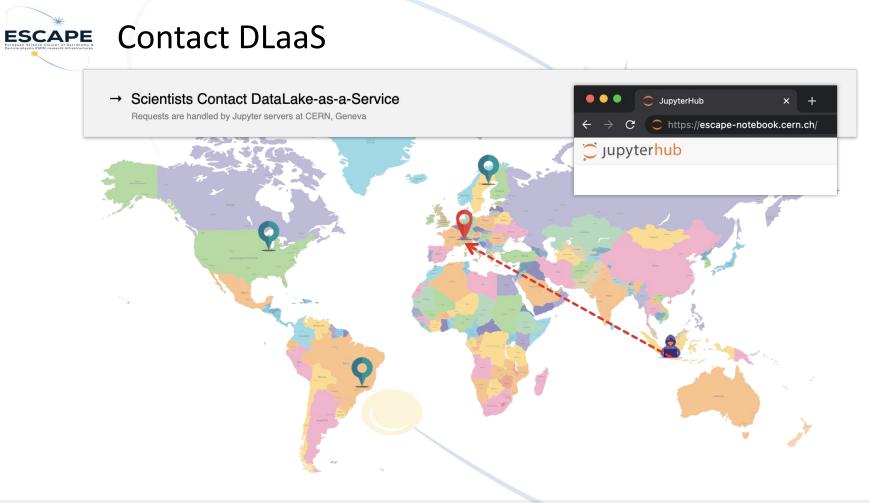
- Deployed in Kubernetes, using Zero-to-JupyterHub Helm chart 
   <u>https://escape-notebook.cern.ch</u>
- OAuth authentication using ESCAPE IAM (X509 still supported)



### **ESCAPE** DataLake-as-a-Service for Open Science









# **ESCAPE** Sign in with OAuth 2.0

••• JupyterHub × +	and the states of the states o		S. 1. 199	
← → C △ C https://escape-notebook.cern.ch		0	. 🐵 🔍 🔋 🖪 🗉 🤤	* = 🛛 🌒 🗄
💢 Jupyter <mark>hub</mark>				
	Sign in with OAuth 2.0			
https://escape-notebook.cern.ch/hub/oauth_login?next=%2Fhub%2F				



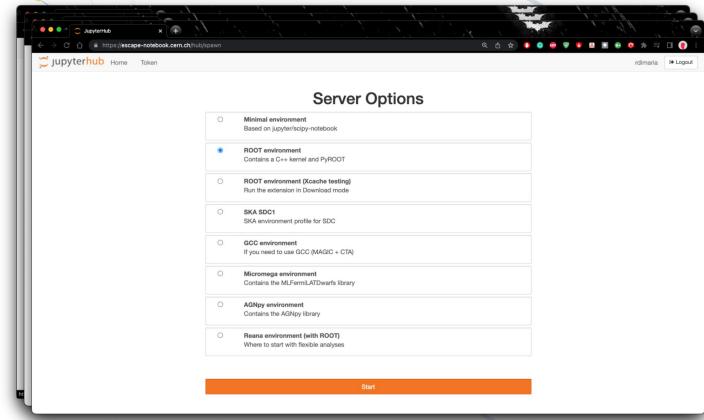
#### **ESCAPE Indigo IAM for Auth**

••• • JINDIGO IAM for escape-Log in x	
← → C A A https://iam-escape.cloud.cnaf.infn.it/login	
	*
	ESCAPE
	Welcome to <b>escape</b>
	Sign in with your escape credentials
	1 rdimaria
	······
	Sign in
	Forgot your password2
	Or sign in with Your X.509 certificate
	G Google
	SeduGAIN
	Not a member?
	Apply for an account
	Privacy policy
M	You have been successfully authenticated as CN=Riccardo Di Iaria,CN=770219,CN=rdimaria,OU=Users,OU=Organic

Funded by the European Union's Horizon 2020 - Grant N° 824064



#### **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

File Edit View Run Kernel Tabs	Launcher
P	Notebook
Search Everything •	Python 3 ROOT C++
	Console
	Python 3 R R R R R R R R R R R R R R R R R R
	\$_ Other
	Terminal     Text File     Markdown File     Show Contextual Help

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

JupyterLab x	a dhean a' an	
← → C △ A https://escape-notebook		≡≀ 🔲
<ul> <li>File Edit View Run Kernel Tabs</li> <li>RUCIO</li> </ul>	Settings Help 23 Launcher	
EXPLORE NOTEBOOK     t	Notebook	
IP     Active Instance       ESCAPE Data Lake     ✓       Image: Second seco	Python 3 ROOT C++	
DpenID Connect           OpenID Connect           X.509 User Certificate           X.509 Proxy Certificate	Console	
Username & Password	\$_ Other	
	S_     Text File       Terminal     Text File	
Save Settings		

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.

14



RUCIO     EXPLORE NOTE	воок 🗢	Notebook	
IP Sear Available scope Available scope Availa	es × T PP_JEZEQUEL PP_SP D_EDU ARGOED_DATA 4_DCIANGOT	Python 3 R Console Python 3 R Python 3 R R ROOT C++	
E ESCAPE_C	CIN2P3_RAHAL_test	S Other	

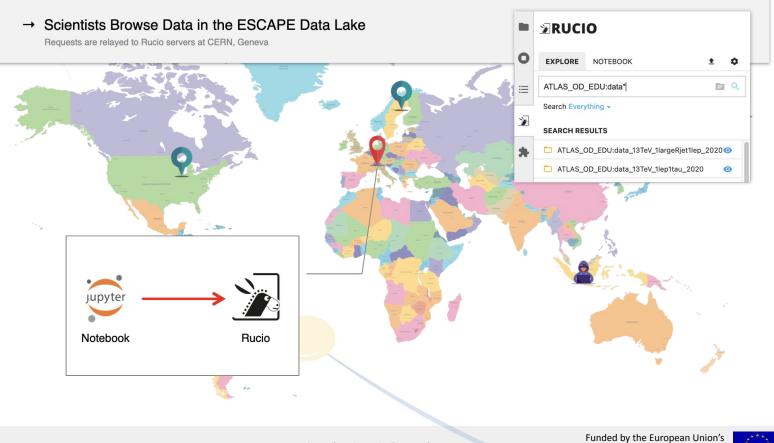
uropean Union's Horizon 2020 - Grant N° 824064



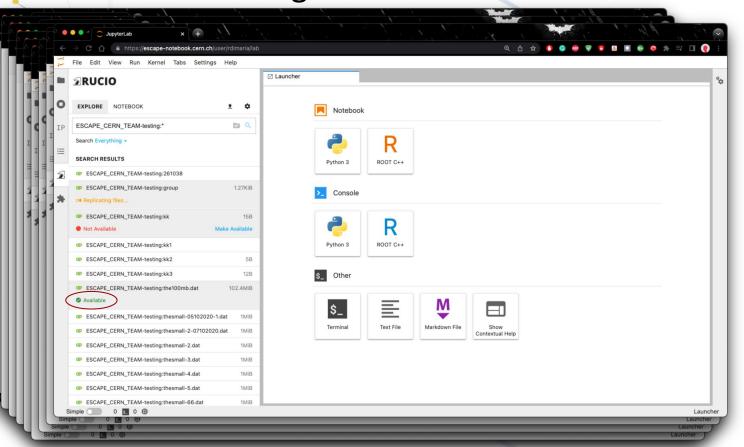
File Edit View Run Kernel Tabs	Settings Help Launcher	
	Laurune	
EXPLORE NOTEBOOK	Notebook	
I I IP ATLAS_OD_EDU:data*	n 🔁 🤁	
Everything	Python 3 ROOT C++	
Datasets Datasets	Console	
Containers Files	🥐 R	
	Python 3 ROOT C++	
	\$_ Other	
	S_     Terminal       Terminal     Text File       Markdown File     Show Contextual Help	

16









18

Riccardo.Di.Maria@cern.ch

Funded by the European Union's Horizon 2020 - Grant N° 824064

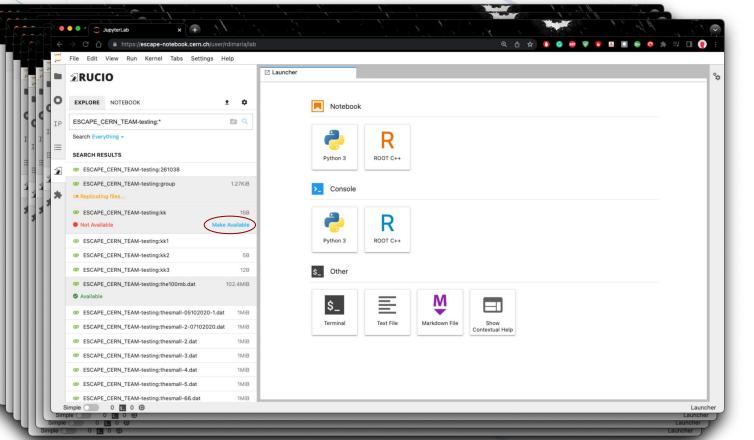


#### **ESCAPE** Redirection to ESCAPE Rucio WebUI

Ru	Icio UI Monitoring * Data Transfers (R2D2) * Admin * pattern OR name OR rule id Search	ୟ 🍐 🖈 🚺 💿 😕 👽 👫 🚨 💽 🐵 🧔 🗮 🏹 🗔 Utilgaccount:
You	are here: Rule [71f827534e314c86af8c5d57d21c3dbe:]	Rucio Version ( WebUI / Server ): 1.25
	Rule metadata	
	account	espinal
	activity	User Subscriptions
	copies	1
I I	created_at	Thu, 01 Oct 2020 13:41:36 UTC
III	did_type	FILE
- = =	expires_at	never + ×
	grouping	DATASET
	id	71f827534e314c86af8c5d57d21c3dbe
	ignore_account_limit	false
1 1	ignore_availability	false
1.1	locked	false
1	locks_ok_cnt	1
	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).

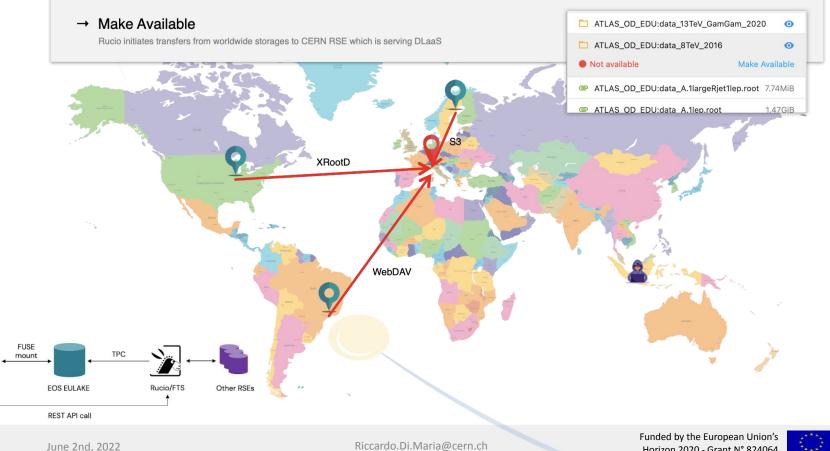
Once replication status is OK, extension translates PFN into local path.

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

20



#### Make Data Available "Locally"

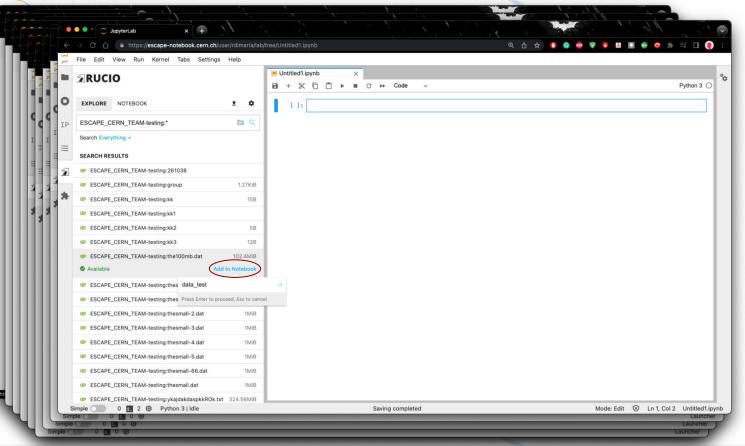


upyte

Jupyter



#### **ESCAPE** Add Data to Notebook



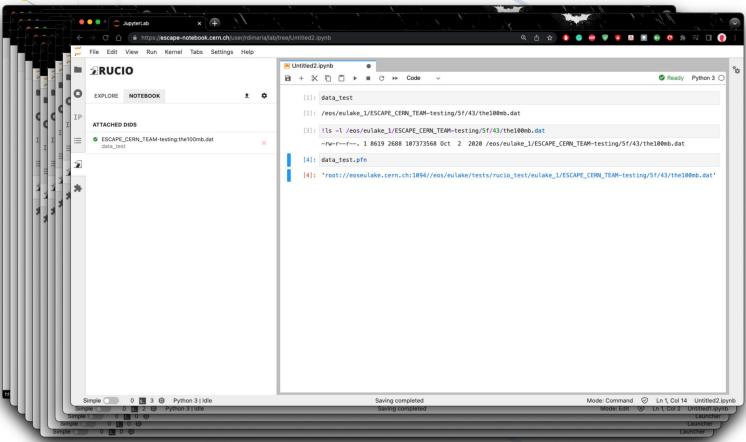
June 2nd, 2022

Riccardo.Di.Maria@cern.ch

Funded by the European Union's Horizon 2020 - Grant N° 824064



### **ESCAPE** Use Data for Analysis



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

Funded by the European Union's Horizon 2020 - Grant N° 824064



June 2nd, 2022

#### **ESCAPE** DataLake-as-a-Service for Open Science

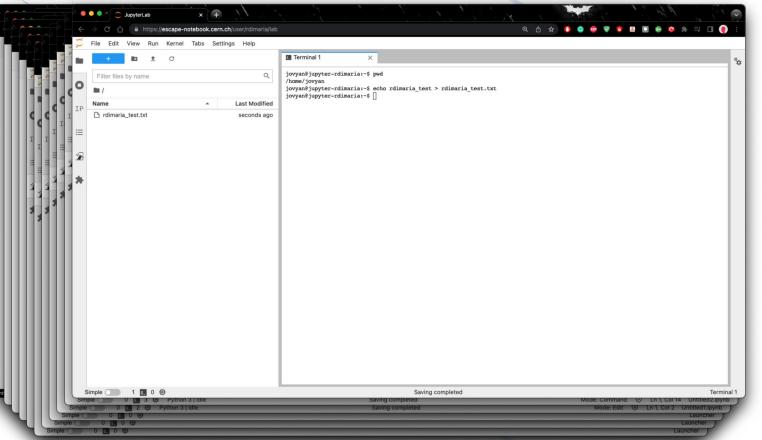
#### → Scientists' Analysis Workflows Read Data

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





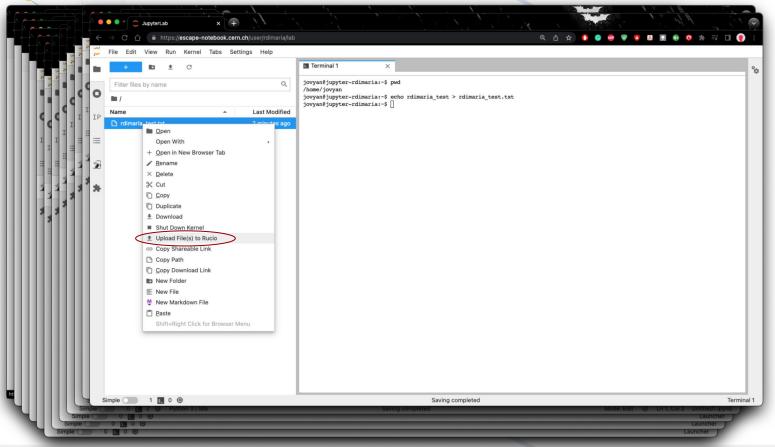
## **ESCAPE** Output of Analysis (Small-Sized Files)



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

Riccardo.Di.Maria@cern.ch



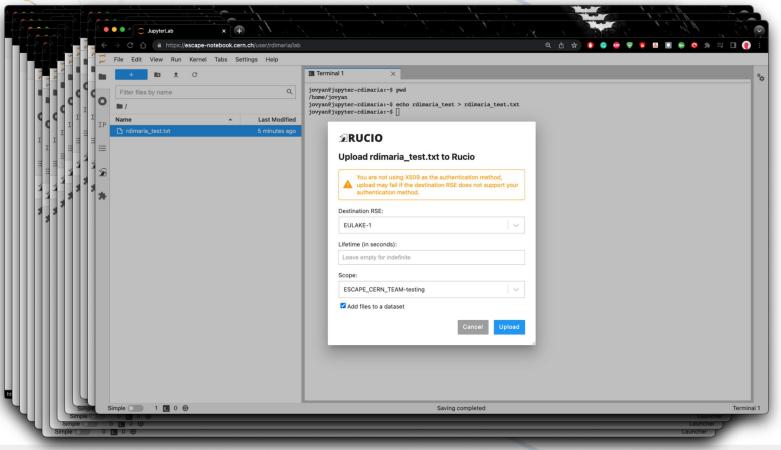


26

Riccardo.Di.Maria@cern.ch

Funded by the European Union's Horizon 2020 - Grant N° 824064





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.



	yupyterLab x		
	← → C ☆ a https://escape-notebook.cern.ch/user/rdin		🔋 🖪 💽 💀 🧔 🌧 🗐 🔲 🌔 :
N N N	File Edit View Run Kernel Tabs Settings Help	p Terminal 1 ×	
	■ <b>ZRUCIO</b>	jovyan@jupyter-rdimaria:-\$	\$
	C EXPLORE NOTEBOOK	joryanejugyez-zuzmazza. V	
	I IP UPLOAD JOBS		
	ESCAPE_CERN_TEAM-testing:rdimaria_test.txt rdimaria_test.txt → EULAKE-1	×	
	2		
3 3 3 3 3 3 Singal	*		
Simple Simple	Simple 1 5 0 @	Saving completed	Terminal 1
Simple O			Launcher

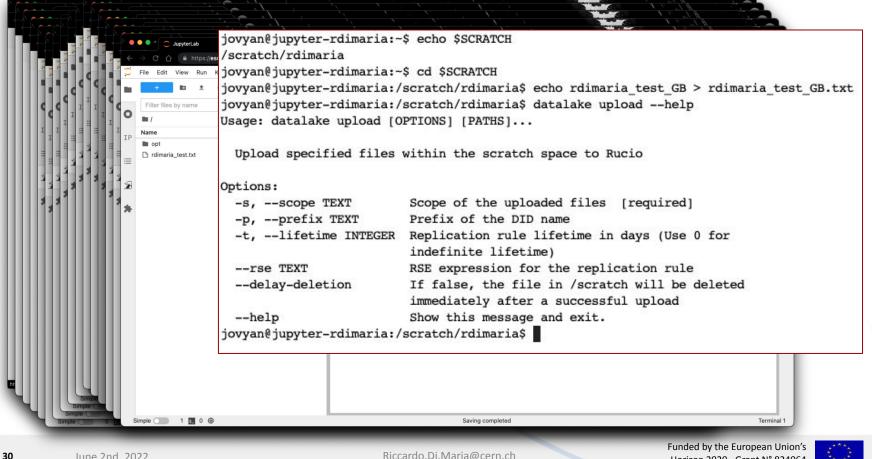


C A https://escape-notebook.cern.ch/user/rdimaria/lab	아 Q 合 ☆) 🚺 🧔 🥹 😵 😫 🔝 🕼 🧔 🐎 🖘 🗔 🌒 :
File Edit View Run Kernel Tabs Settings Help	I Terminal 1 X
RUCIO	1
	jovyan@jupyter-rdimaria:-\$ []
I I I I I I I I I I I I I I I I I I I	
Search Everything -	
SEARCH RESULTS	
ESCAPE_CERN_TEAM-testing:rdimaria_test.txt	
Available	
Simple 0 1 0 0	Saving completed Terminal 1

29



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





### **ESCAPE** Data Preparation and Processing Use Case

← ← → C 介 â https://escape-notebook.cern.ch/user/rdimaria	ajlab 🗢 Q 습 ☆ 🚺 😨 😰 😨 😰 😨 🧐 🖉 🤌 🗐	II 🥊 i
	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.

31

Riccardo.Di.Maria@cern.ch

Funded by the European Union's Horizon 2020 - Grant N° 824064



### **ESCAPE** Data Preparation and Processing Use Case

JupyterLab ← → C △ ê https://escap	× + e-notebook.cern.ch/user/rdimaria/lab rel Tabs Settings Help	()	File Edit View Run Kernel Tabs Settings Help
Filer files by name / IIIIIIIIIIIIIIIIIII HIIIIIIIIIIIII	Last Modified     joyyanë jupytez- /scratch/rdinar joyyanë jupytez- joyyanë jupytez- joyyanë jupytez- joyyanë jupytez- joyyanë jupytez- joyyanë jupytez- joyranë jupytez- joyranë jupytez- joyranë jupytez- joyranë jupytez- ioyranë jupytez- ioyranë jupytez- ioyranë jupytez- 	■ 0 IP	EXPLORE NOTEBOOK   ESCAPE_CERN_TEAM-testing:rdimaria_test_GB.txt   Search Everything ~   SEARCH RESULTS
Simple Simple 1 D 0 D	joryane jogycez -	2	ESCAPE_CERN_TEAM-testing:rdimaria_test_GB.txt

### **ESCAPE** Rucio CLI Available

JupyterLab x (+)	
$ \langle \dot{c} \rangle = C \land (a \text{ https://escape-notebook.cern.ch/user/rdimaria/lab} $	i 🌗 🗉 🖬 🌒 i
File Edit View Run Kernel Tabs Settings Help	
	%
JOYARĚJUPYT-rdimaria:/scratch/rdimaria\$ rucio whoami created_at: 2019-12-05T16:43:26 account : rdimaria status : ACTIVE	
IIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIIII	
I     I     I     I     I     I       I     I     I     I     I     I   Search Everything - Search Everything - Search Everything -	
Suspended at : None joyvarder-rdimaria*/scratch/rdimaria\$ rucio list-rses ALPANED-DPM	
ESCAPE_CERN_TEAM-testing:rdimaria_test_GB.txt 178 ANS_WEBDONV CERNBOX-CS3	
CNA-STON-TAPE CNA-STON-TAPE CNA-STON-TAPE DEST-OCACHE-NDR DEST-OCACHE-NDR DEST-OCACHE-NDR DEST-OCACHE-NDR DEST-OCACHE-NDR EULARE-SC FAIL-NOOT GSI-ROOT IN2P3-OC-LSST-BOORCE IN2P3	
Simple 1 1 0 0 Saving completed	Terminal 1
Simple 0 1 B 0 0 Saving completed	Terminal 1

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

33



<b>ESCAPE</b> XCache Integration	
Server Options	💭 File Edit View Run Kernel Tabs Settings Help
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	<ul> <li>EXPLORE NOTEBOOK</li> <li>EXPLORE NOTEBOOK</li> <li>Active Instance</li> <li>ESCAPE Data Lake</li> <li>ESCAPE Data Lake (Download)</li> <li>ESCAPE Data Lake</li> </ul>
Untitled4.ipynb × HyyAnalysis.ipynb × I Terminal 1	×
rucio_test/eulake_1/ATLAS_LAPP_JEZEQUEL/bd/8f/data.root	EQUEL:data.rootprotocol root ache-redirector.cern.ch//root://eoseulake.cern.ch:1094//eos/eulake/tests/ /xcache-redirector.cern.ch//root://lapp-testse01.in2p3.fr:1094//dpm/in2p3

×





- 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

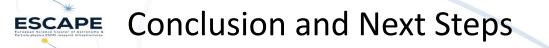




## **ESCAPE** Future Developments

- 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

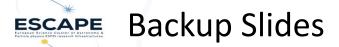




- **DLaaS** hides the complexities of the Data Lake from the end users (so that they are happy and productive!)
  - interesting for both **aficionados** and **newcomers** of **Rucio**
  - o community-driven development, hence driven by the needs of different experiments and sciences
- ESCAPE managed 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









Riccardo.Di.Maria@cern.ch

Funded by the European Union's Horizon 2020 - Grant N° 824064



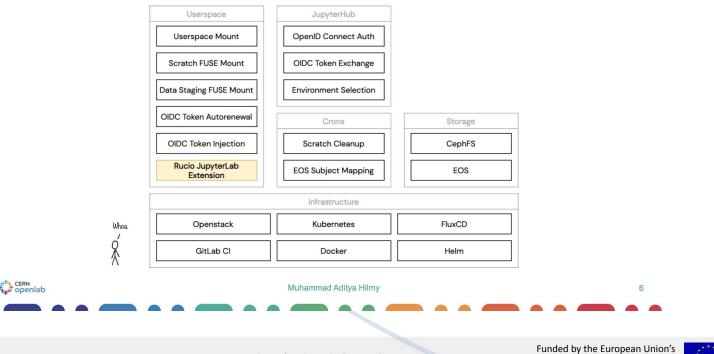
#### **ESCAPE** DataLake-as-a-Service for Open Science

1 C + escape ruce webs com de service, auf antiente service de la servic			st 🕫 🙆 manganta 🖡
a Ul Muntaveg - Data Transfors (1950) - Admin -	James Of Lines (	Non of County of	Dising account: multiliny
e fere Rule (1967/05912+600296481ac02005c6481)			Ratio Version (WebCR) Server 3:125.8/126.8 -
luie metadata			
account		muhitray	
activity		User Subscriptions	
ooples		*/	
breated, at		Wed. 15 5ep 2021 07:24:14 UTC	
did.1yp+		FLE	
ospires, at		Wed, 15 Sep 2021 08:24:14 UTG 🔶 🕷	
Burringelo		DADABET	
inf		7768/70c491da4d828d49cac5302ca644	
ignore account limit		Mine -	
grow, availability		Salary .	
incked		Autom	
licks_sk_crt		10	
woké, replicating, cm		1	
likka, stuck_ovt		a	
name		ggH125 gamper, roal	
netBeation		NO	

39



## Tine Unite As a Service





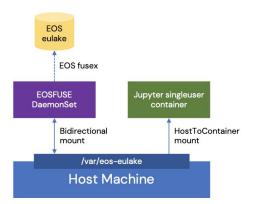
Horizon 2020 - Grant N° 824064

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





Riccardo.Di.Maria@cern.ch

ESCAPE

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

