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Big Data and Quantum Computing

Extending Rucio to support external metadata catalog

Luca Pacioselli (INFN Perugia) on behalf of IDL

"ICSC and Spoke 2 - Where Are We Now?"
Catania, December 10-12 2024

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- What’s next?

Introduction

- One key point of the interoperable Data Lake (IDL) project:
  - develop an interoperable, distributed **Data Lake** service with **state-of-the-art open-source technologies**

See Nicolò Magini's talk

Interoperable Data Lake (IDL)
Nicolò Magini

"ICSC and Spoke2 – Where Are We Now?",
Catania, 10-12 December 2024

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- The presented work focuses on WP1@IDL: developing an **end-to-end prototype** for DM in a distributed environment and on the extension of Rucio to **support external metadata catalogs**

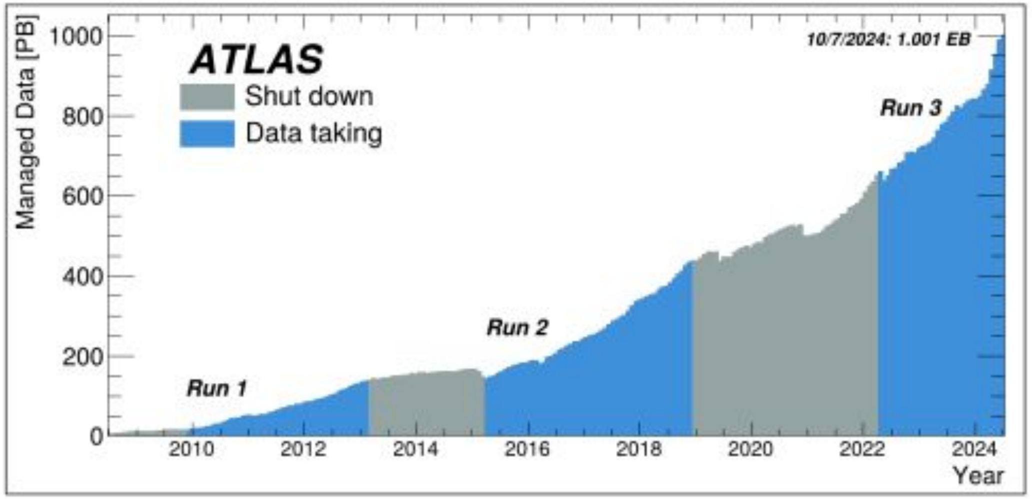
Data Management solution: Rucio

SCIENTIFIC DATA MANAGEMENT
RUCIO

- Rucio is an open-source software for large-scale DM:
  - initially developed by CERN for ATLAS experiment's needs
  - now widely adopted across HEP experiments and beyond (CMS, Belle II, DUNE, etc...)
- Key features:
  - handles large volumes O(ExaBytes) of data
  - data can be stored in geographically distributed storage endpoints
- For IDL we need to **extend** its standard functionality:
  - external metadata database (DB) and tailored client

Proven to work in very challenging environments

Rucio@ATLAS: 1+ Exabyte, 120 data centres



"Volume of Data managed by Rucio: source"

Implementation Strategy: a quick overview

❑ To develop an **automated deployment of a Rucio server** Kubernetes (k8s) cluster

- this include the deployment of **S3 cloud storage** endpoint(s)

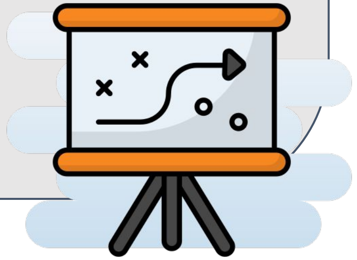
❑ To **extend** the **Rucio** support for external **metadata catalogs** and confine the interactions with the external DB to the server layer:

- strict control on the Rucio-DB interactions (AuthN/Z and atomicity of the operations)

❑ To prototype a **Rucio client wrapper for IDL**-specific requirements :

- to manage data and metadata in a coherent manner
- tailored query system to interrogate the external DB

❑ To provide documentation outlining the steps of the work



Where are we?

✓ Deployed an automated (custom Docker image) Rucio server instance on a k8s cluster (nginx, HTTPS over TLS)

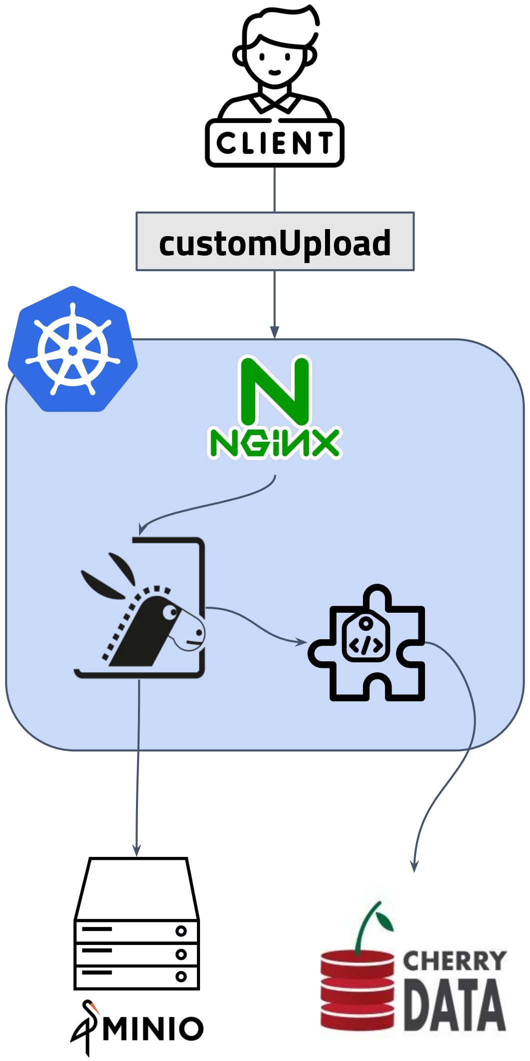
- Configured a storage endpoint with MinIO as an S3-compatible RSE

✓ Functional prototype in Python of a **DID-metadata plugin** to communicate with an external database: AyraDB

✓ Tailored **Rucio client**:

- custom methods to seamlessly interact with the external DB via the DID-metadata plugin
- Python binding to use all the standard methods of Rucio

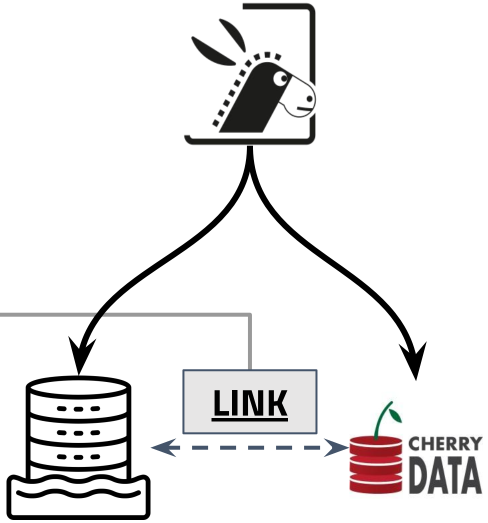
~ Documentation will be available on a Spoke2 github repository



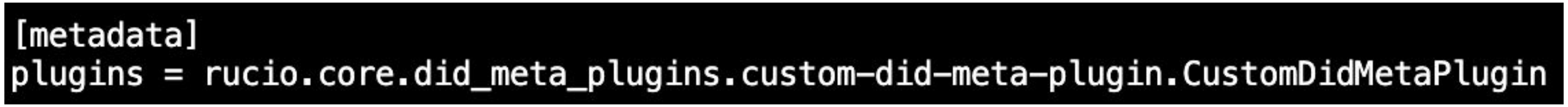
Extension to external metadata catalog: AyraDB

In the IDL project, Rucio plays a central role in the ingestion phase:

- **data** are stored in the **Data Lake**
- **metadata** are stored in the metadata DB, implemented with **AyraDB**
- associates a **LINK**, Data IDentifier (DID), that links the data with its metadata



The concept of **DID-metadata plugins** exists in Rucio:



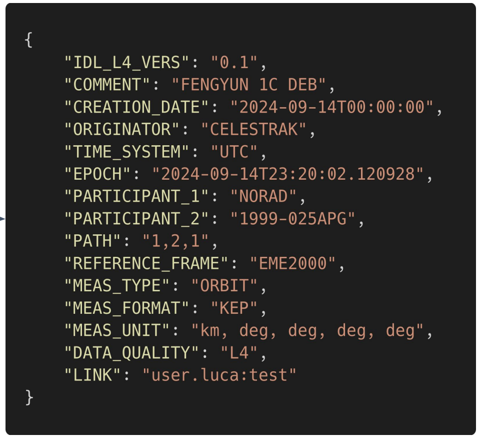
```
[metadata]
plugins = rucio.core.did_meta_plugins.custom-did-meta-plugin.CustomDidMetaPlugin
```

AyraDB, provided by CherryData:

- is a high-throughput DB
- manages read- and write-intensive workloads with all types of data (e.g. JSON files)

Custom DID-metadata plugin

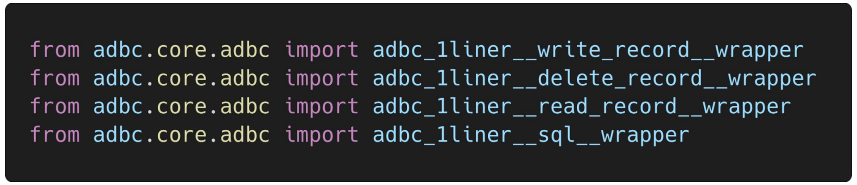
- To **extend metadata catalog** we designed a DID-metadata plugin that allows for external databases to be integrated



```
{
    "IDL_L4_VERS": "0.1",
    "COMMENT": "FENGYUN 1C DEB",
    "CREATION_DATE": "2024-09-14T00:00:00",
    "ORIGINATOR": "CELESTRAK",
    "TIME_SYSTEM": "UTC",
    "EPOCH": "2024-09-14T23:20:02.120928",
    "PARTICIPANT_1": "NORAD",
    "PARTICIPANT_2": "1999-025APG",
    "PATH": "1,2,1",
    "REFERENCE_FRAME": "EME2000",
    "MEAS_TYPE": "ORBIT",
    "MEAS_FORMAT": "KEP",
    "MEAS_UNIT": "km, deg, deg, deg, deg",
    "DATA_QUALITY": "L4",
    "LINK": "user.luca:test"
}
```

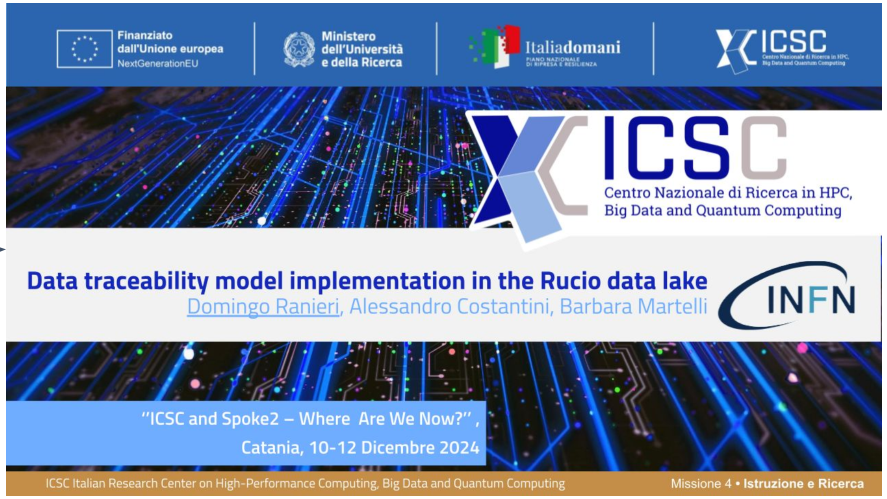
Example of IDL metadata

- The **AyraDB Connector** (**ADBC**) client, by CherryData, allows smooth implementation to perform operations on metadata



```
from adbc.core.adbc import adbc_1liner__write_record__wrapper
from adbc.core.adbc import adbc_1liner__delete_record__wrapper
from adbc.core.adbc import adbc_1liner__read_record__wrapper
from adbc.core.adbc import adbc_1liner__sql__wrapper
```

  - Custom DID-metadata plugin developed also to support interactions with the **blockchain** (see Domingo Ranieri's talk)



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Data traceability model implementation in the Rucio data lake

Domingo Ranieri, Alessandro Costantini, Barbara Martelli

INFN

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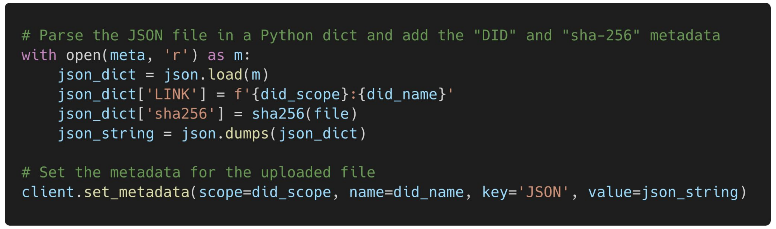
Dedicated Rucio client

- To ensure seamless interactions with the plugin, a dedicated **Rucio client** is needed
- **Python bindings** to include Rucio's default methods for a unified client experience



```python
# Parse the JSON file in a Python dict and add the "DID" and "sha-256" metadata
with open(meta, 'r') as m:
    json_dict = json.load(m)
    json_dict['LINK'] = f'{did_scope}:{did_name}'
    json_dict['sha256'] = sha256(file)
    json_string = json.dumps(json_dict)

# Set the metadata for the uploaded file
client.set_metadata(scope=did_scope, name=did_name, key='JSON', value=json_string)
```

customUpload:

- **combines** upload and set-metadata
- **whole JSON files** as metadata

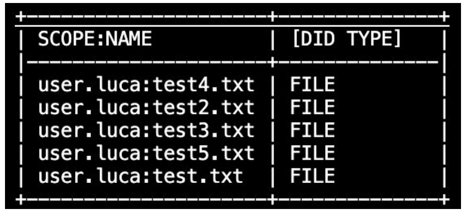
- Queries **AyraDB** via Rucio **without** needing **direct access**

customListDids:

- retrieve the **DIDs** satisfying user-defined filters

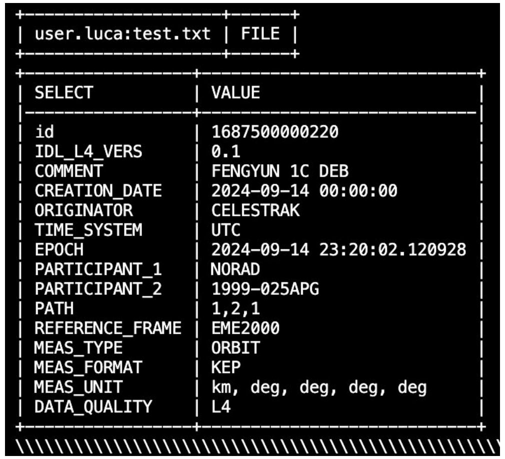
customQuery:

- retrieve a user-defined **list of metadata keys**



```
+----------------------+-------------+
| SCOPE:NAME           | [DID TYPE]  |
|----------------------+-------------|
| user.luca:test4.txt  | FILE        |
| user.luca:test2.txt  | FILE        |
| user.luca:test3.txt  | FILE        |
| user.luca:test5.txt  | FILE        |
| user.luca:test.txt   | FILE        |
+----------------------+-------------+
```

Output: customListDids

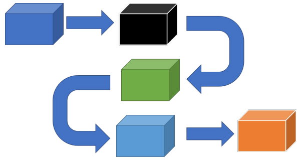


```
+---------------------+------+
| user.luca:test.txt  | FILE |
+---------------------+------+
+-----------------+------------------------------+
| SELECT          | VALUE                        |
|-----------------+------------------------------|
| id              | 1687500000220                |
| IDL_L4_VERS     | 0.1                          |
| COMMENT         | FENGYUN 1C DEB               |
| CREATION_DATE   | 2024-09-14 00:00:00          |
| ORIGINATOR      | CELESTRAK                    |
| TIME_SYSTEM     | UTC                          |
| EPOCH           | 2024-09-14 23:20:02.120928   |
| PARTICIPANT_1   | NORAD                        |
| PARTICIPANT_2   | 1999-025APG                  |
| PATH            | 1,2,1                        |
| REFERENCE_FRAME | EME2000                      |
| MEAS_TYPE       | ORBIT                        |
| MEAS_FORMAT     | KEP                          |
| MEAS_UNIT       | km, deg, deg, deg, deg       |
| DATA_QUALITY    | L4                           |
+-----------------+------------------------------+
\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\
```

Output: customQuery

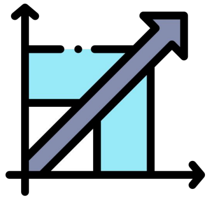
Future Plans: what's next?

- **End-to-End Testing**: Validate the solution using domain-specific datasets to meet real-world scenarios.



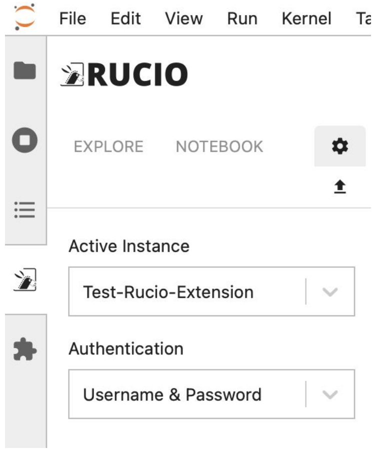
End to End Testing

- **Scalability Test**: Perform stress tests to evaluate the system's scalability as more data is ingested into the Data Lake and AyraDB.



Scalability Test

- **JupyterHub Integration**: Deploy a JupyterHub instance over a k8s cluster to enable seamless interaction between the Rucio based Data Lake and data analysis workflows



Active Instance

Test-Rucio-Extension

Authentication

Username & Password

Thank you for your attention!

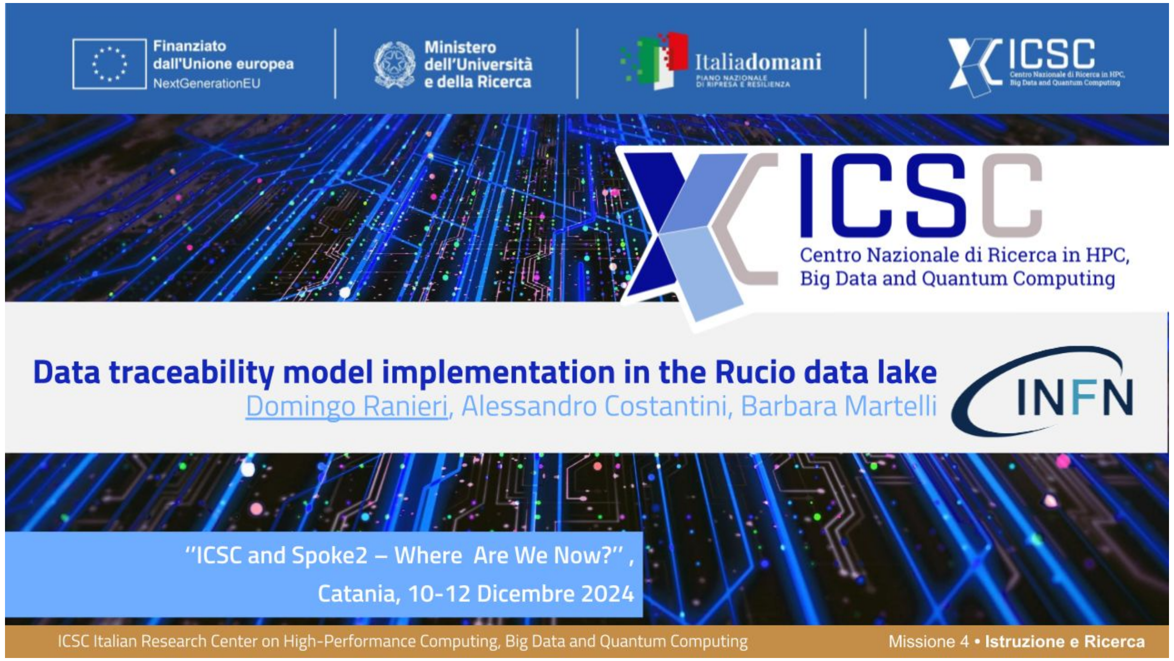
luca.pacioselli@pg.infn.it

Backup

Blockchain implementation

Blockchain functionality, in collaboration with Domingo Ranieri:

- **Hashes Storing**: blockchain stores SHA-256 hashes of data and metadata
- **Data Validation**: when file uploaded, hashes of data and metadata are stored in the blockchain
- **Verification Process**: when files retrieved, both metadata and data hashes are compared against blockchain-stored hashes



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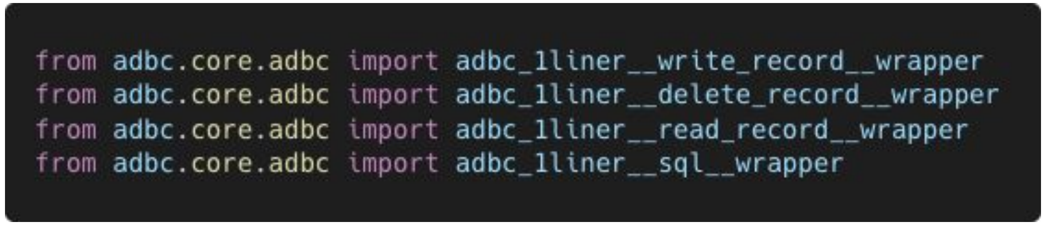
Custom DID-metadata plugin

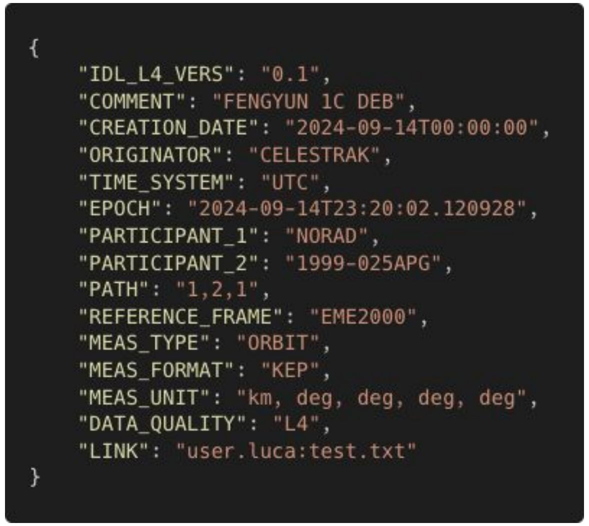
To **extend** the Rucio **metadata catalog** we designed a DID-metadata plugin that allows for external databases to be integrated for storing and querying metadata: AyraDB in our case

Functional methods for metadata handling are: set-, get-, delete-metadata and list-dids

The **AyraDB Connector** (ADBC) client, by CherryData, allows smooth implementation to perform operations like writing, deleting, or querying metadata:



```python
from adbc.core.adbc import adbc_1liner__write_record__wrapper
from adbc.core.adbc import adbc_1liner__delete_record__wrapper
from adbc.core.adbc import adbc_1liner__read_record__wrapper
from adbc.core.adbc import adbc_1liner__sql__wrapper
```

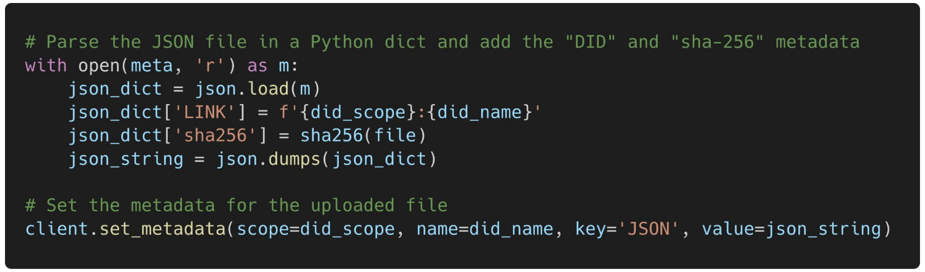


```json
{
    "IDL_L4_VERS": "0.1",
    "COMMENT": "FENGYUN 1C DEB",
    "CREATION_DATE": "2024-09-14T00:00:00",
    "ORIGINATOR": "CELESTRAK",
    "TIME_SYSTEM": "UTC",
    "EPOCH": "2024-09-14T23:20:02.120928",
    "PARTICIPANT_1": "NORAD",
    "PARTICIPANT_2": "1999-025APG",
    "PATH": "1,2,1",
    "REFERENCE_FRAME": "EME2000",
    "MEAS_TYPE": "ORBIT",
    "MEAS_FORMAT": "KEP",
    "MEAS_UNIT": "km, deg, deg, deg, deg",
    "DATA_QUALITY": "L4",
    "LINK": "user.luca:test.txt"
}
```

Example of IDL metadata

Dedicated Rucio client

- To ensure seamless communication between users, the plugin, and the blockchain, a dedicated **Rucio client** is needed
- Extended functionalities to upload, get-metadata, list-dids methods and new sql method to do custom queries
- **Python bindings** to include Rucio's default methods for a unified client experience



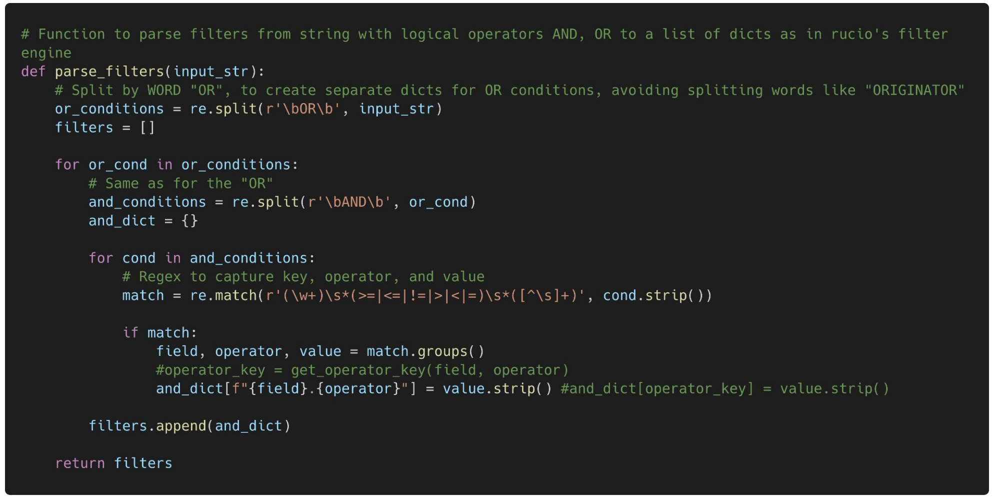
```python
# Parse the JSON file in a Python dict and add the "DID" and "sha-256" metadata
with open(meta, 'r') as m:
    json_dict = json.load(m)
    json_dict['LINK'] = f'{did_scope}:{did_name}'
    json_dict['sha256'] = sha256(file)
    json_string = json.dumps(json_dict)

# Set the metadata for the uploaded file
client.set_metadata(scope=did_scope, name=did_name, key='JSON', value=json_string)
```

customUpload:

- Rucio uploads data first, then sets metadata
- customUpload **combines** the two steps
- Handles specific integration needs with the plugin and AyraDB, e.g. passing **JSON file** content as a **whole**

Improves user experience and efficiency, ensuring smooth interaction with AyraDB

Dedicated Rucio client (cont.)

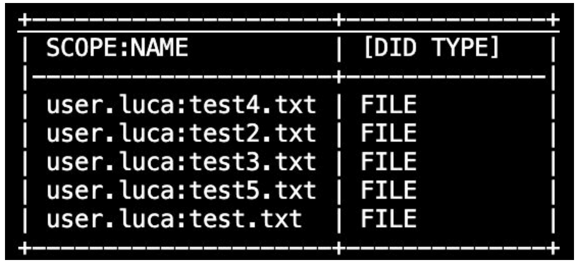


```python
# Function to parse filters from string with logical operators AND, OR to a list of dicts as in rucio's filter
engine
def parse_filters(input_str):
    # Split by WORD "OR", to create separate dicts for OR conditions, avoiding splitting words like "ORIGINATOR"
    or_conditions = re.split(r'\bOR\b', input_str)
    filters = []

    for or_cond in or_conditions:
        # Same as for the "OR"
        and_conditions = re.split(r'\bAND\b', or_cond)
        and_dict = {}

        for cond in and_conditions:
            # Regex to capture key, operator, and value
            match = re.match(r'(\w+)\s*(>=|<=|!=|>|<|=)\s*([^\s]+)', cond.strip())

            if match:
                field, operator, value = match.groups()
                #operator_key = get_operator_key(field, operator)
                and_dict[f"{field}.{operator}"] = value.strip() #and_dict[operator_key] = value.strip()

        filters.append(and_dict)

    return filters
```

Methods for Database Interaction:

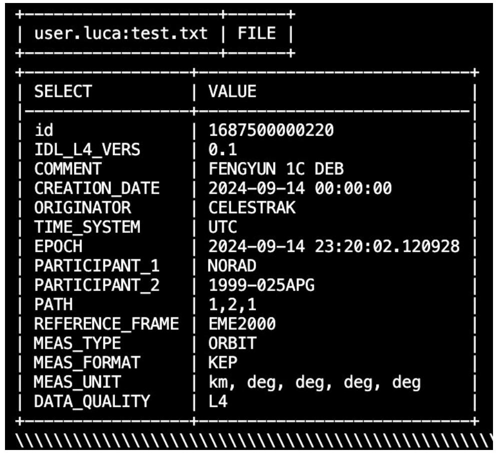
1. **customListDids** (extension of “rucio list-dids”)
   - Interrogates AyraDB through the plugin to retrieve a **list of DIDs** based on user-specified filters
2. **customQuery** (added functionality to Rucio)
   - Queries AyraDB via the plugin to retrieve a user-defined **list of keys** (DIDs are included by default)

Users can query **database queries through Rucio** to interact with the external database **without** needing **direct access**



```
+----------------------+--------------+
| SCOPE:NAME           | [DID TYPE]   |
|----------------------+--------------|
| user.luca:test4.txt  | FILE         |
| user.luca:test2.txt  | FILE         |
| user.luca:test3.txt  | FILE         |
| user.luca:test5.txt  | FILE         |
| user.luca:test.txt   | FILE         |
+----------------------+--------------+
```

Output: customListDids



```
+---------------------+------+
| user.luca:test.txt | FILE |
+---------------------+------+

+------------------+-----------------------------+
| SELECT           | VALUE                       |
|------------------+-----------------------------|
| id               | 1687500000220               |
| IDL_L4_VERS      | 0.1                         |
| COMMENT          | FENGYUN 1C DEB              |
| CREATION_DATE    | 2024-09-14 00:00:00         |
| ORIGINATOR       | CELESTRAK                   |
| TIME_SYSTEM      | UTC                         |
| EPOCH            | 2024-09-14 23:20:02.120928 |
| PARTICIPANT_1    | NORAD                       |
| PARTICIPANT_2    | 1999-025APG                 |
| PATH             | 1,2,1                       |
| REFERENCE_FRAME | EME2000                     |
| MEAS_TYPE        | ORBIT                       |
| MEAS_FORMAT      | KEP                         |
| MEAS_UNIT        | km, deg, deg, deg, deg      |
| DATA_QUALITY     | L4                          |
+------------------+-----------------------------+
\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\\
```

Output: customQuery

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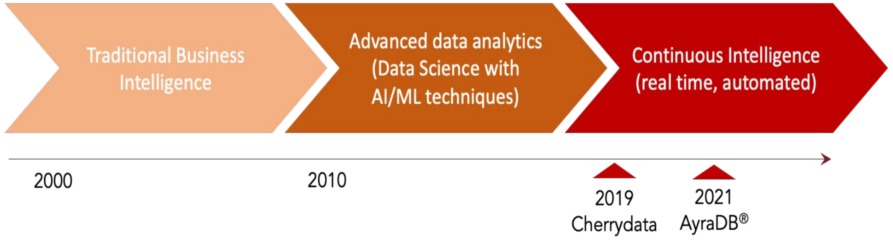
AyraDB as a metadata database for the “space debris” use case, objectives

Original slide by: Nicolò Magini (thanks!)

- In the IDL system, data are stored on a data lake, while **metadata** are stored on a **dedicated database**
- AyraDB (high-performance database designed by **Cherrydata**, **www.ayradb.com**) has been chosen as metadata DB
- The objective is to **maximise query performance** by executing SQL queries on the metadata database (AyraDB) and retrieving from the data lake only the requested data

Cherrydata is a startup (and a spinoff of PoliMi), offering consulting, innovation, and research services on big data and analytics.


Traditional Business Intelligence
Advanced data analytics (Data Science with AI/ML techniques)
Continuous Intelligence (real time, automated)
2000
2010
2019 Cherrydata
2021 AyraDB®

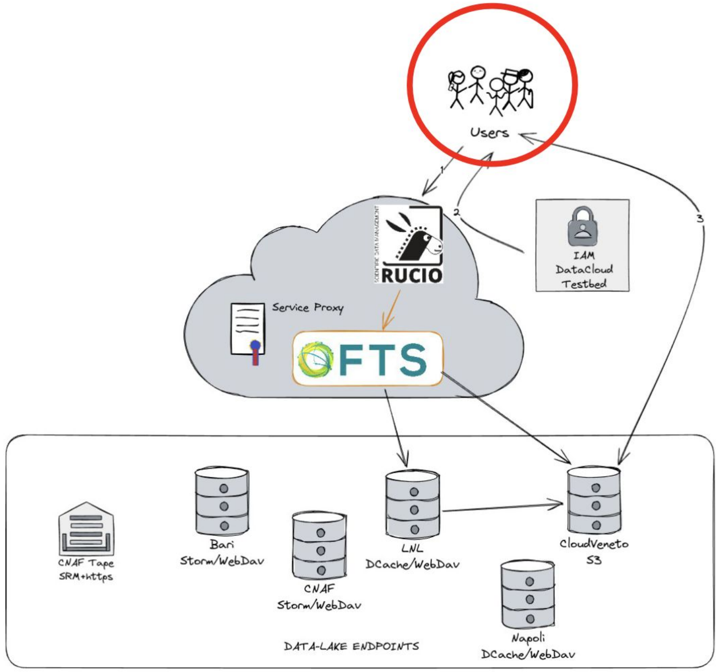
- *AyraDB has been tested on Leonardo Davinci-1 supercomputer in 2022, as part of Euro NCC project.*
- *Cherrydata is involved in IDL as technology provider, to test AyraDB in the context of storing and querying astrophysical data and satellite measurements.*

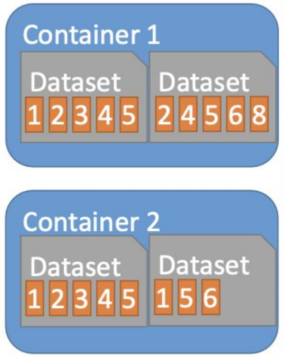
- The implementation of AyraDB has been designed to **minimise response time** to queries operating **on large tables**
- Preliminary tests have been performed on synthetic metadata (1 billion records)

Rucio in a nutshell

Data Management tool:

- manages data **transfers**, **deletions** and **storage**
- integrates with **many storage solutions**
- data can be stored across **multiple sites**, with diverse **setups** and **protocols**
- **data can be anything**: scientific observations, measurements, objects, events, images saved in files, etc…

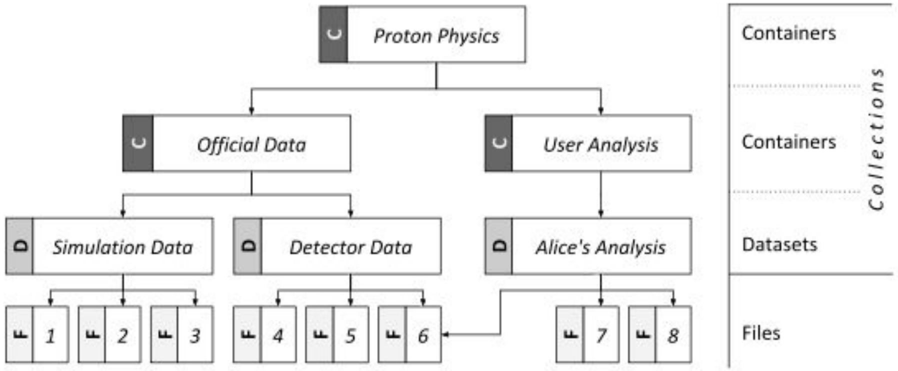




Rucio **Files**, **Datasets** and **Containers**:

- Files can be replicated using **rules**
- Files are grouped in **datasets** (can belong to multiple datasets)
- **Containers** are collections of datasets and containers

Rucio in a nutshell (cont.)



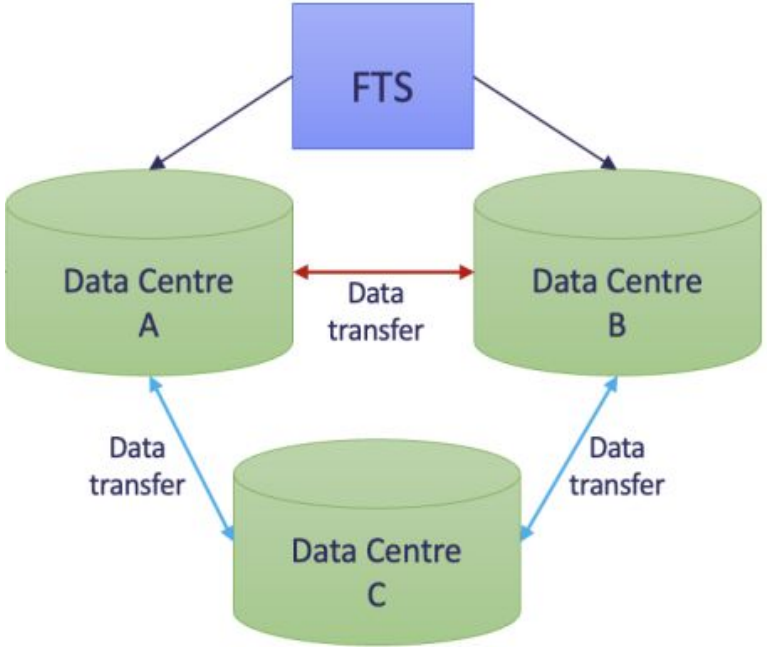
1. **Namespace** handling:
   - Data are organized using Data IDentifiers (**DIDs**)
     - three levels of granularity: files, datasets, and containers
   - DIDs are globally **unique**
     - **identified forever**: cannot reuse names of deleted DIDs
     - name change when data have been changed
   - Global namespace containing all DIDs can be partitioned into **scopes**
   - DIDs are always tuples **<scope>:<name>**
     - names are unique in a scope, whereas DIDs are globally unique

2. **Storage** abstraction:
   - Rucio associates physical location of DIDs with Rucio Storage Elements (**RSEs**)
   - RSE holds **all attributes** to **access** the **storage** space: hostname, port, protocol, and local file system path
   - No software needed to run at the data centers providing storage as RSE configs are in Rucio

Data transfer between multiple RSEs

FTS : File Transfer Service responsible for Bulk data movement

- Open-source software for large-scale queuing and reliable execution of file transfers
- Efficiently **schedules data transfers**
- **Maximizes** use of available **network** & **storage** resources whilst respecting any limits



WP1@IDL enhances the existing services

- to provide a seamless integration with external metadata
- to integrate datalake and compute enviroment

WP1@IDL in a nutshell

- **Test solutions for managing data in a geographically distributed environment (aka the DataLake)** by building end-to-end prototype and testbeds to demonstrate the capability to analyze the astrophysical observations and simulations available data in a cloud environment.

- **The Data Management capability**
  - Store/inject data (meant as files or data objects) in the DataLake
- **The data and compute integration for a effective processing and analysis**
  - deploy Platform as a Service (PaaS) services for the actual processing of the data ingested into the Datalake.

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