The ESCAPE Project: Data Lake and Science Platform

Yan Grange
grange@astron.nl

Klaas Kliffen
kliffen@astron.nl

John Swinbank
swinbank@astron.nl

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

Introductions & ESCAPE Overview

John Swinbank

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

Overview

- Introductions: who are we?
- Context: the ESCAPE project, its environment, its acronyms.
- Other ESCAPE deliverables: software repository, VO, citizen science
- Deep dive: DIOS — the “Data Lake”
- Deep dive: ESAP — the “Science Platform”

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

ESCAPE Goals & Fast Facts

- **Develop common “e-infrastructure” solutions that benefit a wide range of particle physics & astronomy research facilities.**
- ~30 different partners across 8 countries.
- Operating in partnership with four other “cluster” projects covering environmental research (ENVRI), neutron & photon science (PaNOSC), life sciences (EOSC-Life), and social sciences and humanities (SSHOC).
- Project runs from 2019 until 2023.

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

ESCAPE Consortium

ASTRON · CWI · MAX-PLANCK-GESELLSCHAFT · FAU · Heidelberger Institut für Theoretische Studien · THE UNIVERSITY OF EDINBURGH · DESY · UNIVERSIDAD COMPLUTENSE MADRID · university of groningen · IFAE · INFN · Nikhef · Trust-IT Services communicating to markets · INSTITUTO NACIONAL DE TÉCNICA AEROESPACIAL · Royal Observatory of Belgium · CSIC · GSI · AIP Leibniz-Institut für Astrophysik Potsdam · INAF · Leibniz-Institut für Sonnenphysik (KIS) · cnrs · CERN · UNIVERSITÄT HEIDELBERG ZUKUNFT SEIT 1386 · Università di Roma Tor Vergata · OROBIX TOOLS WITH A MIND · The Open University · SURF SARA

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

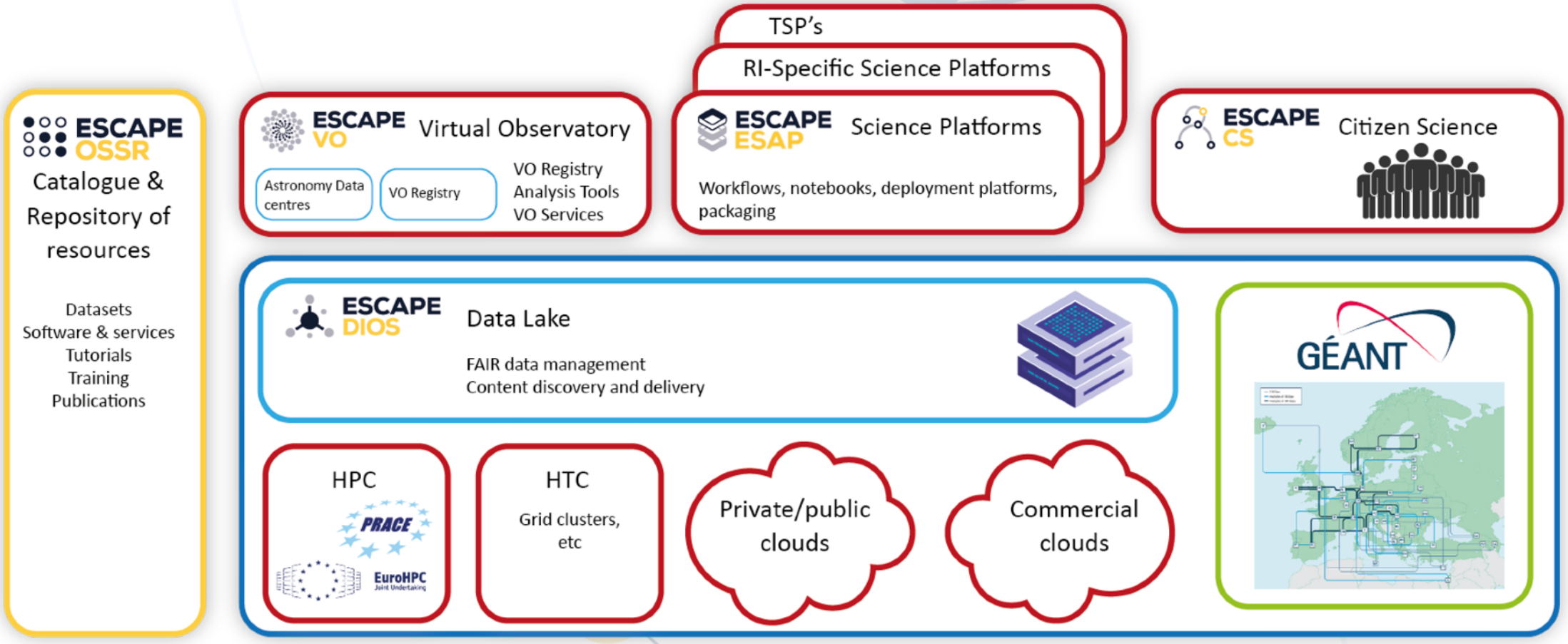
Acronyms

- **ESCAPE**: **E**uropean **S**cience **C**luster of **A**stronomy and **P**article physics **E**SFRI research infrastructures
- **ESFRI**: **E**uropean **S**trategy **F**orum on **R**esearch **I**nfrastructures
- **EOSC**: **E**uropean **O**pen **S**cience **C**loud
- **DIOS**: **D**ata **I**nfrastructure for **O**pen **S**cience (Yan's presentation)
- **ESAP**: **E**SFRI **S**cience **A**nalysis **P**latform (Klaas' presentation)

- So that means that “ESCAPE ESAP” is the European Science Cluster of Astronomy and Particle physics European Strategy Forum on Research Infrastructures research infrastructures European Strategy Forum on Research Infrastructures Science Analysis Platform.
  - …watch out for a quiz later!

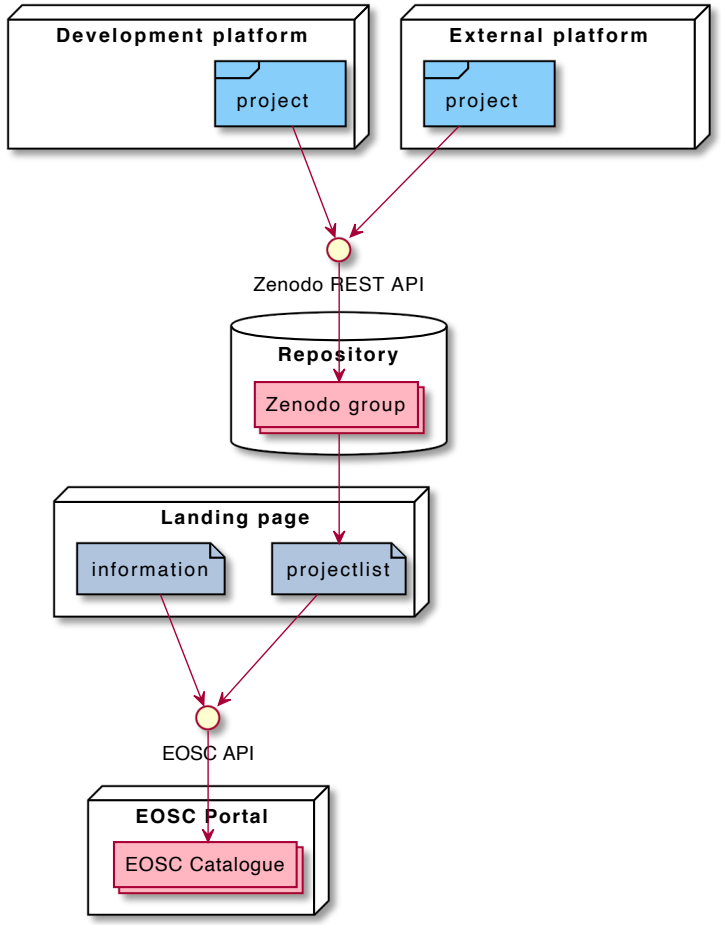
Funded by the European Union’s Horizon 2020 - Grant N° 824064

ESCAPE Work Packages

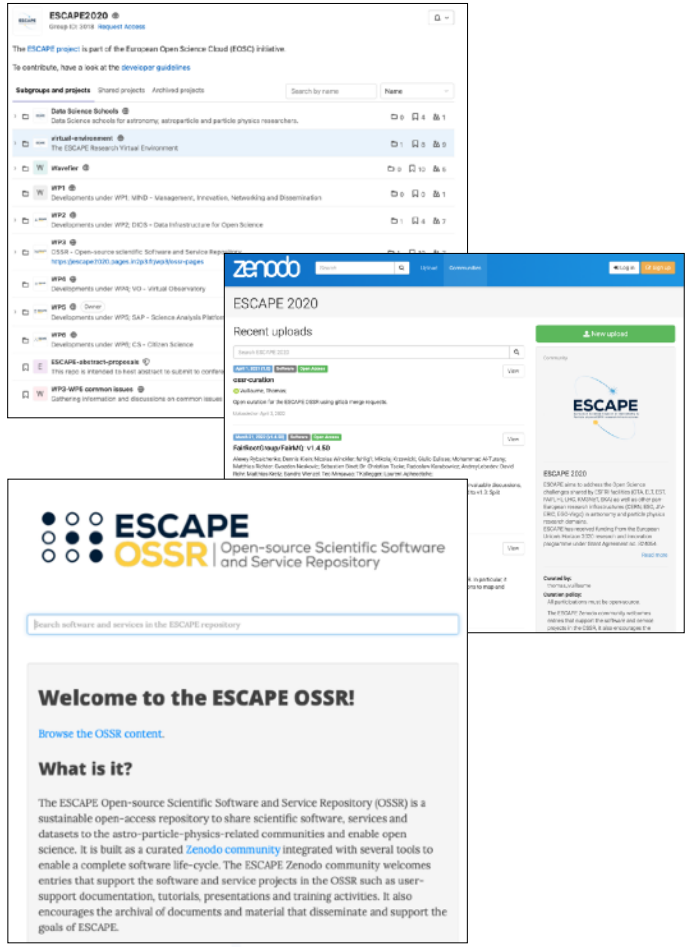


Funded by the European Union's Horizon 2020 - Grant N° 824064

Software & Services Repository



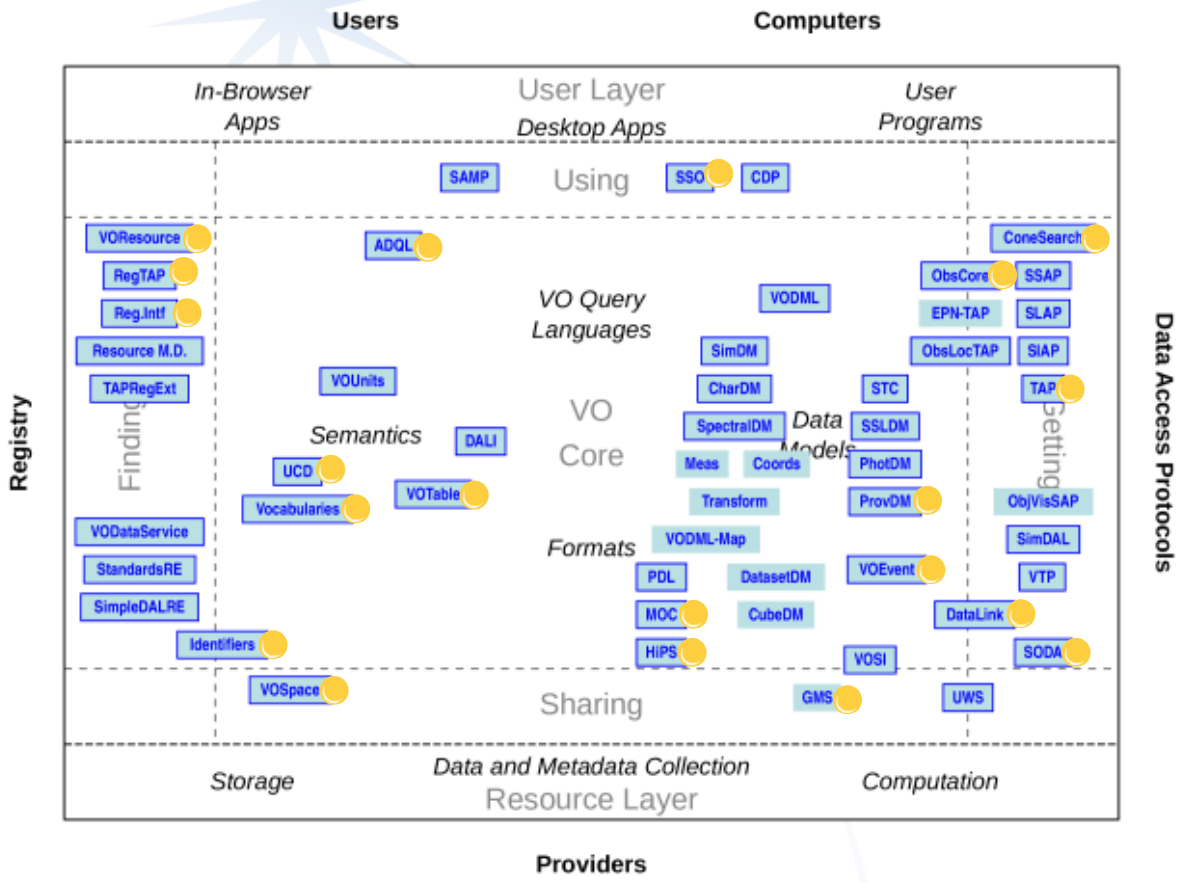
- A common repository for software across the various ESCAPE infrastructures.
- Designed both to *make software available* to practising scientists and to *preserve* software for future reproducibility.
- Built-in to common CI/CD systems (GitLab, Hub, etc).
- Built around the Zenodo system for long-term stability and preservation.
- Programmatic access through the eOSSR library.
- Integrated with the ESAP platform... see later.



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

Pushing on open standards: the Virtual Observatory

- ESCAPE aims to build around open standards wherever possible.
- We have used and contributed to a bunch of IVOA standards. In particular, the project has pushed on:
  - Using IVOA semantic UCD metadata for solar physics.
  - Developing IVOA standards for radio astronomy metadata.
  - Deploying IVOA-compliant services in the ESO science archive.
- Education, education, education, ...



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

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

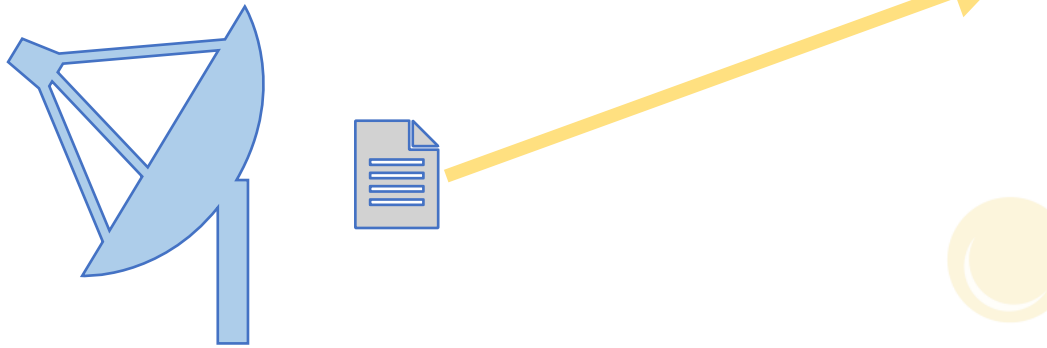
The Scientific Data Lake

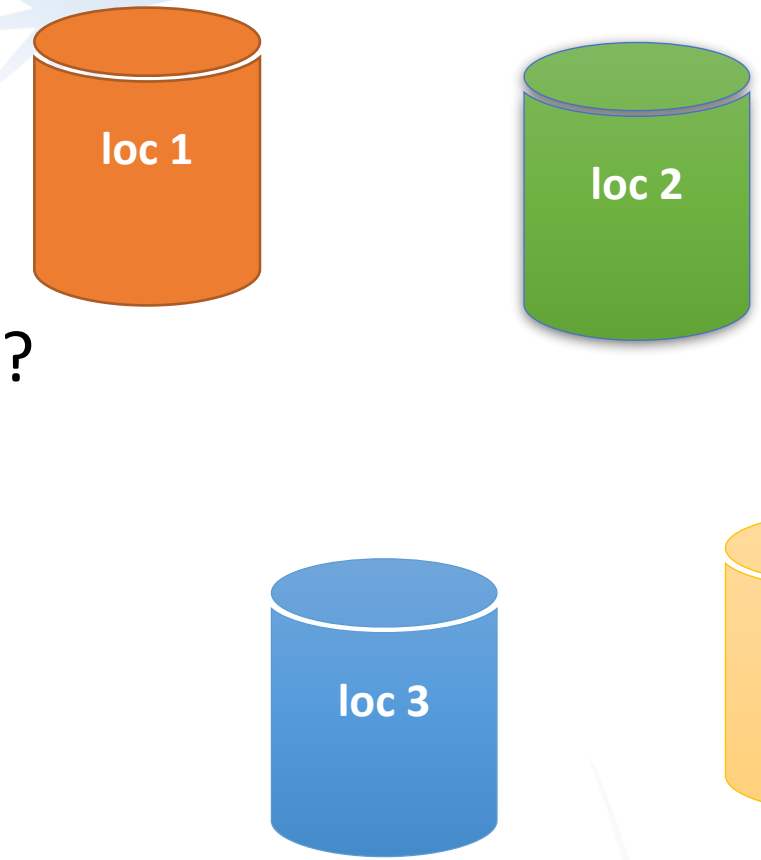
Yan Grange

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

Current situation

- Data sizes are increasing
- Distributed, federated storage
- Need to know what data is where
- Manual data management, database, ?
- Doesn't scale too well…





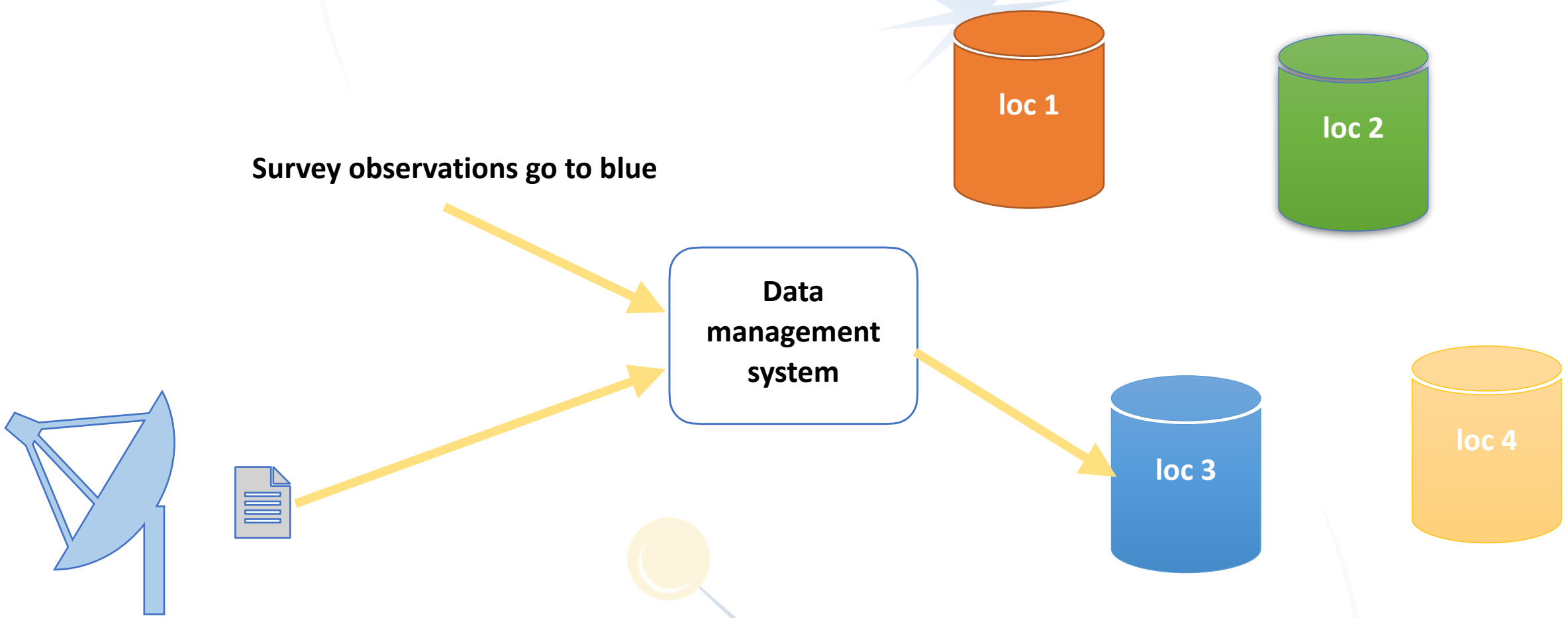
Funded by the European Union's Horizon 2020 - Grant N° 824064

Scientific Data Lake (ESCAPE WP2)

- CERN experiments generate large data volumes, as does radio astronomy (especially SKA), and astronomy in general.
- In both cases, the data is provided to users using distributed infrastructure
- ATLAS experiment has developed an architecture for data management at this scale, which we will refer to as the Scientific Data Lake
- Of course, the domains do also have some significant differences; one of the goals of the DIOS WP is to investigate the architecture and find how it maps on the different domains, and feed it back to the Rucio development team.

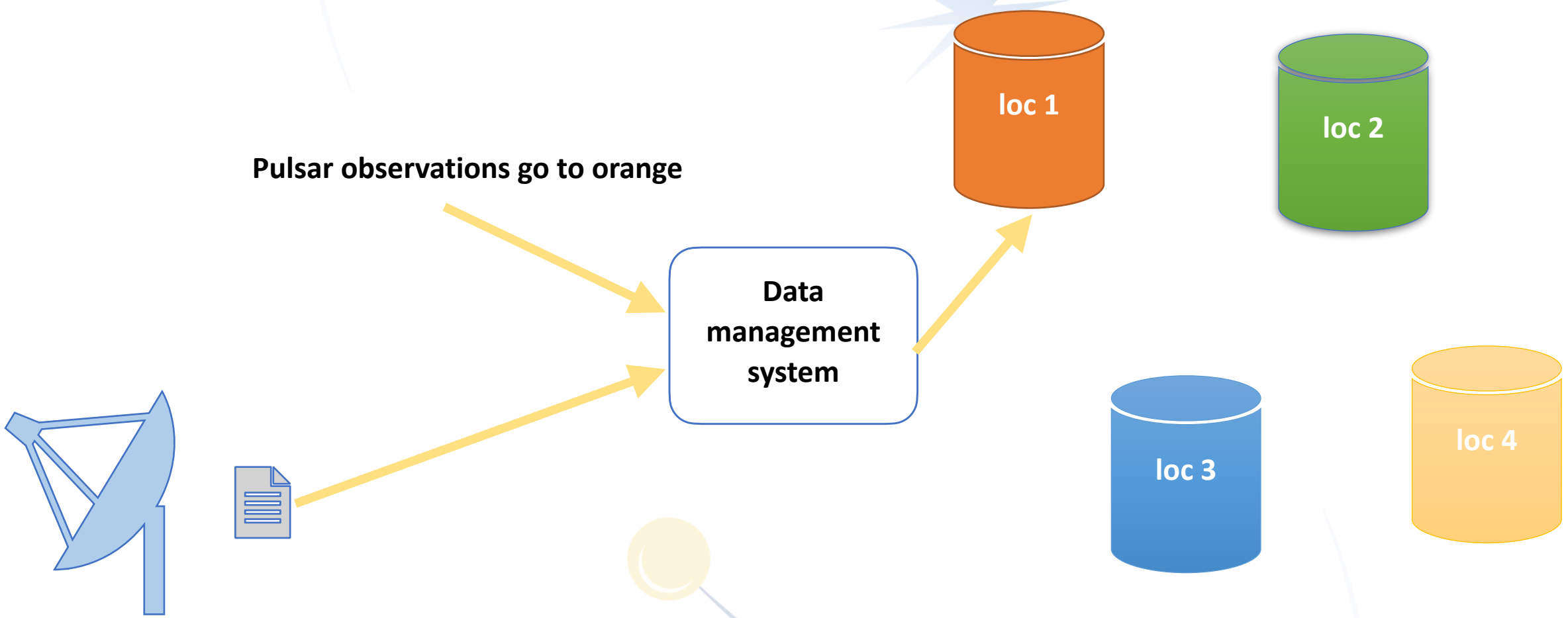
Funded by the European Union's Horizon 2020 - Grant N° 824064

Rule-based data management



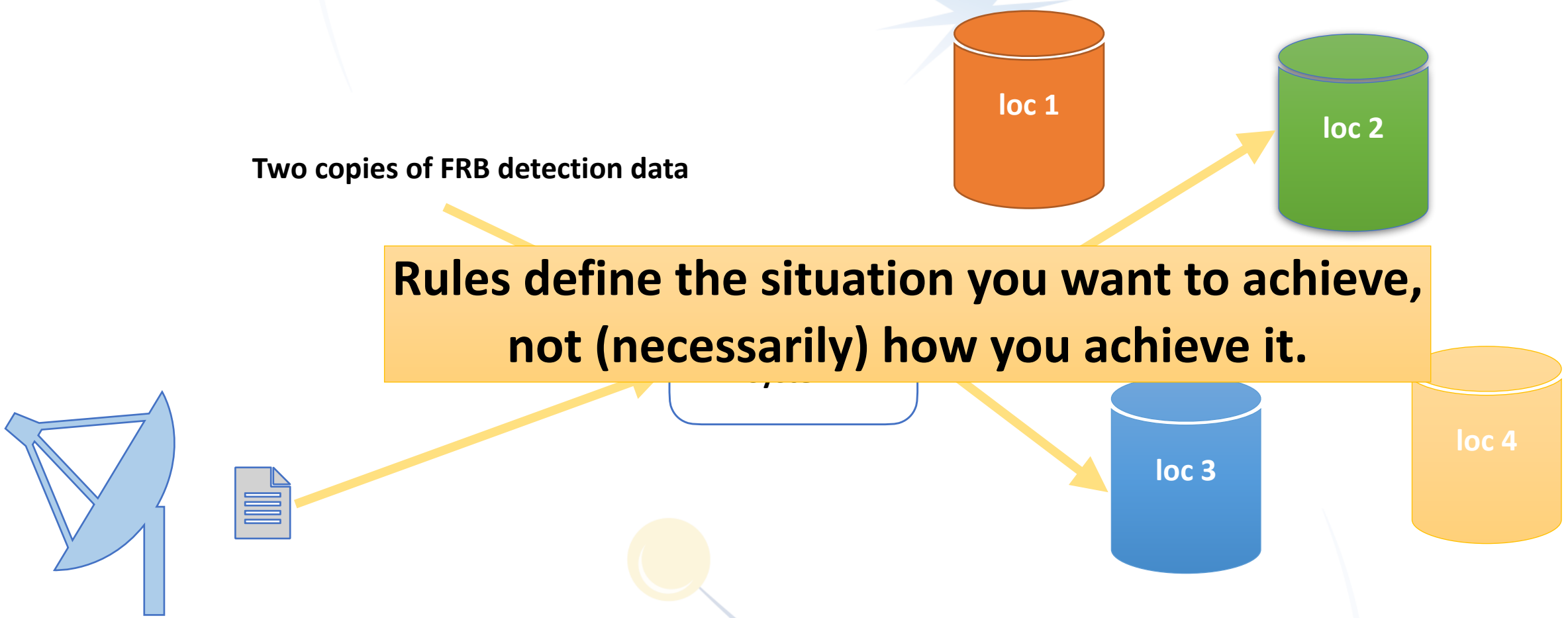
Funded by the European Union's Horizon 2020 - Grant N° 824064

Rule-based data management



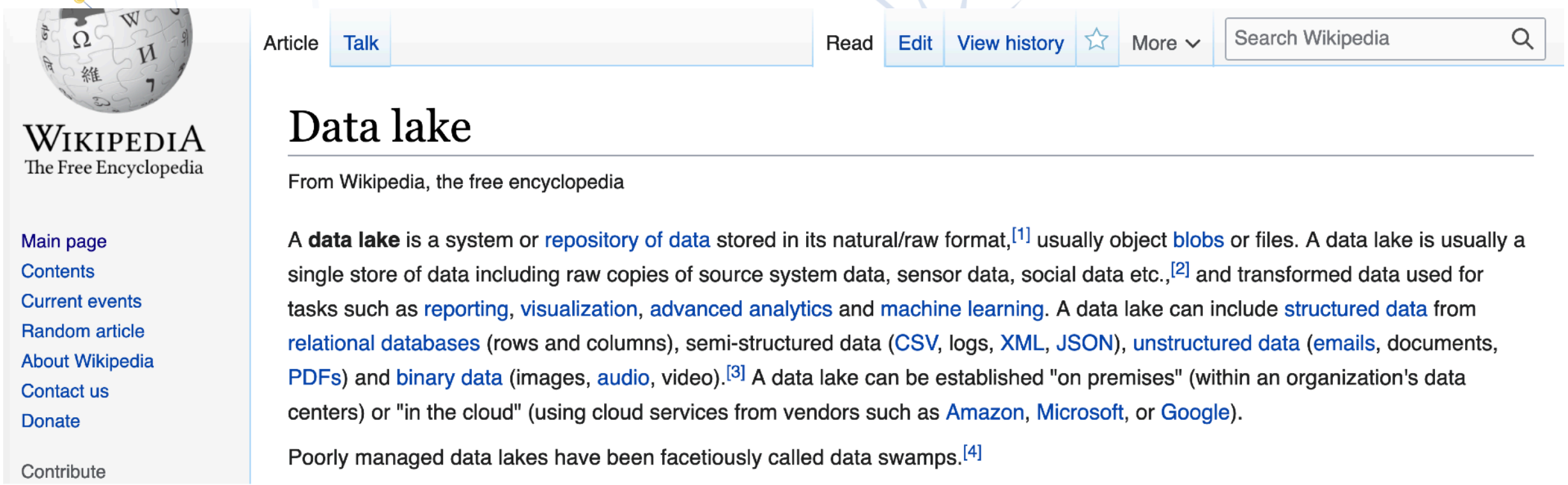
Funded by the European Union's Horizon 2020 - Grant N° 824064

Rule-based data management



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

Intermezzo: naming



WIKIPEDIA
The Free Encyclopedia

Main page
Contents
Current events
Random article
About Wikipedia
Contact us
Donate

Contribute

Article | Talk | Read | Edit | View history | More | Search Wikipedia

Data lake

From Wikipedia, the free encyclopedia

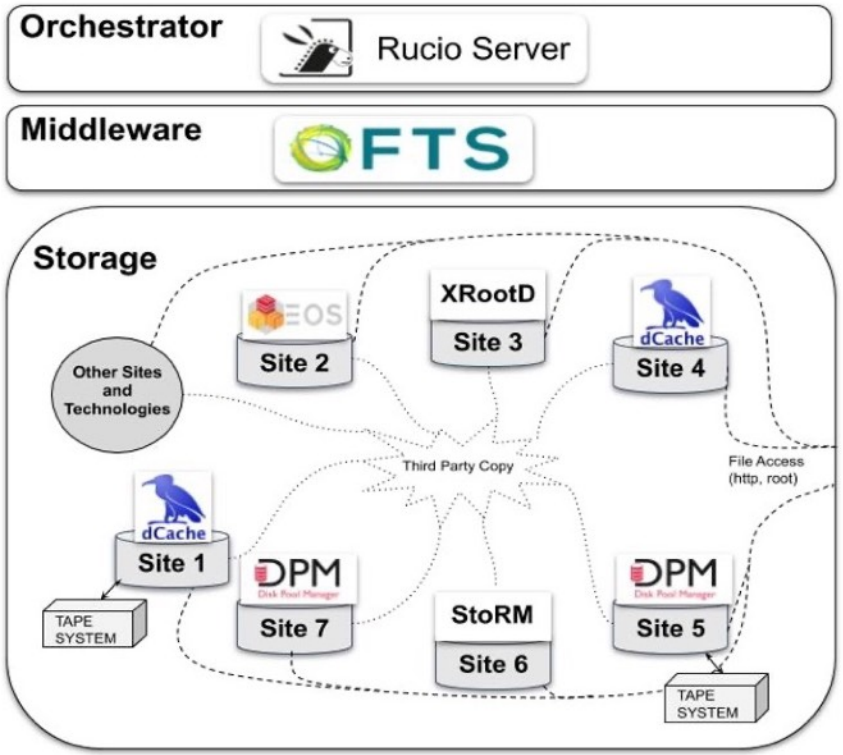
A **data lake** is a system or repository of data stored in its natural/raw format,[1] usually object blobs or files. A data lake is usually a single store of data including raw copies of source system data, sensor data, social data etc.,[2] and transformed data used for tasks such as reporting, visualization, advanced analytics and machine learning. A data lake can include structured data from relational databases (rows and columns), semi-structured data (CSV, logs, XML, JSON), unstructured data (emails, documents, PDFs) and binary data (images, audio, video).[3] A data lake can be established "on premises" (within an organization's data centers) or "in the cloud" (using cloud services from vendors such as Amazon, Microsoft, or Google).

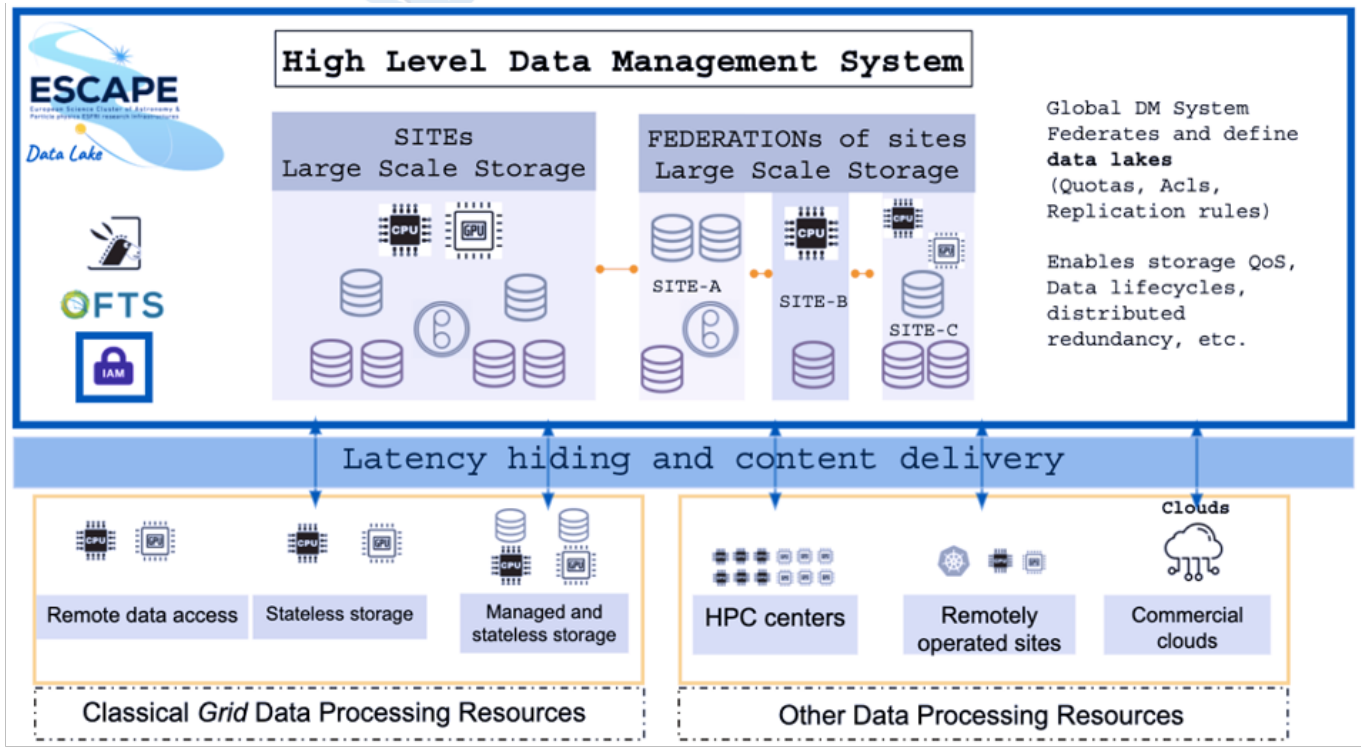
Poorly managed data lakes have been facetiously called data swamps.[4]

- Naming can be somewhat confusing. I may say Data Lake, but what I mean is this concept of a Scientific Data Lake.

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

Scientific Data Lake architecture





Data management and orchestration: **Rucio**
File transfer and data movement: **FTS**
Content delivery and latency hiding: **XCache**

Data Lake Information System: **CRIC**
AAI: Indigo **IAM**

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

Rucio community

From: Martin Barisits (2020)

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

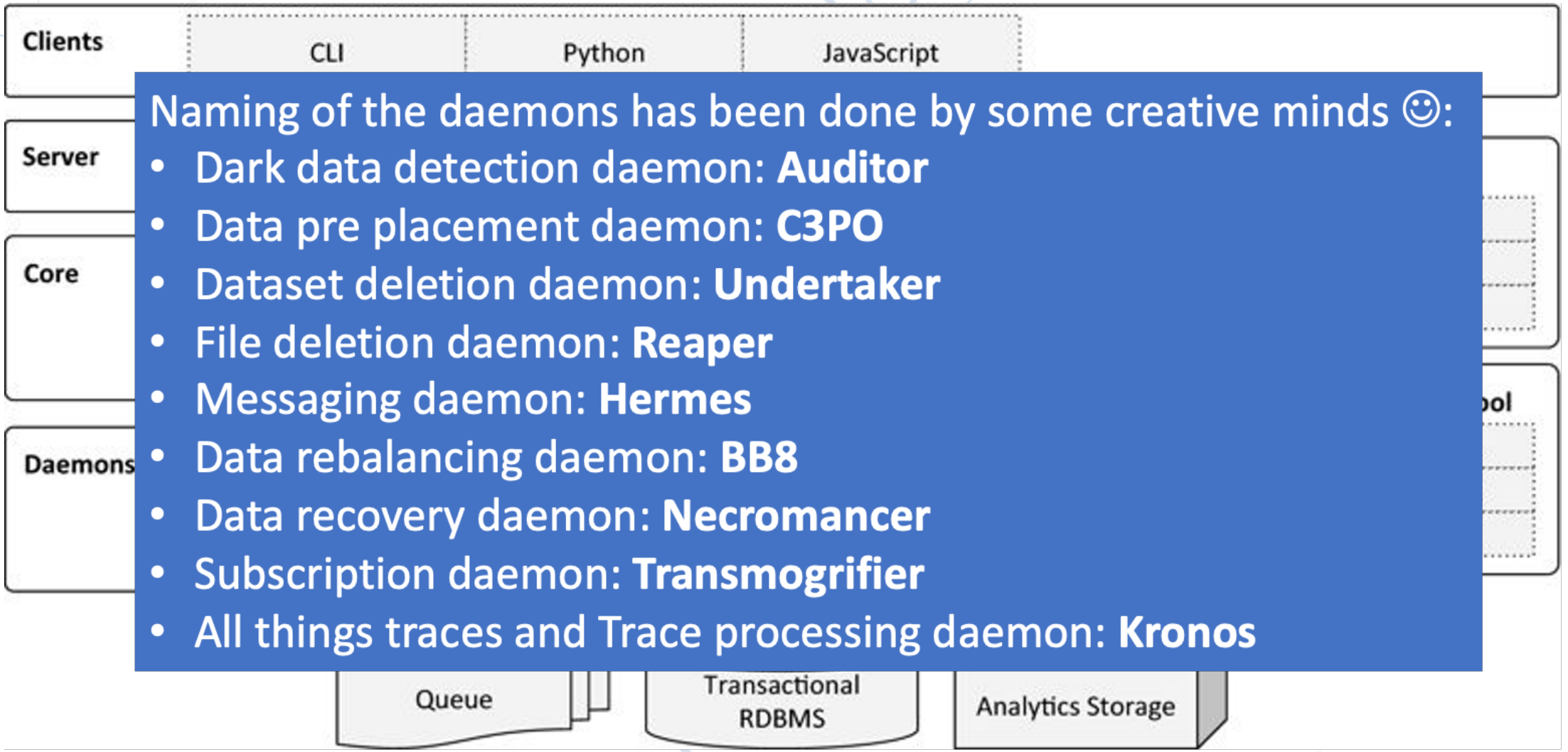
Rucio features

- Provides many features that can be enabled selectively
  - File and dataset catalog
  - Transfers between facilities including disk, tapes, clouds, HPCs
  - Web-UI, CLI, and API to discover/download/upload/transfer/annotate data
  - Extensive monitoring for all dataflows
  - Support for caches
  - Expressive policy engines with rules and subscriptions
  - Automated corruption identification and recovery
  - Data popularity based replication
  - …

More advanced

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

Rucio



Naming of the daemons has been done by some creative minds ☺:

- Dark data detection daemon: **Auditor**
- Data pre placement daemon: **C3PO**
- Dataset deletion daemon: **Undertaker**
- File deletion daemon: **Reaper**
- Messaging daemon: **Hermes**
- Data rebalancing daemon: **BB8**
- Data recovery daemon: **Necromancer**
- Subscription daemon: **Transmogrifier**
- All things traces and Trace processing daemon: **Kronos**

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

Rucio concepts

- Expressive metadata is key for rule-based management.
- Storage Elements are described by storage type (e.g tape, disk), space properties (e.g. used, free), geographical zone and supported protocol (e.g. https, s3, gridftp)
- Currently, some work is done in moving away from concrete storage device names (tape, disk, ssd) and move towards Quality of Service (fast, cheap, opportunistic) to support more expressive rules and not focus on the “how” but on the “what”.

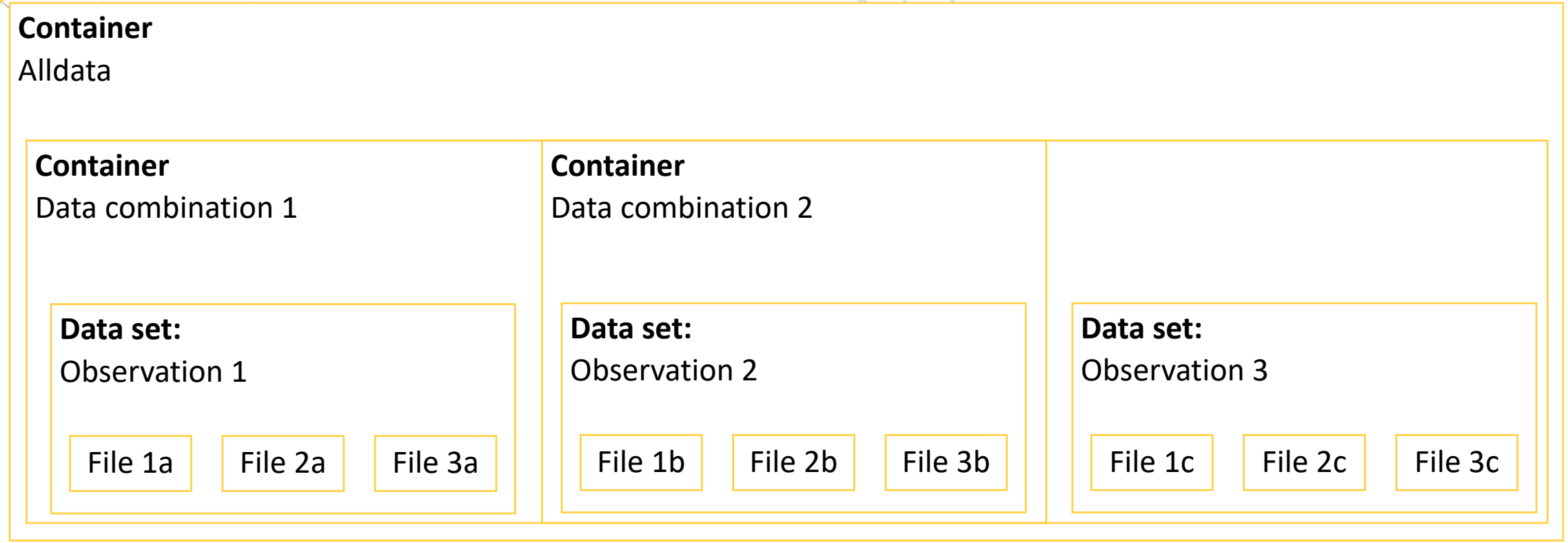
Funded by the European Union’s Horizon 2020 - Grant N° 824064

Data in Rucio

- The metadata of the data is described using three types of attributes
  - System-defined attributes (e.g. file size, checksum)
  - Data attributes. By defaut those are particle-physics based (e.g. number of events, run number, task_id). But there is support for either JSON metadata or plugins.
  - Data management attributes (e.g. whether replicas should be purged if the data is not needed to be on a location anymore)

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

Rucio data hierarchy



- Name space of Rucio is flat. Everything (files, containers, data sets) is a **D**ata **ID**entifier (DID).
  - Names are prepended by a “scope”

LOFAR_IMAGING:L12345_cal.MS.tar

scope name

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

Data management vs access

- Rucio supports data uploads and downloads, but primarily the goal of Rucio is data management (i.e. making sure data gets copied between remote end points)
  - Manual uploads are certainly possible, but then you have to do the registration using either python or the REST API.
- Direct access to the data can be done either via a Download; downloading a DID which, as we saw before can be a file, or a set of files belonging together.
- Alternatively, data can be moved to a place that can be directly mounted (e.g. webdav, or fuse-mountable file system)
  - Here one should keep in mind that by default, Rucio uses an algorithm to distribute files in directories. It can however be configured to behave otherwise.

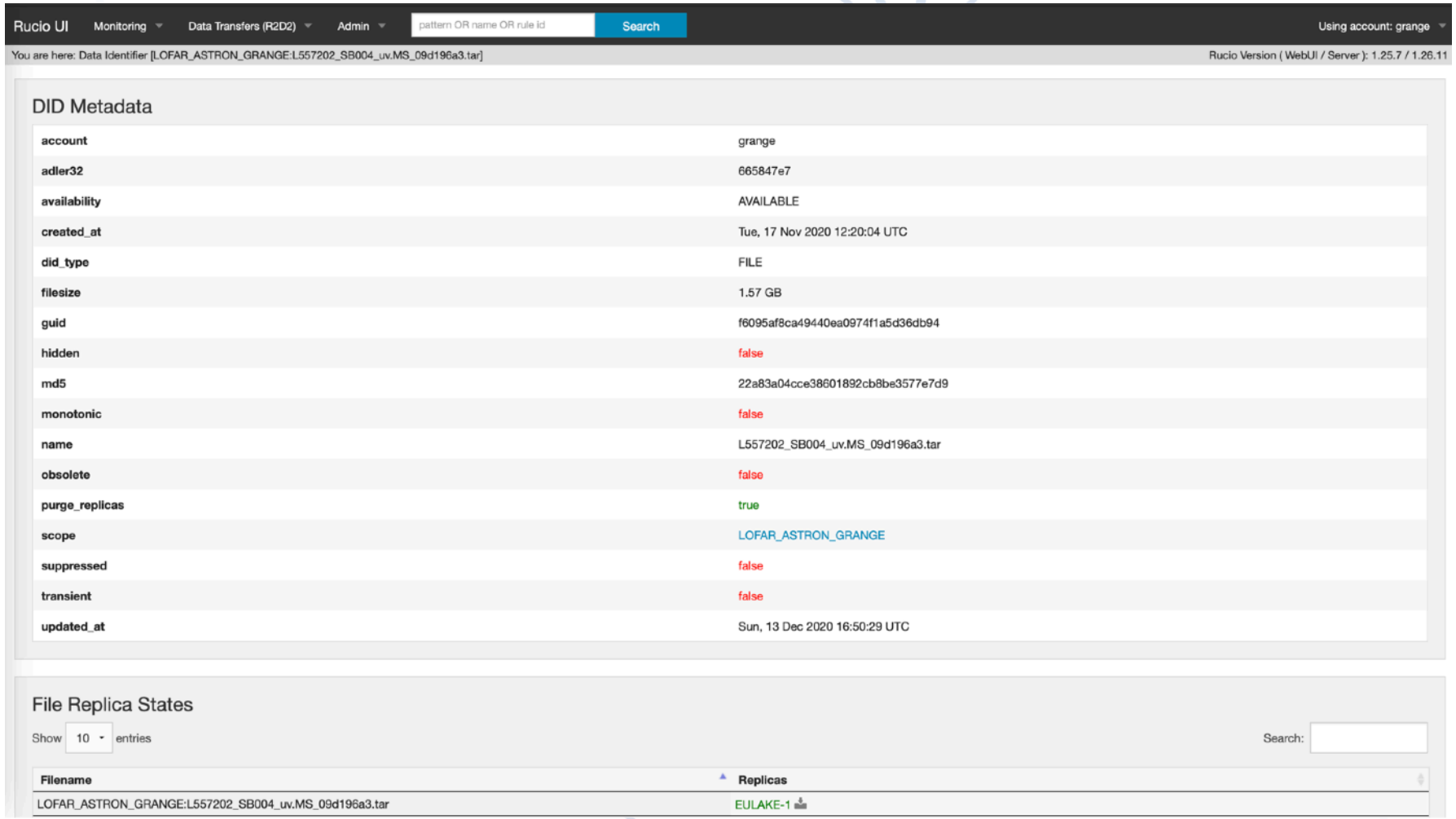
Funded by the European Union's Horizon 2020 - Grant N° 824064

Interacting with Rucio

- Primarily the Rucio daemon provides a REST API
- CLI (which in essence is a wrapper around the python library)
- Python library
  - This can be very neat if you want to integrate data management in your workflow, e.g. to manage the data ingests yourself.
- Web UI
- DataLake as a Service (which is a Jupyer notebook that gives access to a Scientific Data Lake; Klaas will show you more about that).

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

Interacting with Rucio



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

Ongoing developments

- SKA has embedded a developer in the Rucio dev team, also SKA is prototyping with Rucio for the regional centre data management
  - Transmogrifier daemon → making rules based on metadata
    - Implemented that this also works on custom metadata
    - Also implemented that this works with inequality
    - → We could say: “put all data from the Galactic bulge in Amsterdam”
  - Future: looking at performance of taking metadata from database (e.g. observation DB)

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

How to get started

- Requirement on FTS for data transfers. In principle several public FTS services are around, which could save people some head aches.
  - One could point the Rucio server to one of those
  - For the storage system behind it, use one that supports a protocol that FTS speaks (webdav is a safe choice to start with).
- Rucio is fully open source. There are helm charts for deployment on Kubernetes.
  - For development and testing, also a development docker-compose file is present.

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

Some ESCAPE resources

- The ESCAPE team created docker containers (which can be turned in to Singularity) for the Rucio client, including the tooling that can be used to upload and download data (gfal). Of course the default configuration settings point to the ESCAPE instance, but this can easily be changed.
  - https://github.com/ESCAPE-WP2/Rucio-Client-Containers/tree/master/rucio-client-container
- Also on the ESCAPE wiki there are some ‘data challenges’ that were executed by all the instruments
  - e.g. the reports on https://indico.in2p3.fr/event/22501/

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

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

The ESFRI Science Analysis Platform

Klaas Kliffen

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

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

References

John Swinbank

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

References

- ESCAPE:
  - https://www.projectescape.eu
- Software Repository:
  - https://escape2020.pages.in2p3.fr/wp3/ossr-pages/
- ESAP Repositories:
  - https://git.astron.nl/astron-sdc/esap-api-gateway
  - https://git.astron.nl/astron-sdc/esap-gui

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