university of groningen

R3B at project ESCAPE; a case study to practice open science for FAIR/GSI experiments

Maisam M. Dadkan

Posdoc fellow at project ESCAPE

Fairness conference, May 2022

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

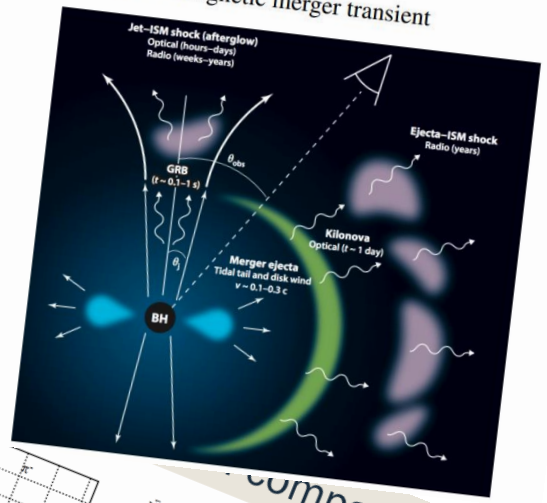
Electromagnetic Counterparts of Neutron Star Mergers: Signatures of Heavy r-Process Nucleosynthesis

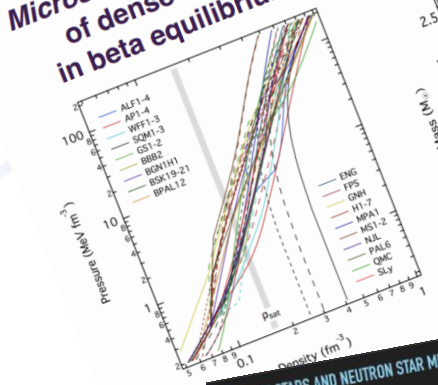
Andreas Flörs (GSI)
Luke Shingles (GSI, QUB), Gerrit Leck (GSI), Gabriel Martínez-Pinedo (GSI)
Ricardo Ferreira da Silva (LIP)

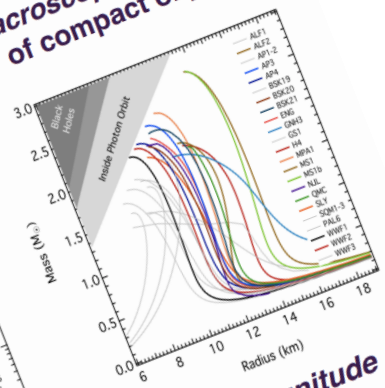
GSI

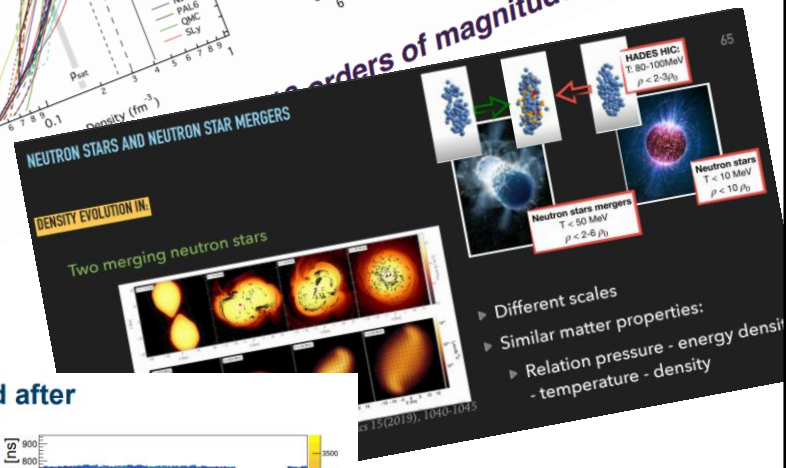
Neutron Star Mergers and Kilonovae

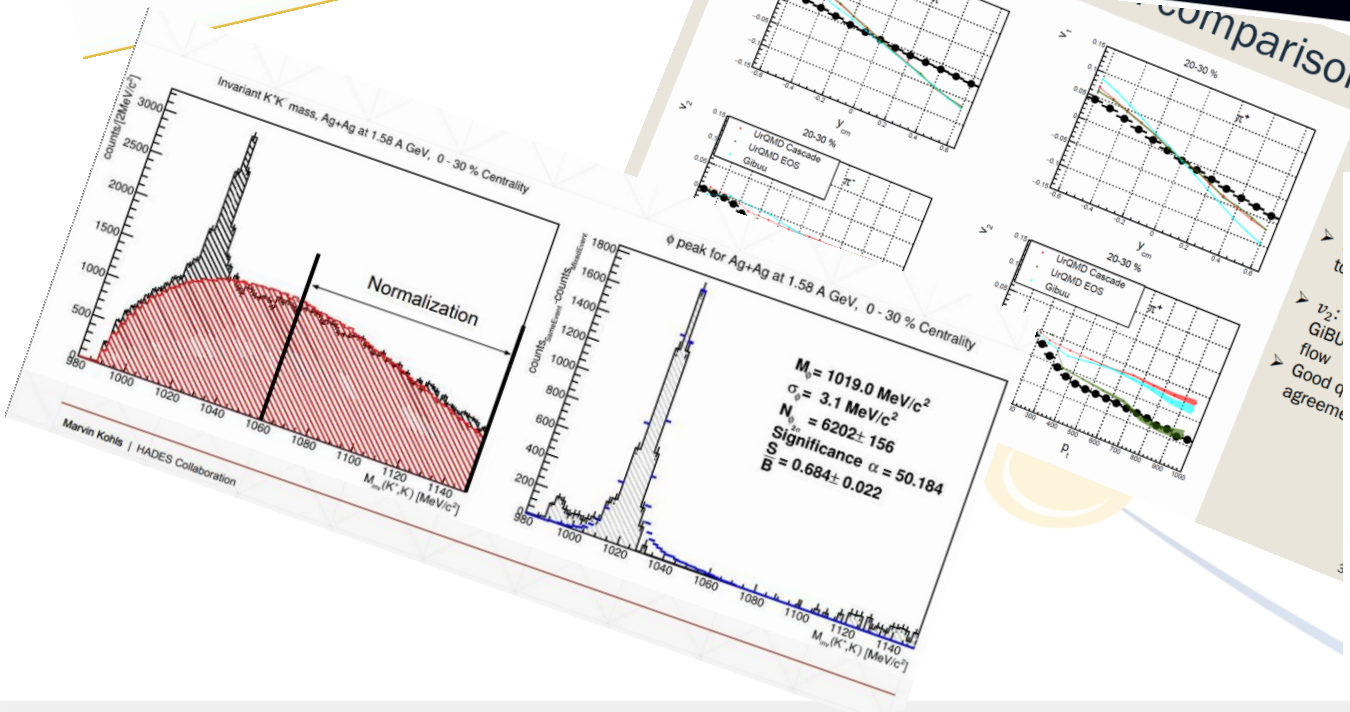
- kilonova: electromagnetic merger transient

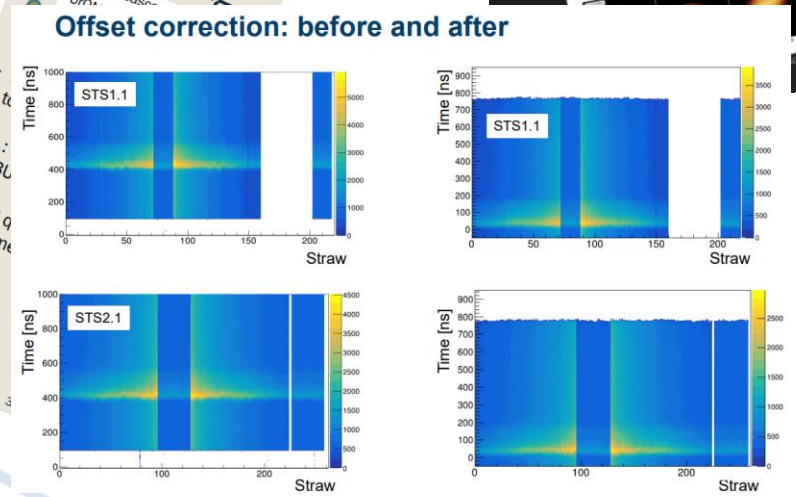












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ESCAPE
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Neutron Star Mergers and Kilonovae

- kilonova: electromagnetic merger transient

Microscopic properties of dense matter in beta equilibrium

Macroscopic properties of compact objects

Partial wave dispersion relation approach:

- $\sigma/f_0(500)$ in $\pi\pi$ scattering (real & lattice data); $f_0(980)$ in $\{\pi\pi, K\bar{K}\}$
- $\kappa/K^*(700)$ in πK scattering (real & lattice data)

Can search for resonances & bound states given the data input

$\sqrt{s_p} = 458(10)^{+7}_{-15} - i\,256(9)^{+5}_{-8}$ MeV

$\sqrt{s_{f_0(980)}} = 993(2)^{+2}_{-1} - i\,21(3)^{+2}_{-4}$ MeV

$\sqrt{s_p} = 498(21)^{+12}_{-19} - i\,138(13)^{+5}_{-10}$ MeV

$\sqrt{s_p} = 758(5)(0)$ MeV bound state

$\bar{B}\bar{B}$ Decomposition in energy scan

- $B\bar{B}$, $B^*\bar{B}$, $B^*\bar{B}^*$ cross section at various energies
- Higher statistic to improve fits
- JHEP06(2021)137

$B\bar{B}$ $B^*\bar{B}$ $B^*\bar{B}^*$

Orders of magnitude

NEUTRON STAR MERGERS

Merging neutron stars

HADES HIC: T: 80-100MeV $\rho < 2\text{-}3\rho_0$

Neutron stars mergers T < 50 MeV $\rho < 2\text{-}6\ \rho_0$

Neutron stars T < 10 MeV $\rho < 10\ \rho_0$

- Different scales
- Similar matter properties:
- Relation pressure - energy density - temperature - density

Yield Extraction

Double Gaussian function is used for signal

$Fit(m) = Ae^{\frac{-1}{2}\frac{(m-m_0)^2}{\sigma_1^2}} + Be^{\frac{-1}{2}\frac{(m-m_0)^2}{\sigma_2^2}} + pol2(m)$

1. Exclude signal region (m_0<0.43485 & m_0>0.56135) and fit background with $pol2(m)$
2. Use background fit parameters as initial values for next iteration, where signal (double Gaussian) fit function has fixed $m_0 = 0.4976$ GeV/c^2 and widths σ_1=0.004 GeV, σ_2=0.007 GeV
3. Use fit parameters as initial values for unconstrained fit to the whole inv. mass range

Normalization

Marvin Kohls | HADES Collaboration

Step 1 Step 2 Step 3

Divide (p_T,y) phase space into 6x6 bins

Offset correction: before and after

STS1.1 STS2.1

Time [ns] Straw

Current results (different collaborations agree within errors):

$T_c(\mu_B = 0) = 158.0 \pm 0.6$ MeV $\kappa_2 = 0.0153 \pm 0.0018$ $\kappa_4 = 0.00032 \pm 0.00067$

T_c [MeV] μ_B [MeV]

crossover line: $\mathcal{O}(\mu_B^4)$ constant: ϵ freeze-out: STAR ALICE

$n_S = 0$, $\frac{n_Q}{n_B} = 0.4$

Analytical continuation NLO Taylor-expansion LO Taylor-expansion

Dyson-Schwinger: hep-ph/1906.11644

Chemical freezeout: nucl-th/0511071v3 nucl-th/1212.2431 hep-ph/1403.4903 nucl-th/1512.08025 nucl-ex/1701.07065

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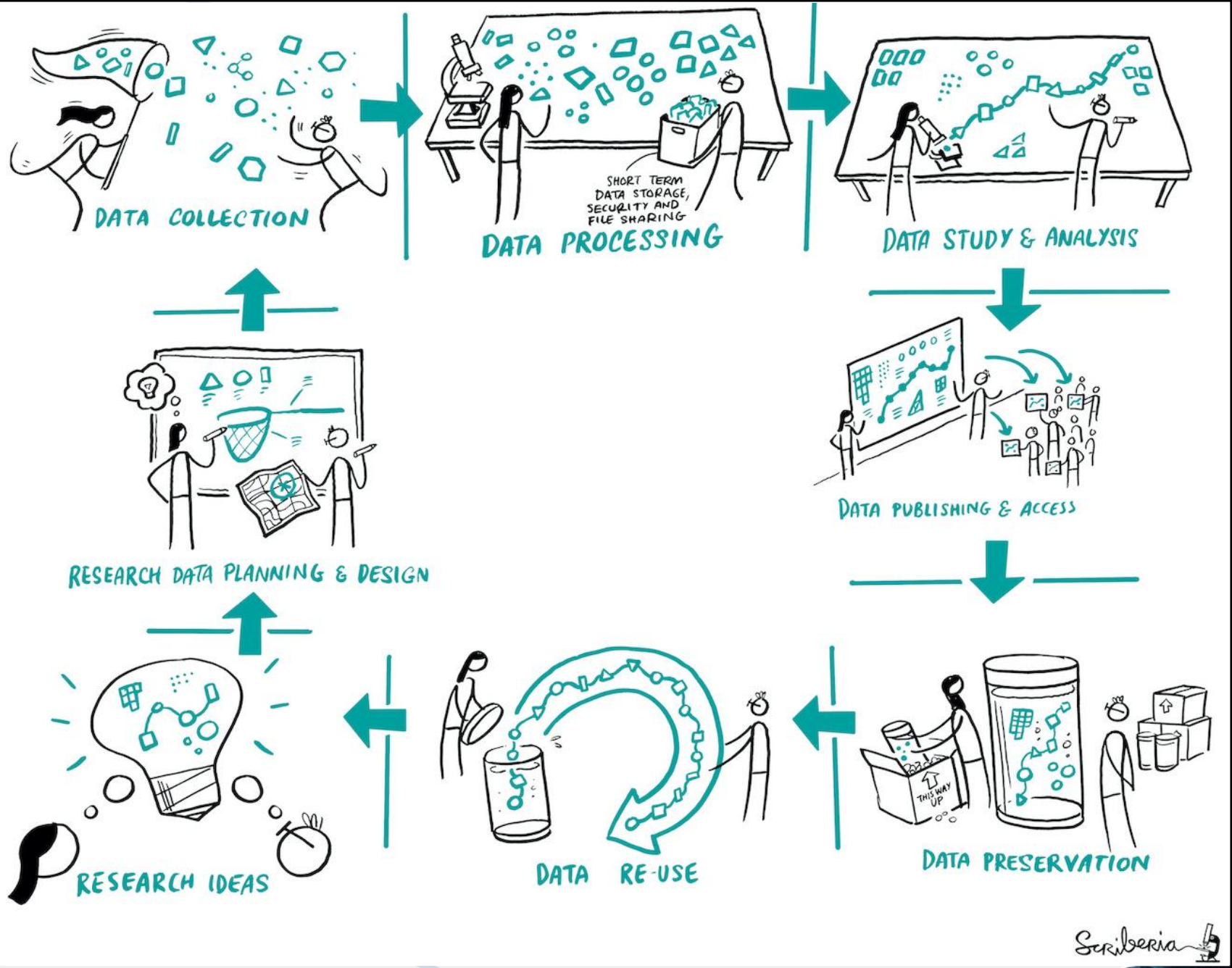
Data = Data+analysis workflow

- Is…
  - your data findable?
  - your data accessible?
  - your data reusable?



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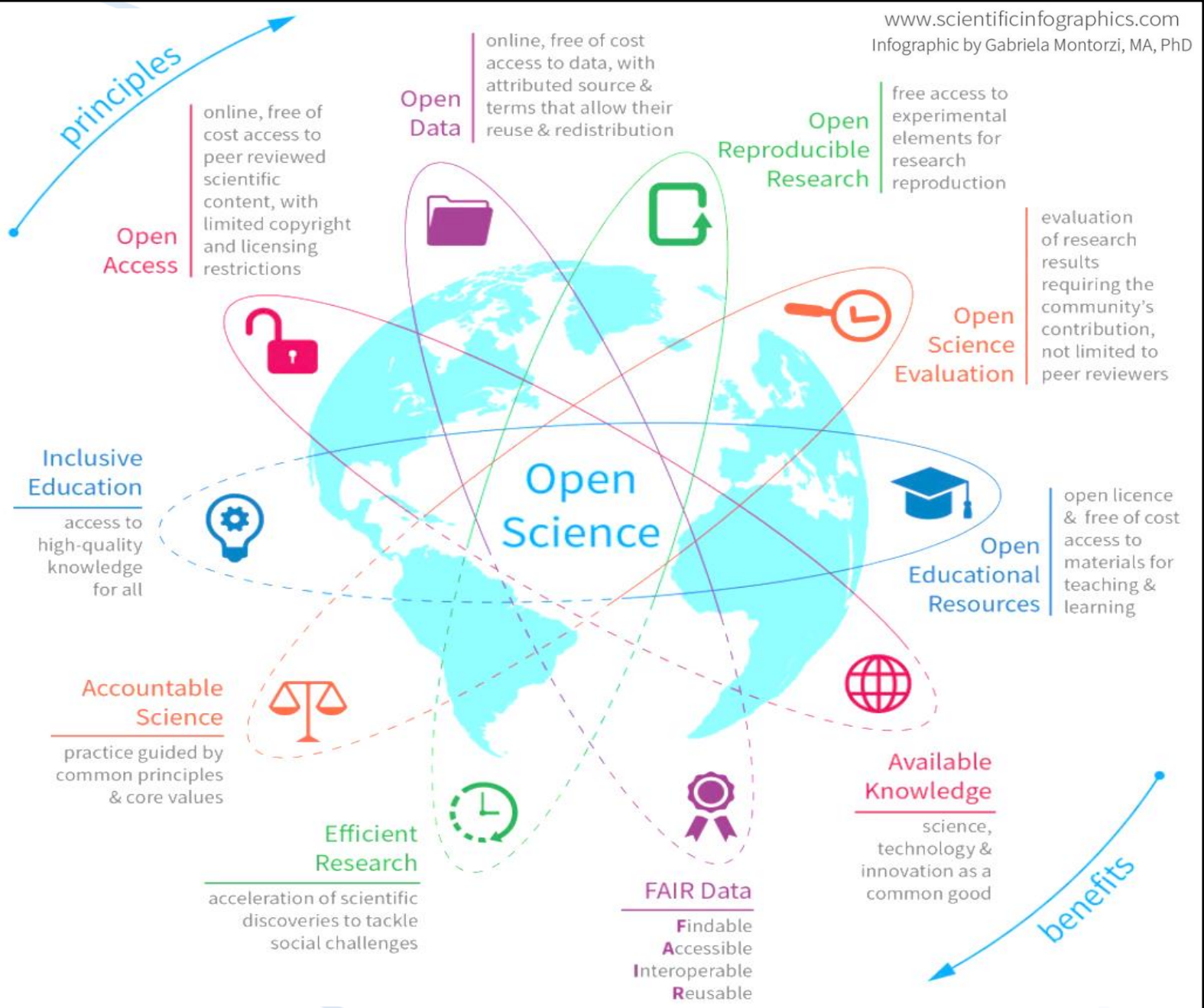

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Time to unlock the potential of the digital age:

- The key is the internet – digitization
- Open science requires systems thinking
- The value is making new knowledge from connections
- Standards to make (machine) interoperable
- Minimize technical, legal, financial and linguistic barriers
- Collaboration not Competition for Global Goods
- A reset for scientific careers; new incentive measures needed

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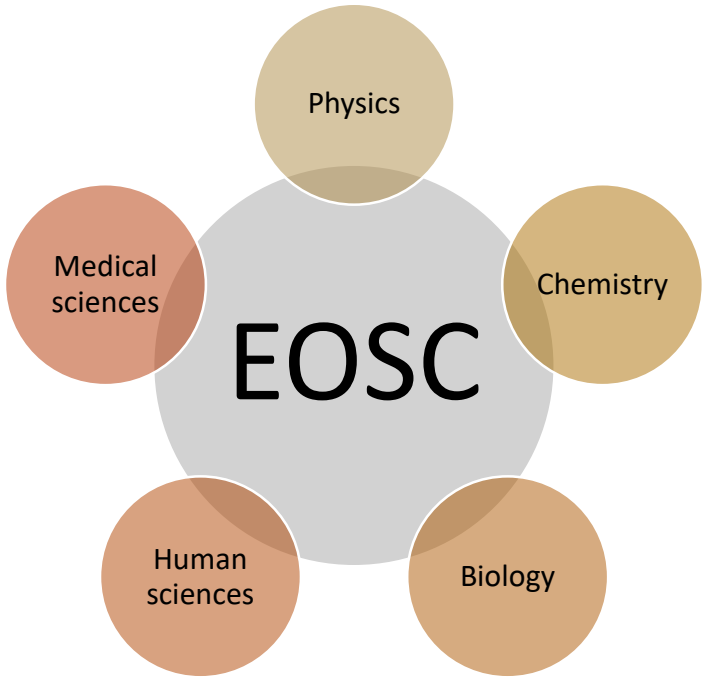
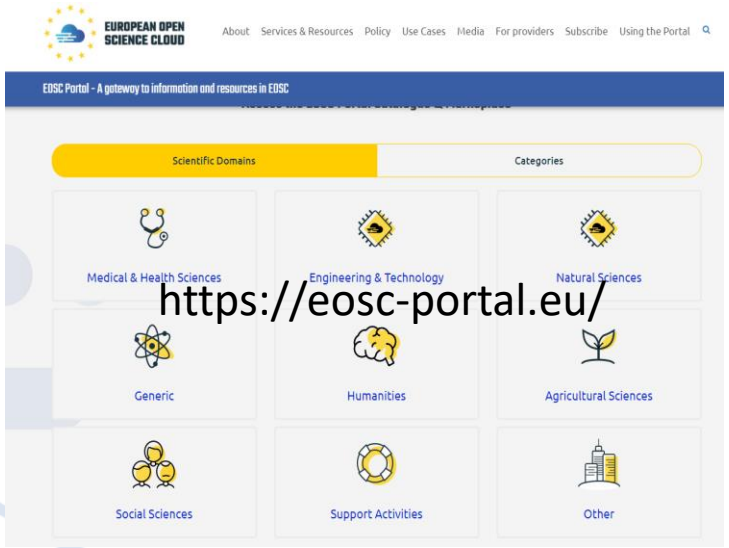
EOSC & ESCAPE

European Open Science Cloud (EOSC)

- Proposed in 2016
- **1.7 million** European researchers
- **€360** million in **48** sub-projects (under Horizon 2020)

- Universal access to data through a **single online platform** based on FAIR
- Make **synergy** between different **scientific research communities** in EU
- **Federating** existing data resources and Research Infrastructures (RIs)
- Accelerating innovations and tools for **computing** and **big-data management**





https://eosc-portal.eu/

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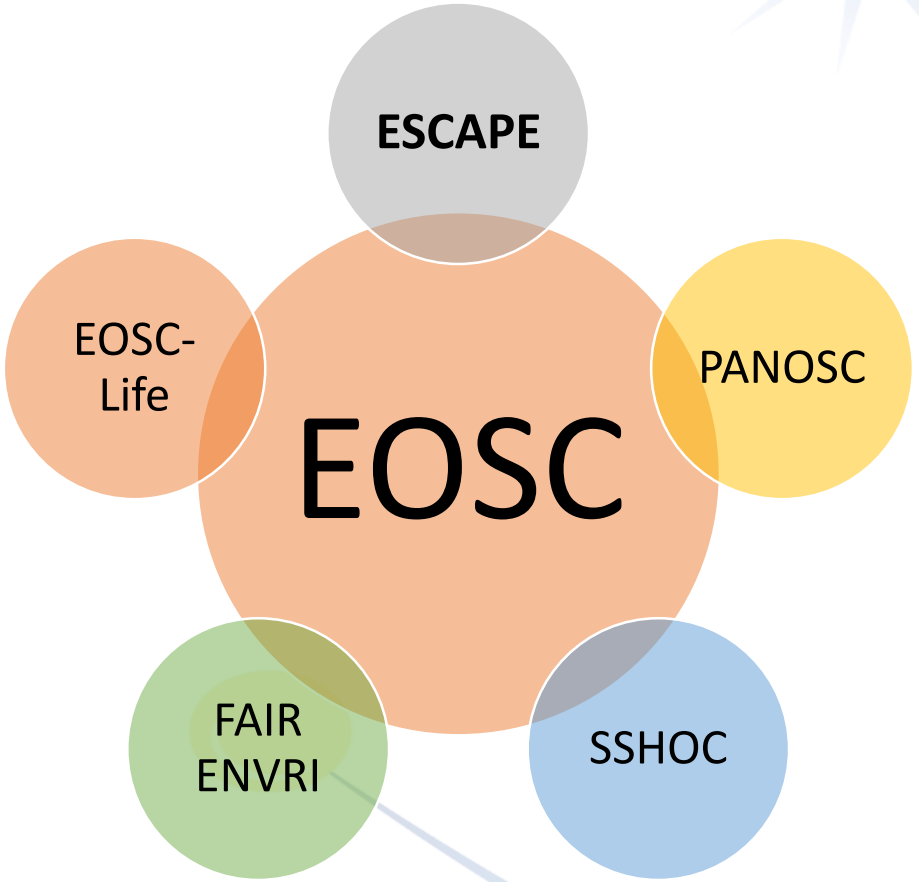
E S C A P E

(**E**uropean **S**cience **C**luster of
Astronomy & **P**article physics **E**SFRIs)



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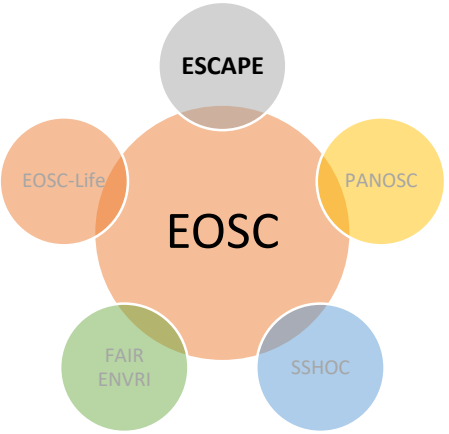
EOSC & ESCAPE



- **31** partners including
- **10** ESFRI projects & landmarks: CTA, EST, FAIR, HL-LHC, KM3NeT, SKA, LSST, VIRGO, ESO, JIVE
- **2** pan-European International Organizations: CERN & ESO with their world-class established infrastructures, experiments and observatories
- **2** European Research Infrastructures: EGO and JIV-ERIC
- **1** involved initiative/infrastructure: EURO-VO
- **4** supporting European consortia: APPEC, ASTRONET, ECFA and NuPECC

- Budget: **16 M€**
- Started: **1/2/2019**
- Duration: **48 months** (end date 31/1/2023)

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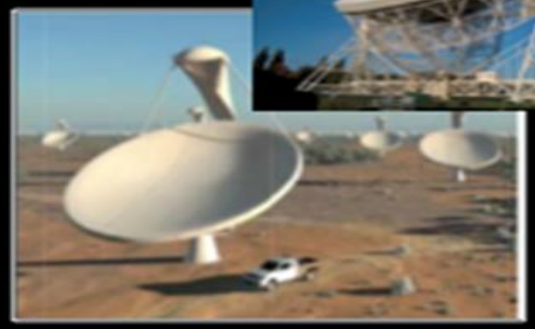
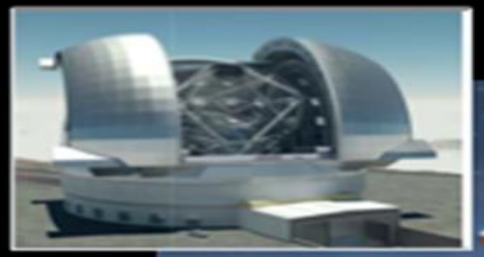
Radio



JIVE-VLBI

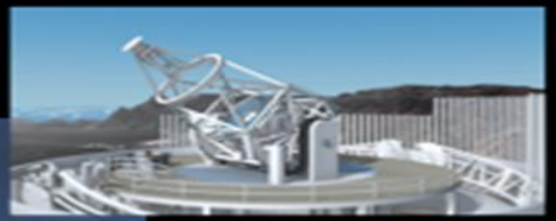
SKA

Visible light



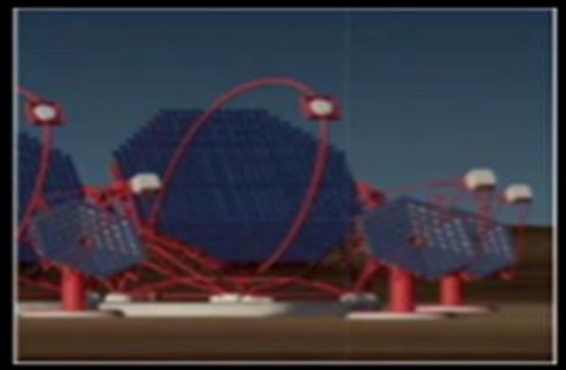
ELT

ESO



EST

Gamma rays



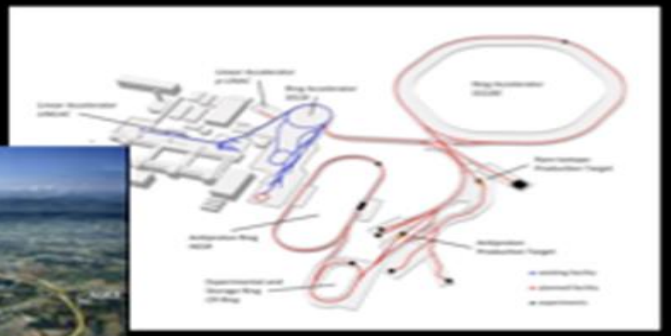
CTA

Accelerator-based
Particle Physics

HL-LHC

CERN

Accelerator-based
Nuclear Physics

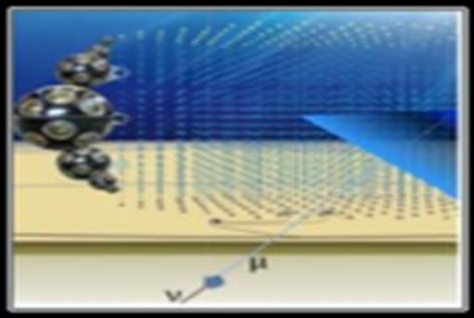


FAIR

Gravitational
Waves

EGO-VIRGO

Cosmic-rays
Neutrinos



KM3NeT

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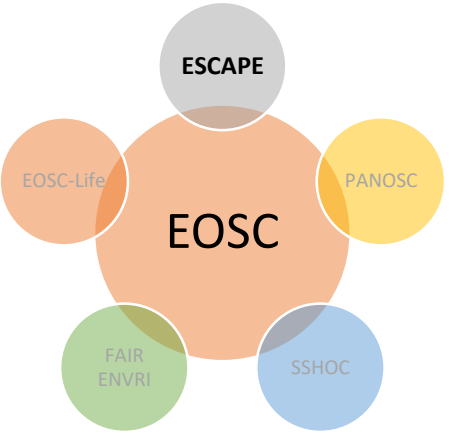
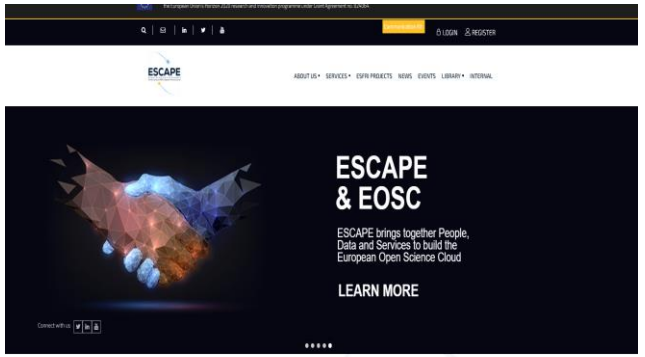
EOSC & ESCAPE



- Address the **Open Science challenges** shared by ESFRIs in **astronomy** and **particle physics**
- Developing solutions for the **large data sets** handled by the ESFRI facilities
- Facilitate **interdisciplinary** and **networked research** between different sciences
- **Connecting** ESFRI's projects to **EOSC**
- **Educate** and **train** the scientific and wider user communities

https://projectescape.eu



Select ESCAPE Services

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EOSC & ESCAPE

Data Lake:
Build a scalable, federated, data infrastructure as the basis of open science for the ESFRI projects within ESCAPE.

Software Repository:
Repository of "scientific software" as a major component of the "data" to be curated in EOSC.

Science Platforms:
Flexible science platforms to enable the open data analysis tailored by and for each facility as well as a global one for transversal workflows.

Citizen Science:
Open gateway for citizen science on ESCAPE data archives and ESFRI community

Virtual Observatory:
Extend the VO *FAIR* standards, methods and to a broader scientific context; prepare the VO to interface the large data volumes of next facilities.

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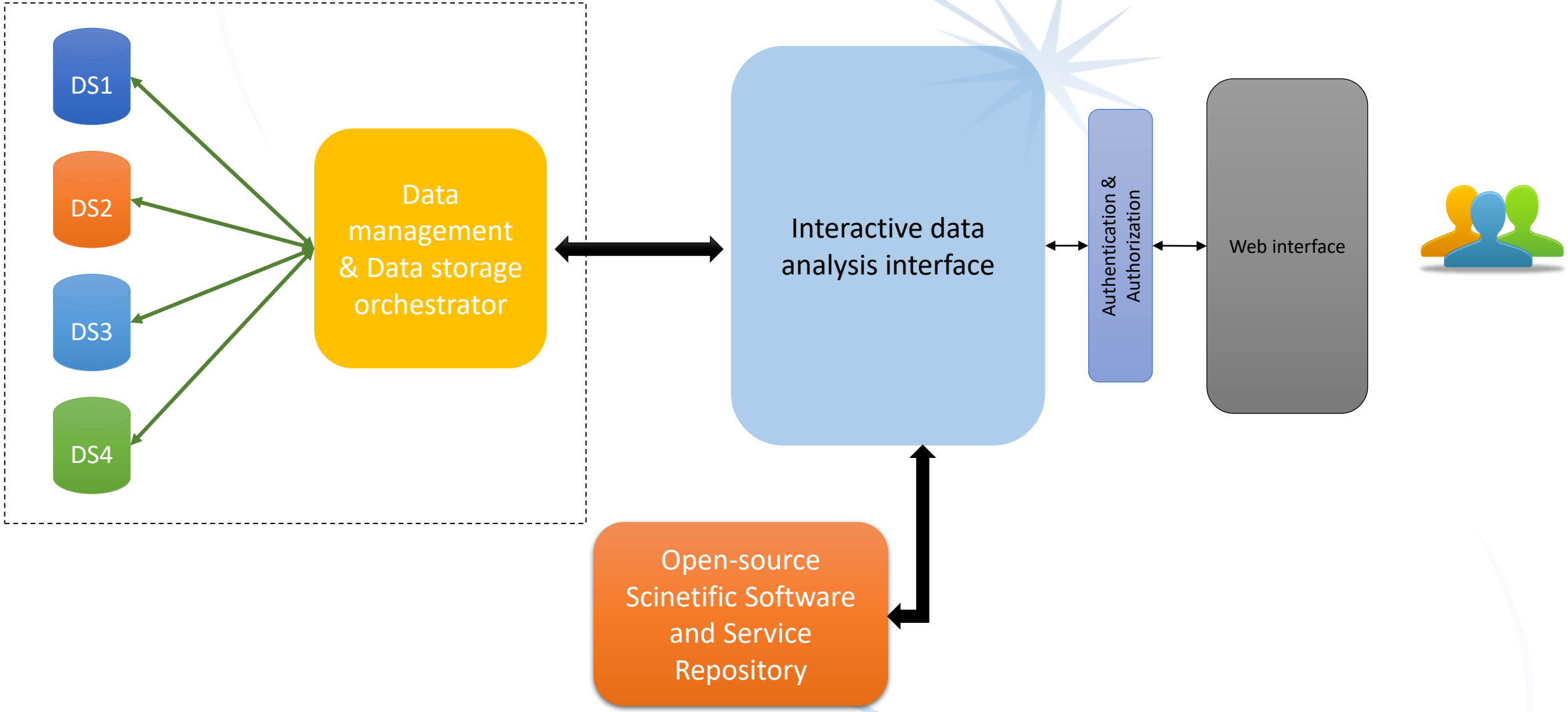
EOSC & ESCAPE



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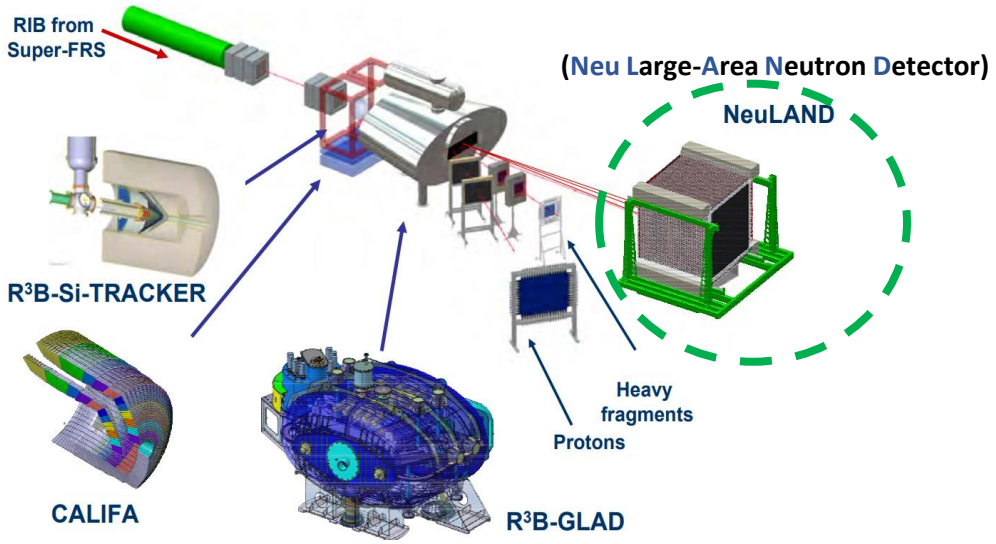
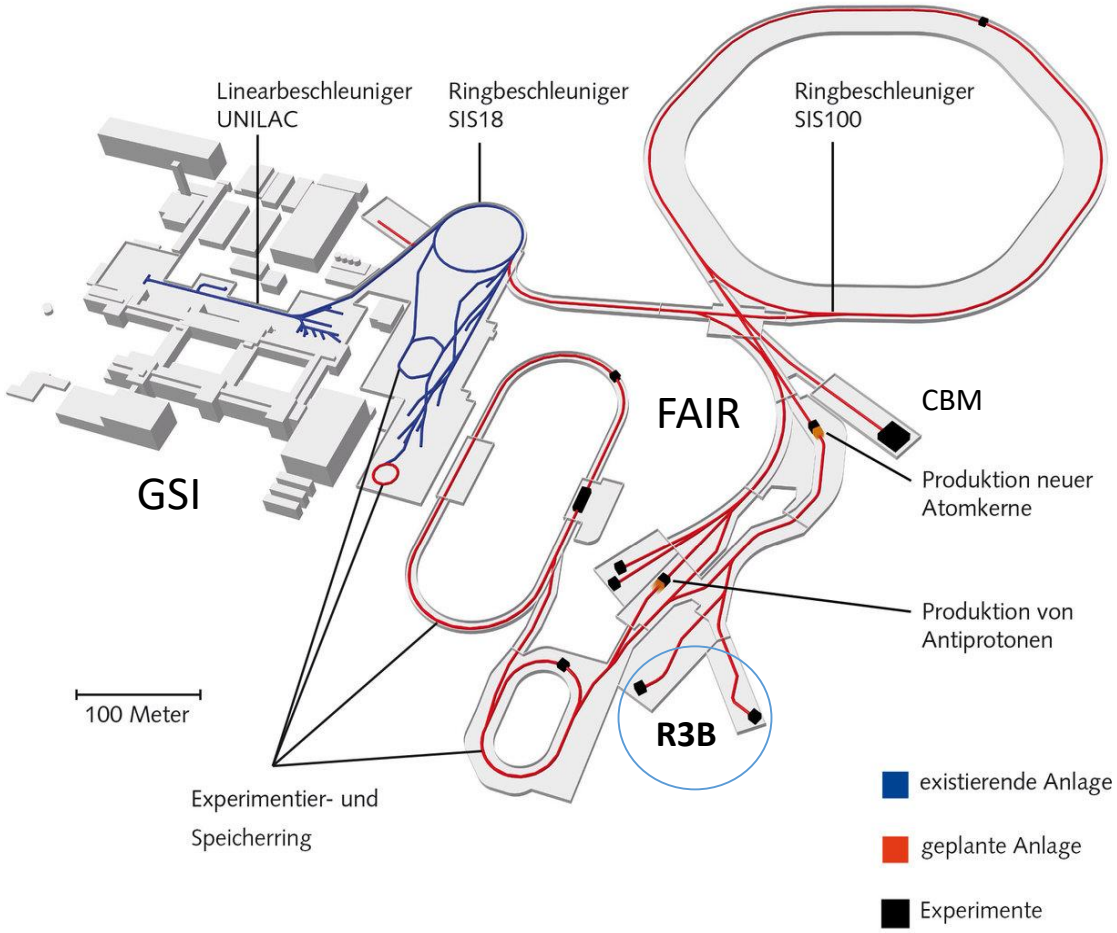
R3B-NeuLAND

R³B

Reactions with Relativistic Radioactive Beams





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R3B-NeuLAND

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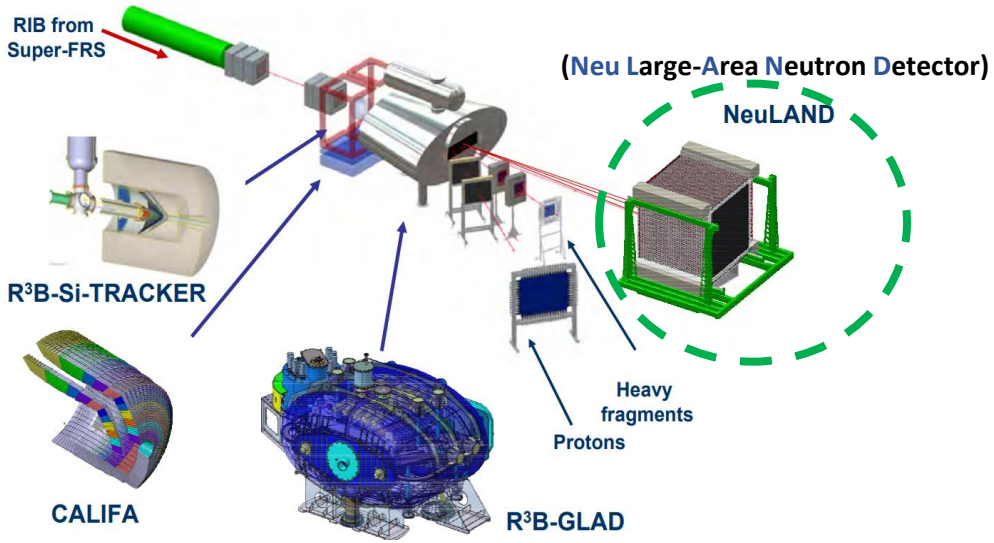

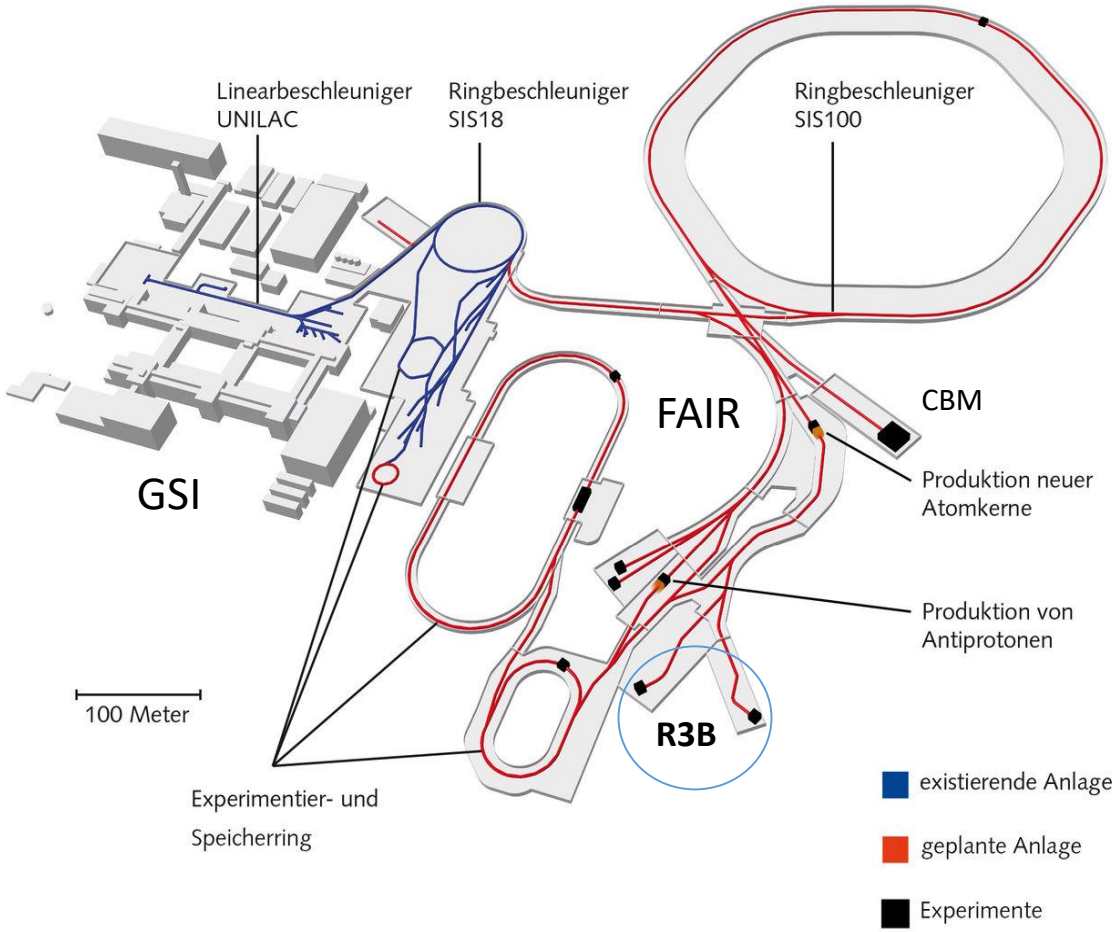

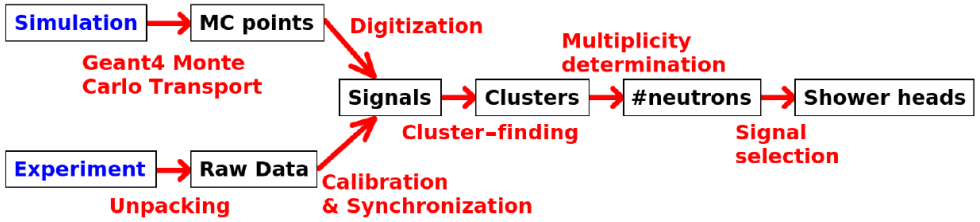

- Multiplicity determination
- Shower head determination

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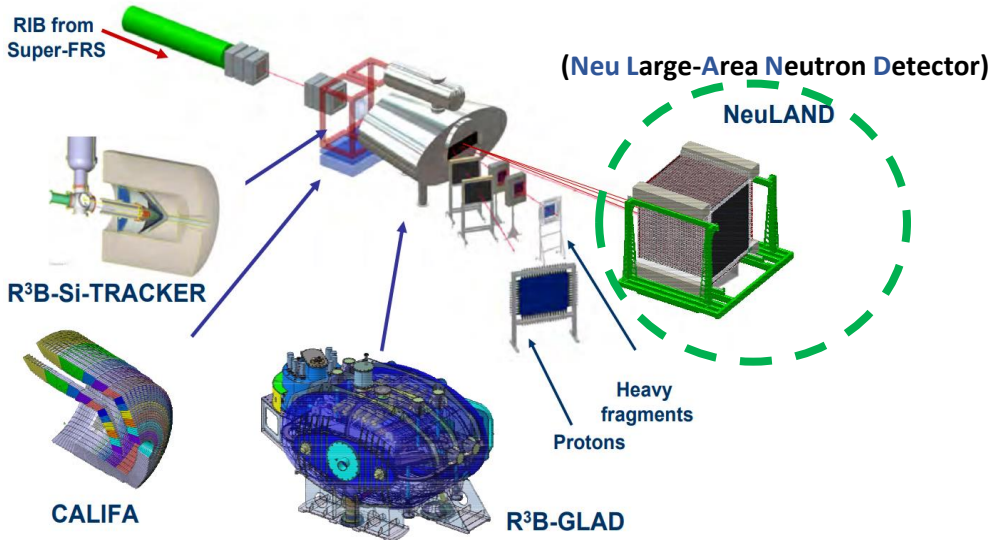
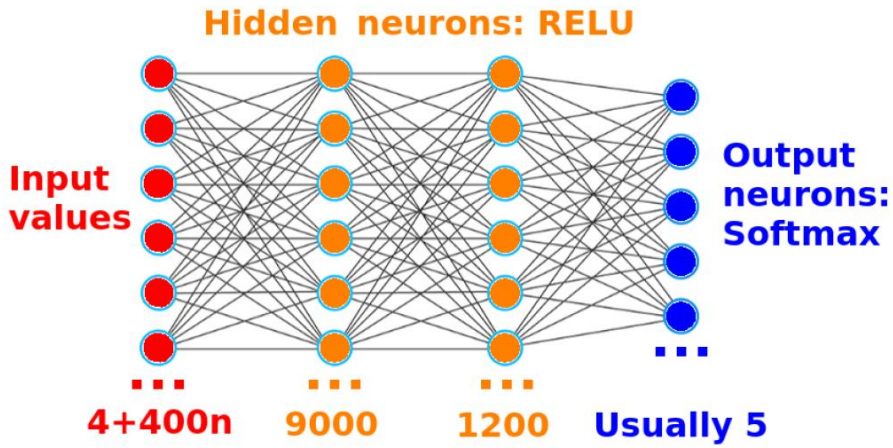
R3B

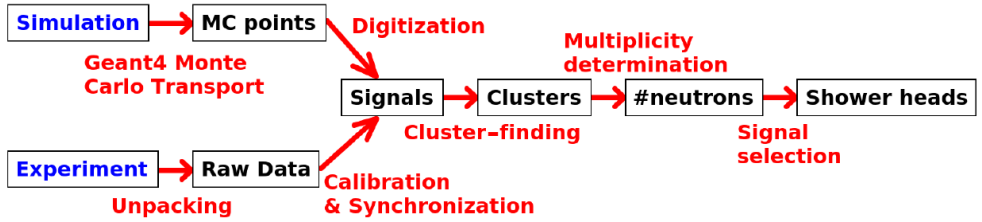
Reactions with Relativistic Radioactive Beams



Analysis methods:

- Technical Design Report (TDR)
- Deep Neural Network (DNN)





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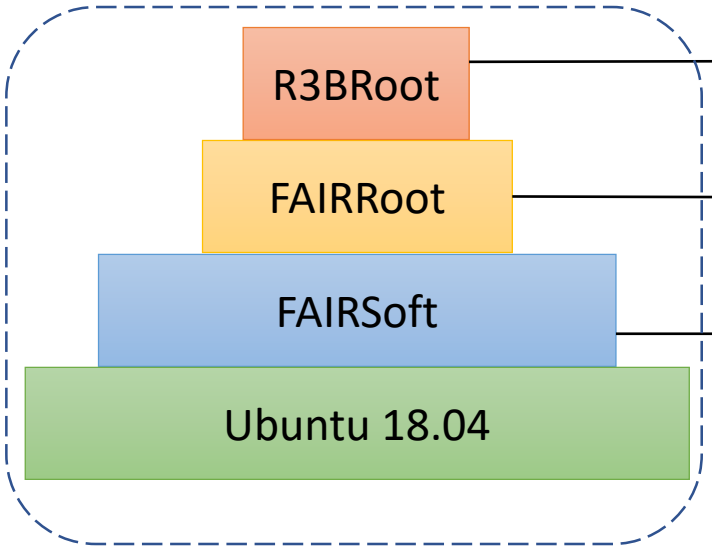

Simulation & analysis libraries for R3B experiment

Simulation libraries for FAIR-GSI experiments

Root, Geant3/4,…

Analysis methods:

- Technical Design Report (TDR)
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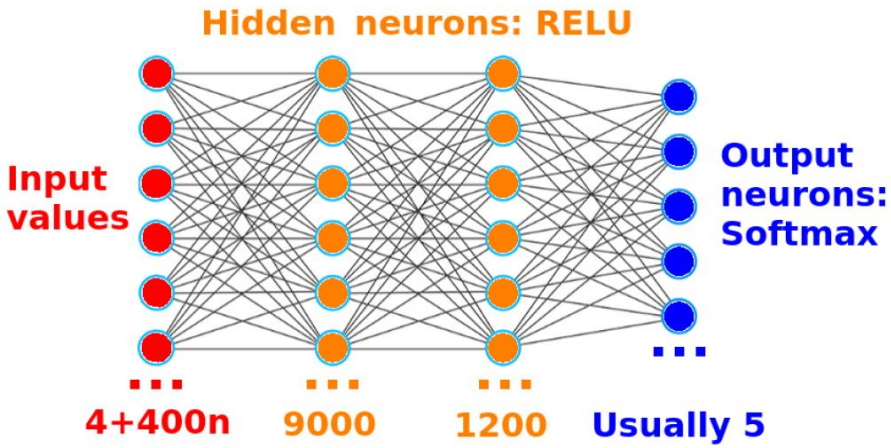

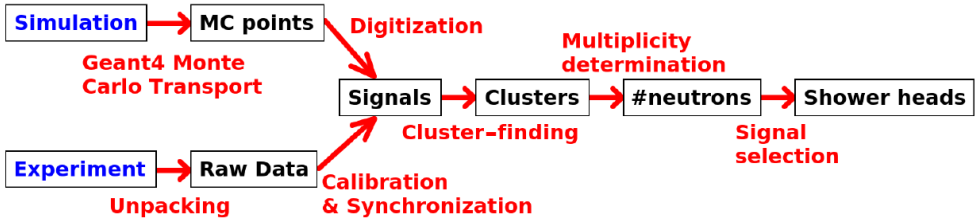

- Multiplicity determination
- Shower head determination

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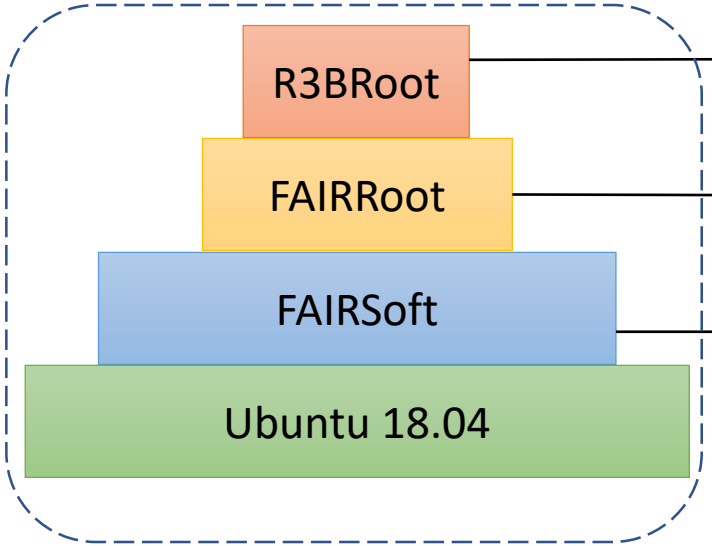
- Complicated installation
- Version conflict
- Difficult to run the simulation
- Not user-friendly



Simulation & analysis libraries for R3B experiment

Simulation libraries for FAIR-GSI experiments

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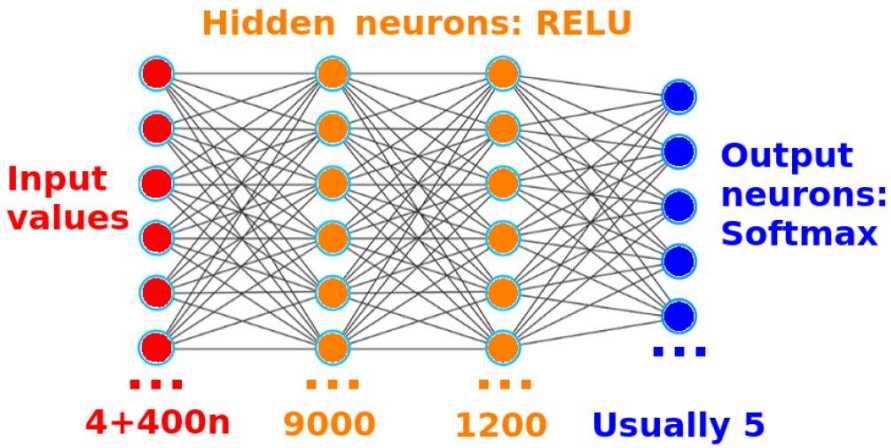

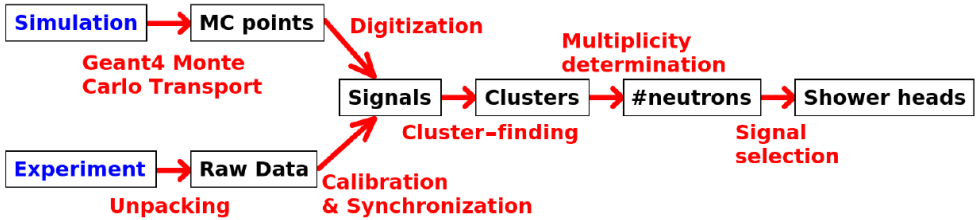

- Multiplicity determination
- Shower head determination

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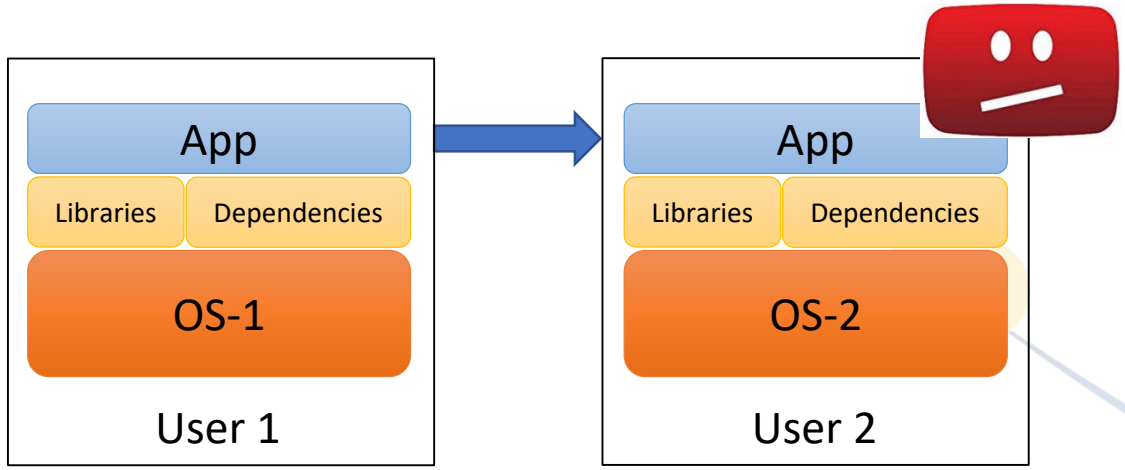
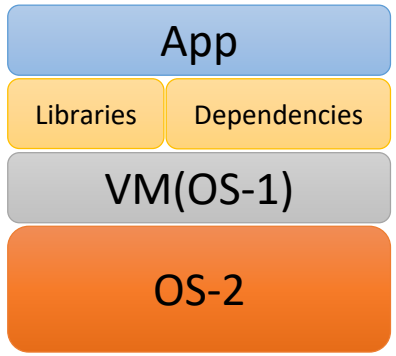
R3BRoot software portability

Compatibility and portability issues



Virtual Machine?!



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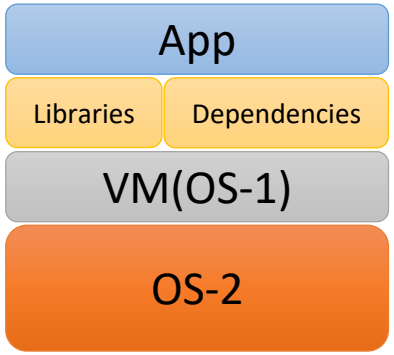
R3BRoot software portability

1. Compatibility and portability issues
2. Configuration is time consuming
3. Scaling
4. Resource utilization

Virtual Machine?!



User 2

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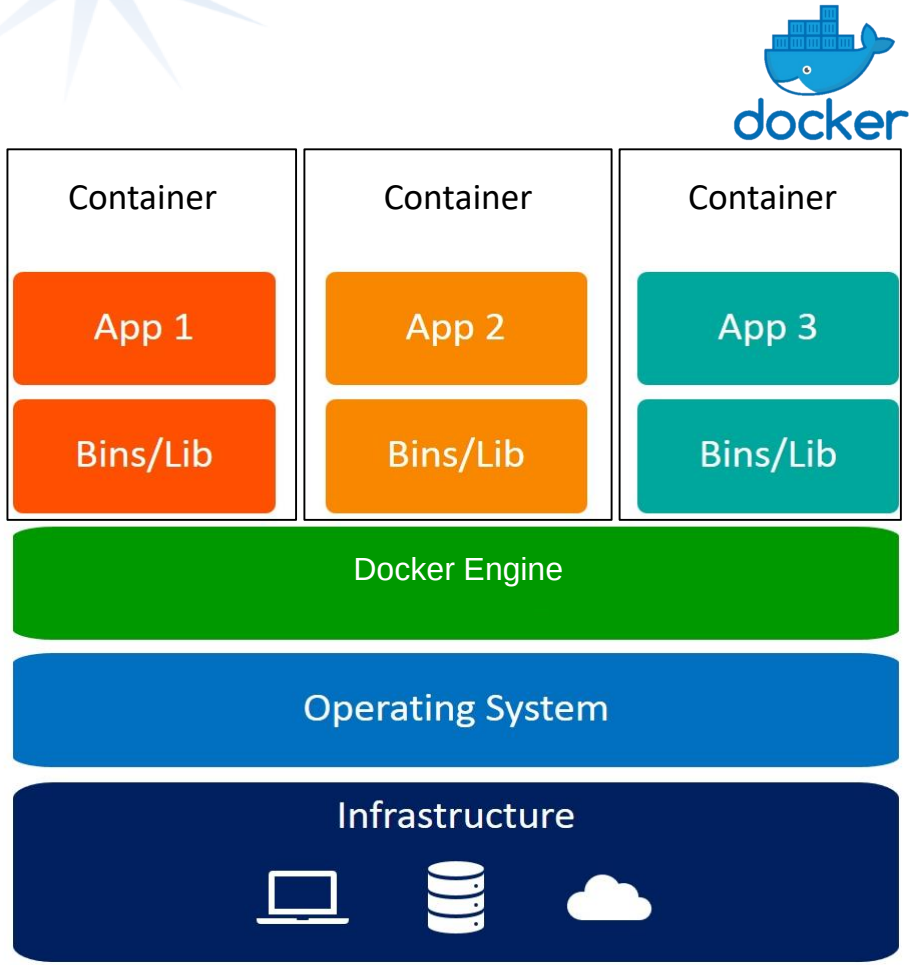
Containerization:

A standard OS-virtualization technology for **packing up software** and all the **dependencies** to **run applications on different environments**.

- Lighter than VM
- Faster configuration
- Less resource utilization
- Portability
- Micro services & Scaling



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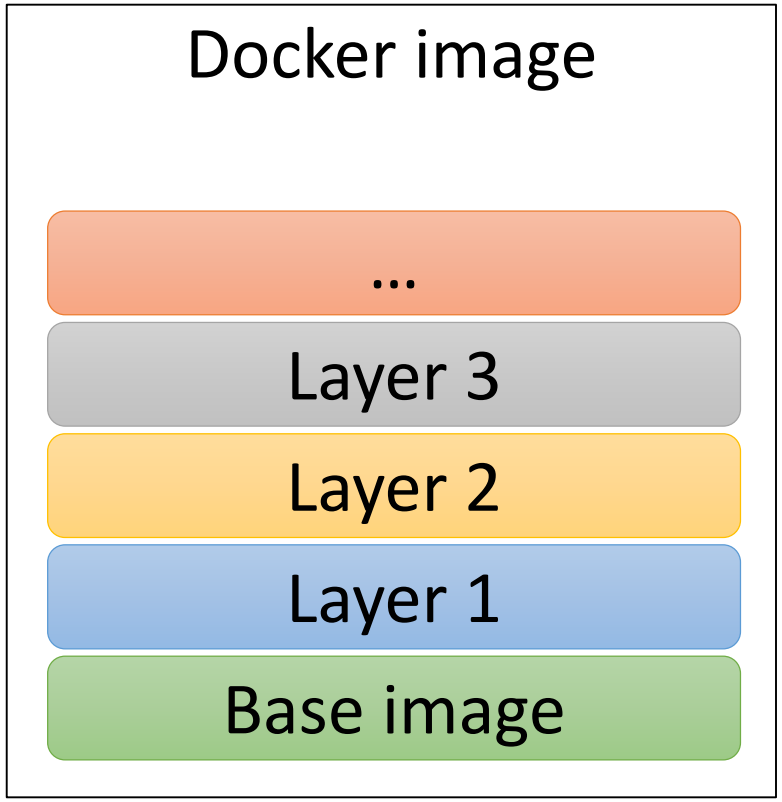
R3BRoot software portability

Containerization:



Docker file

Activities Text Editor di 17:39

Open Fairsoft.Dockerfile
~/r3bdocker/r3bdocker_final/Version1.4

```
1 ARG BASE_IMAGE=ubuntu:18.04
2 FROM $BASE_IMAGE
3
4 MAINTAINER Maisam M. Dadkan, Email:maisam.m.dadkan@gmail.com
5 #
6 # Install dependencies
7 #
8
9 RUN     apt-get update && \
10        apt-get install -y cmake cmake-data g++ gcc gfortran \
11        debianutils build-essential make patch sed \
12        libx11-dev libxft-dev libxext-dev libxpm-dev libxmu-dev \
13        libglu1-mesa-dev libgl1-mesa-dev \
14        libncurses5-dev curl libcurl4-openssl-dev bzip2 libbz2-dev gzip unzip tar \
15        subversion git xutils-dev flex bison lsb-release python-dev python3-dev\
16        libc6-dev-i386 libxml2-dev wget libssl-dev libkrb5-dev \
17        automake autoconf libtool zlib1g-dev \
18        libreadline-dev libsqlite3-dev llvm \
19        libncursesw5-dev xz-utils liblzma-dev python-openssl python3-openssl &&\
20        apt-get clean && rm -rf /var/lib/apt/lists/*
21
22 #
23 # Steal newer CMake
24 #
25 WORKDIR /opt
26 RUN wget https://github.com/Kitware/CMake/releases/download/v3.16.4/cmake-3.16.4-Linux-x86_64.sh -O cmake.sh && chmod +x cmake.sh && \
27     mkdir /opt/cmake-3.16.4 && ./cmake.sh --skip-license --prefix=/opt/cmake-3.16.4 && \
28     rm cmake.sh
29 ENV PATH="/opt/cmake-3.16.4/bin:${PATH}"
30
31 #copy modified source code of fairsoft and install it
32 WORKDIR /tmp/fairsoft-build
33 COPY    ./fairsoft.conf ./fairsoft.conf
34 COPY    ./FairSoft-jun19p2 ./FairSoft
35 RUN     cd FairSoft &&  ./configure.sh ../fairsoft.conf && ./make_clean.sh all && rm -rf /tmp/fair*
36
37 ENV SIMPATH="/opt/fairsoft_jun19p2"\
38     G4INCLDATA="/opt/fairsoft_jun19p2/share/Geant4-10.5.1/data/G4INCL1.0"\
39     G4LEVELGAMMADATA="/opt/fairsoft_jun19p2/share/Geant4-10.5.1/data/PhotonEvaporation5.3"\
40     G4RADIOACTIVEDATA="/opt/fairsoft_jun19p2/share/Geant4-10.5.1/data/RadioactiveDecay5.3"\
41     G4PIIDATA="/opt/fairsoft_jun19p2/share/Geant4-10.5.1/data/G4PII1.3"\
42     G4SAIDXSDATA="/opt/fairsoft_jun19p2/share/Geant4-10.5.1/data/G4SAIDDATA2.0"\
43     G4ABLADATA="/opt/fairsoft_jun19p2/share/Geant4-10.5.1/data/G4ABLA3.1"\
44     G4REALSURFACEDATA="/opt/fairsoft_jun19p2/share/Geant4-10.5.1/data/RealSurface2.1.1"\
45     G4NEUTRONHPDATA="/opt/fairsoft_jun19p2/share/Geant4-10.5.1/data/G4NDL4.5"\
46     G4PARTICLEXSDATA="/opt/fairsoft_jun19p2/share/Geant4-10.5.1/data/G4PARTICLEXS1.1"\
47     G4ENSDFSTATEDATA="/opt/fairsoft_jun19p2/share/Geant4-10.5.1/data/G4ENSDFSTATE2.2"\
48     G4LEDATA="/opt/fairsoft_jun19p2/share/Geant4-10.5.1/data/G4EMLOW7.7"
49
```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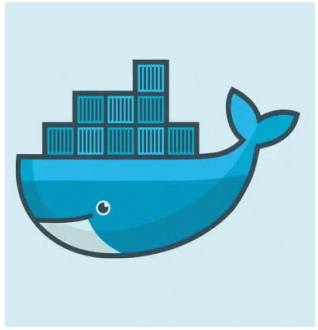
R3BRoot software portability

A standard OS-virtualization platform for **packing up software** and all the **dependencies** to **run applications on different environments**.



- Reusability
- Accessibility
- Interoperability
- Portability
- Micro services & Scaling

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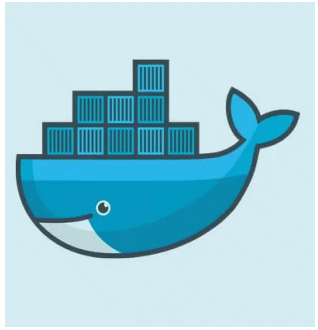

A **Web IDE** for **live code**, equations, **visualizations** and **narrative text (Jupyter Notebook)**

Brings the power of **notebooks** to **groups of users** & handles users access to **computational environments** and ... **(Jupyter Hub)**

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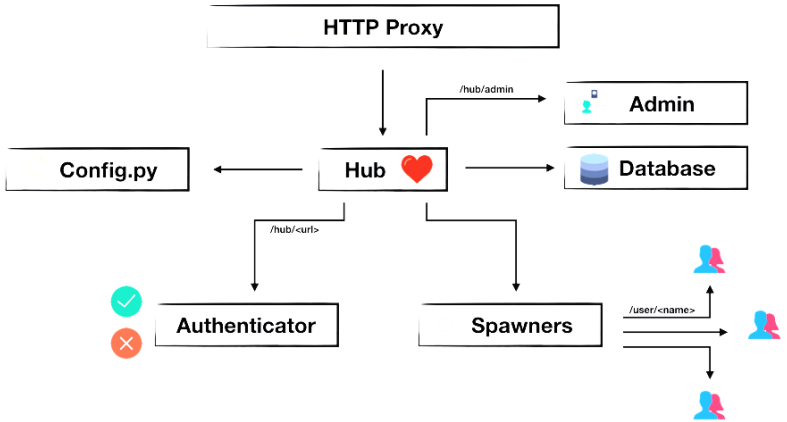
JupyterHub



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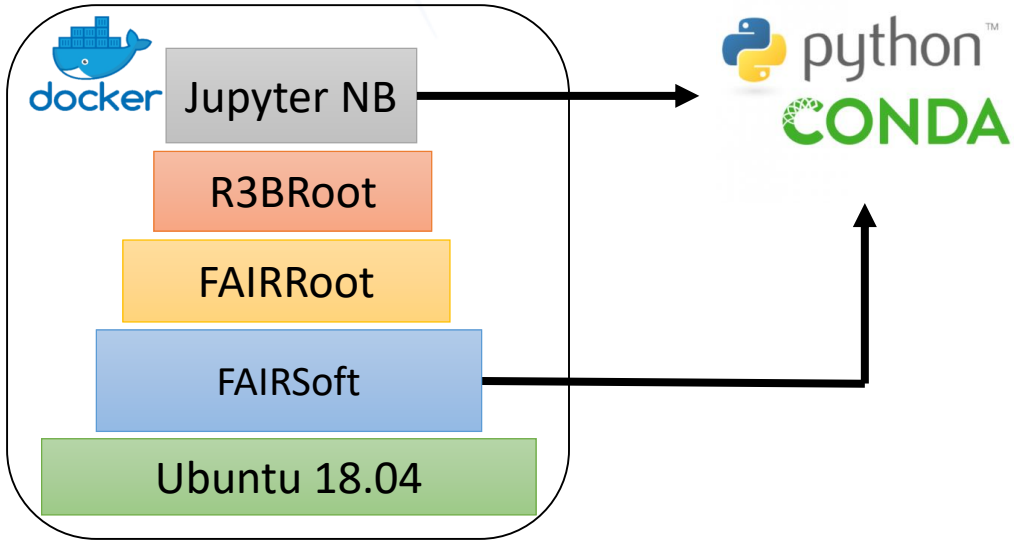
R3BRoot software portability

✓ **Standard Python environment**



- New FAIRSoft (some bugs are fixed)
- PyRoot and Jupyter NB use the same python version (ensure compatibility)
- Docker images are made for each part (can be used in other FAIR projects)
- Some security issues were resolved (root access limited)

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R3BRoot software portability

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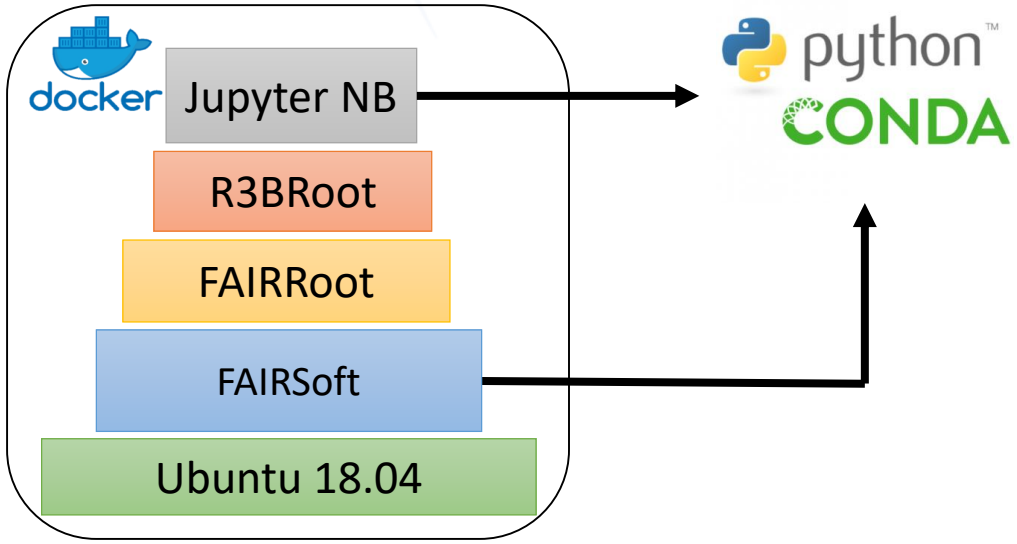

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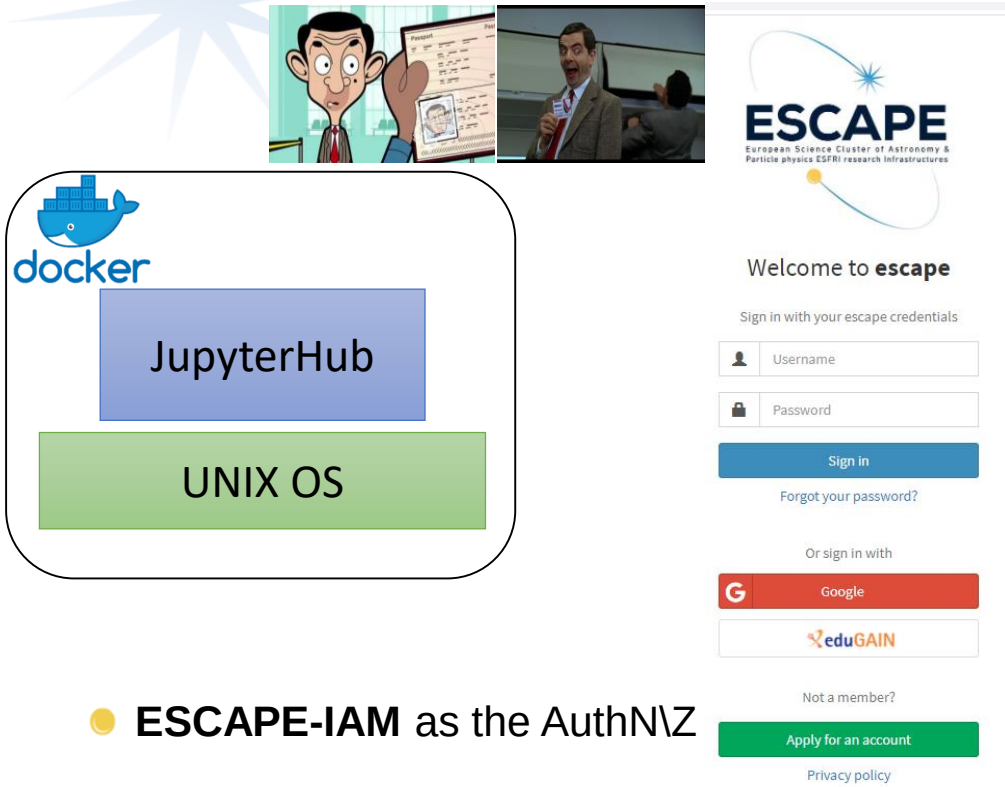
✓ Integrated with ESCAPE AuthN/Z (IAM)



- **ESCAPE-IAM** as the AuthN\Z
- To take advantage of other ESCAPE services
- Enabling the end-to-end AuthN/Z
- Supported **token-based** AuthN/Z

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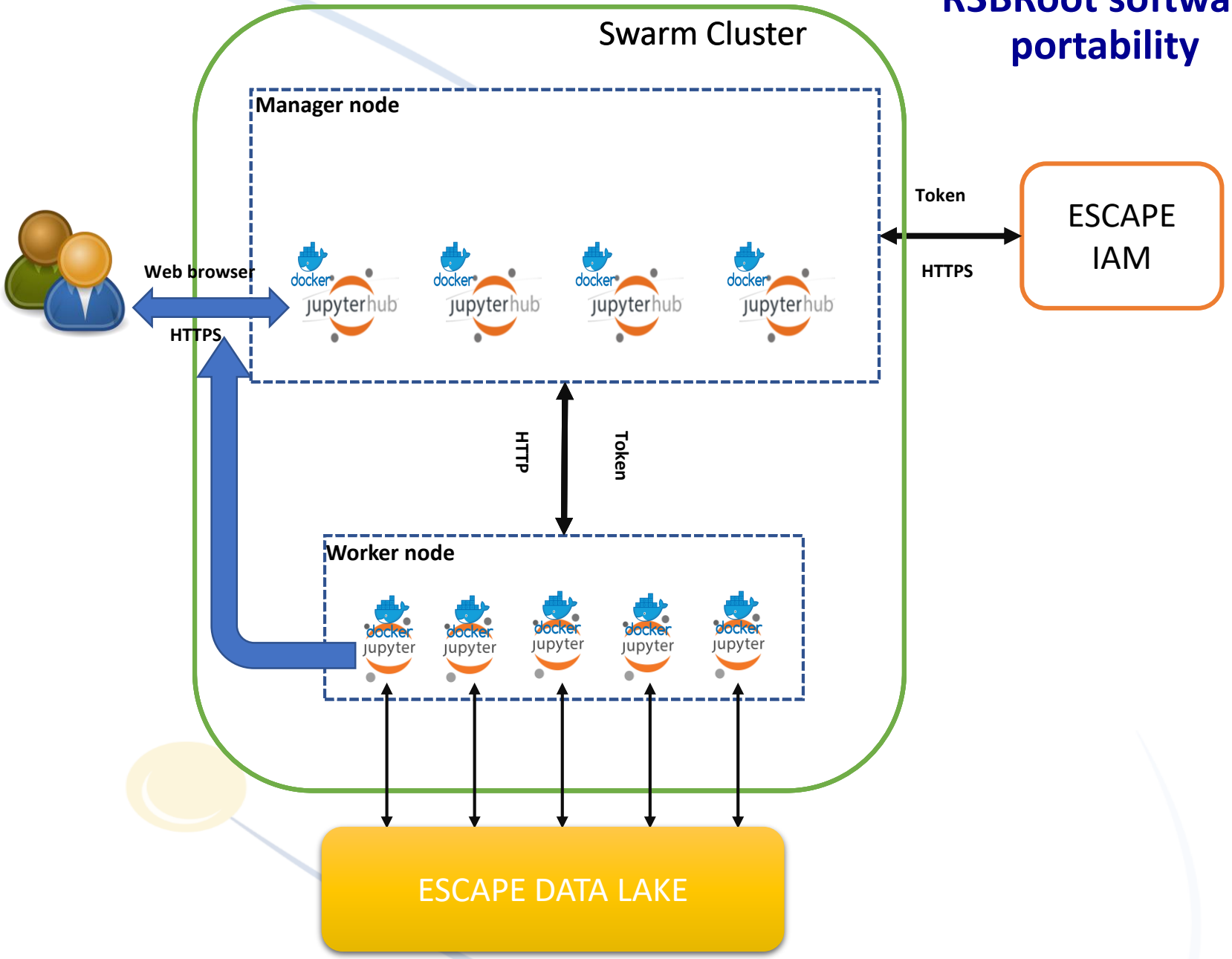
R3BRoot software portability



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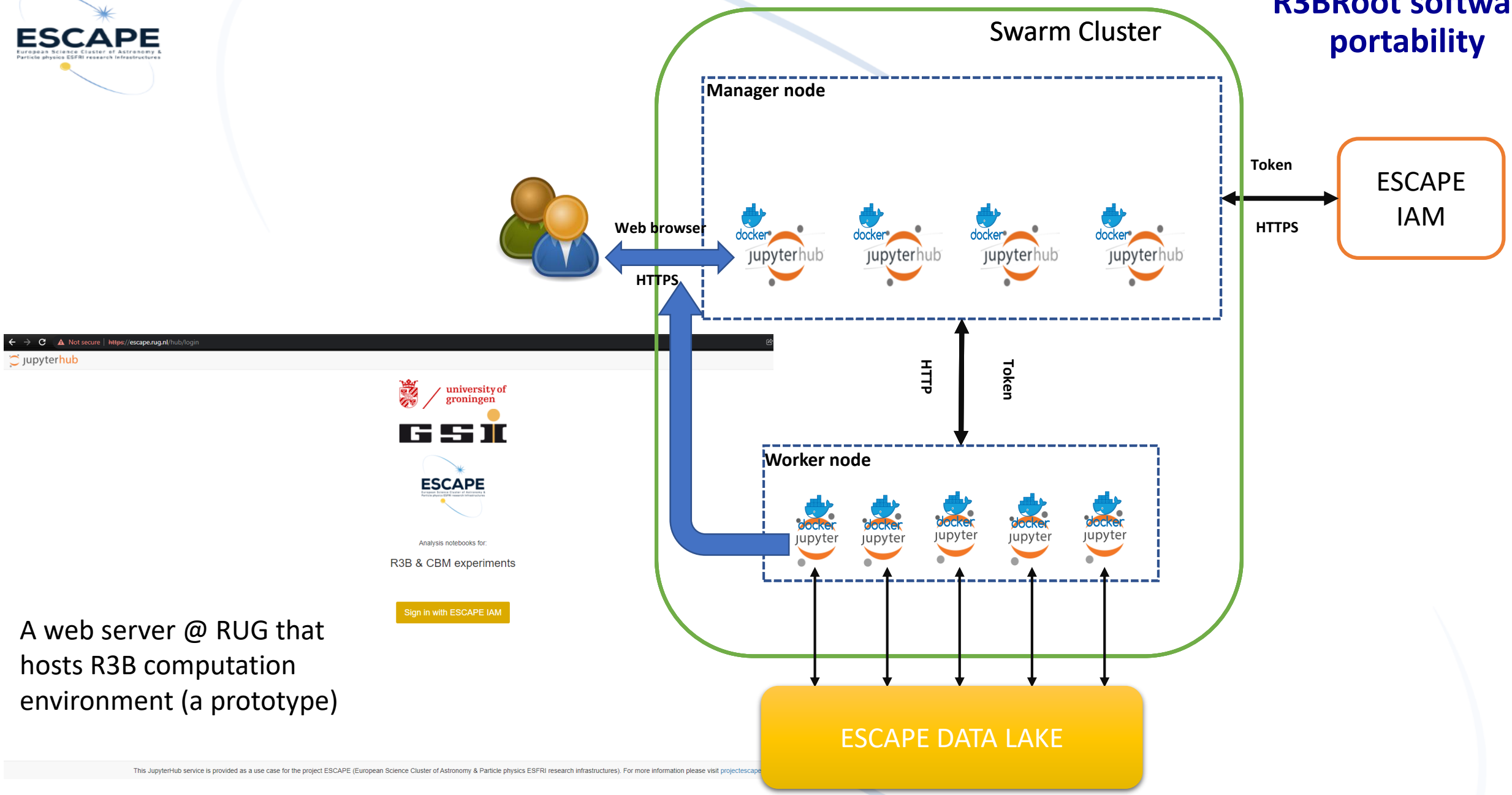
R3BRoot software portability



A web server @ RUG that hosts R3B computation environment (a prototype)

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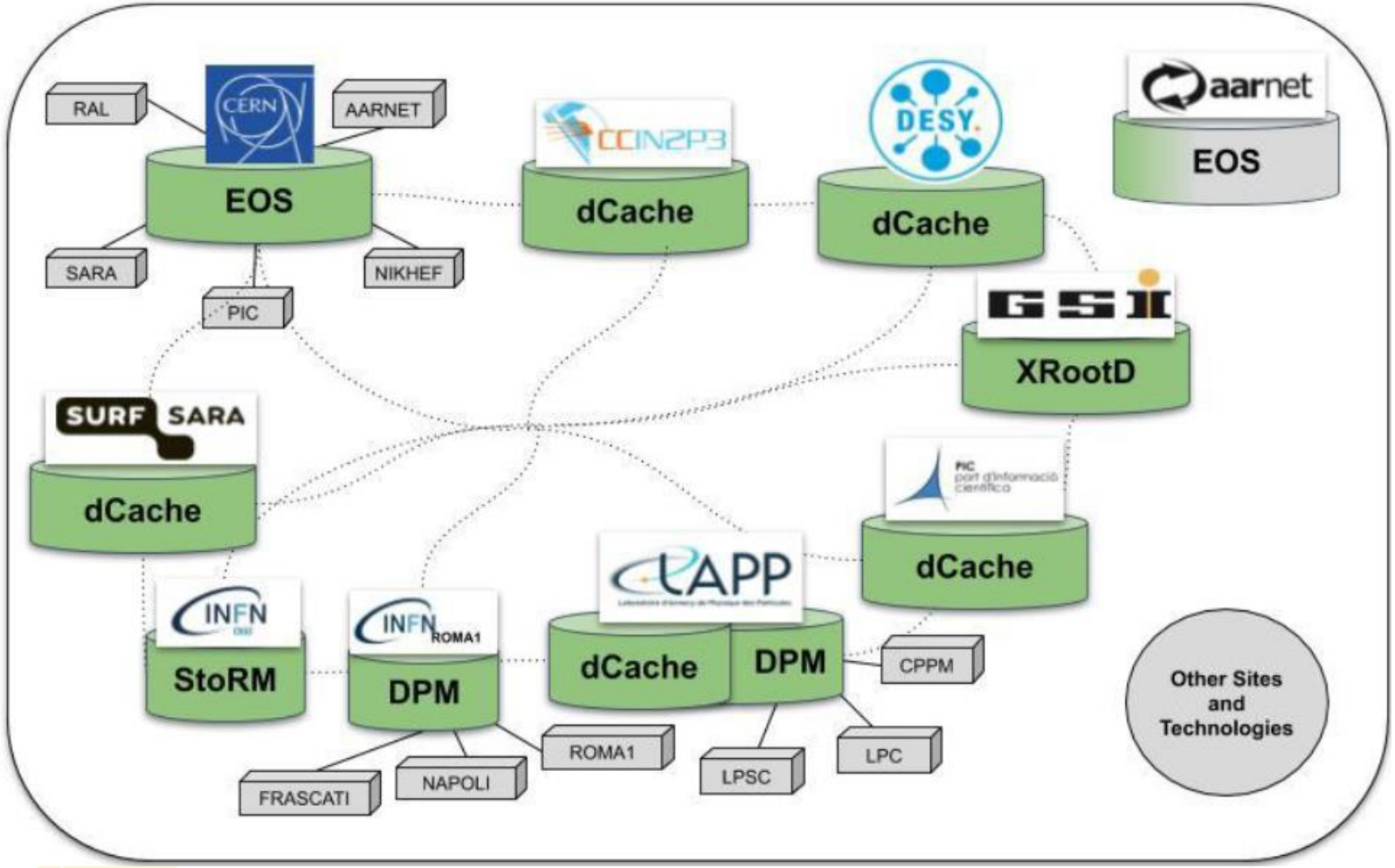
Data Lake



- Distributed across the world
- Using different technologies for data management
- Each one has a different regulation and policy

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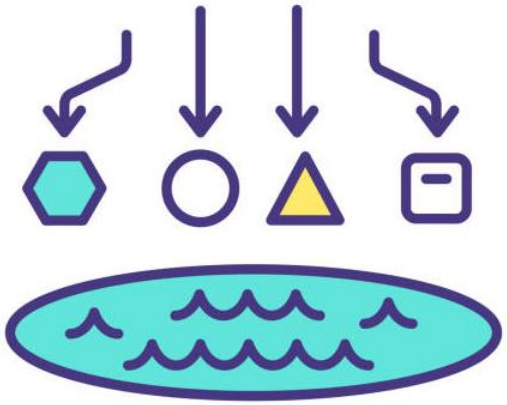
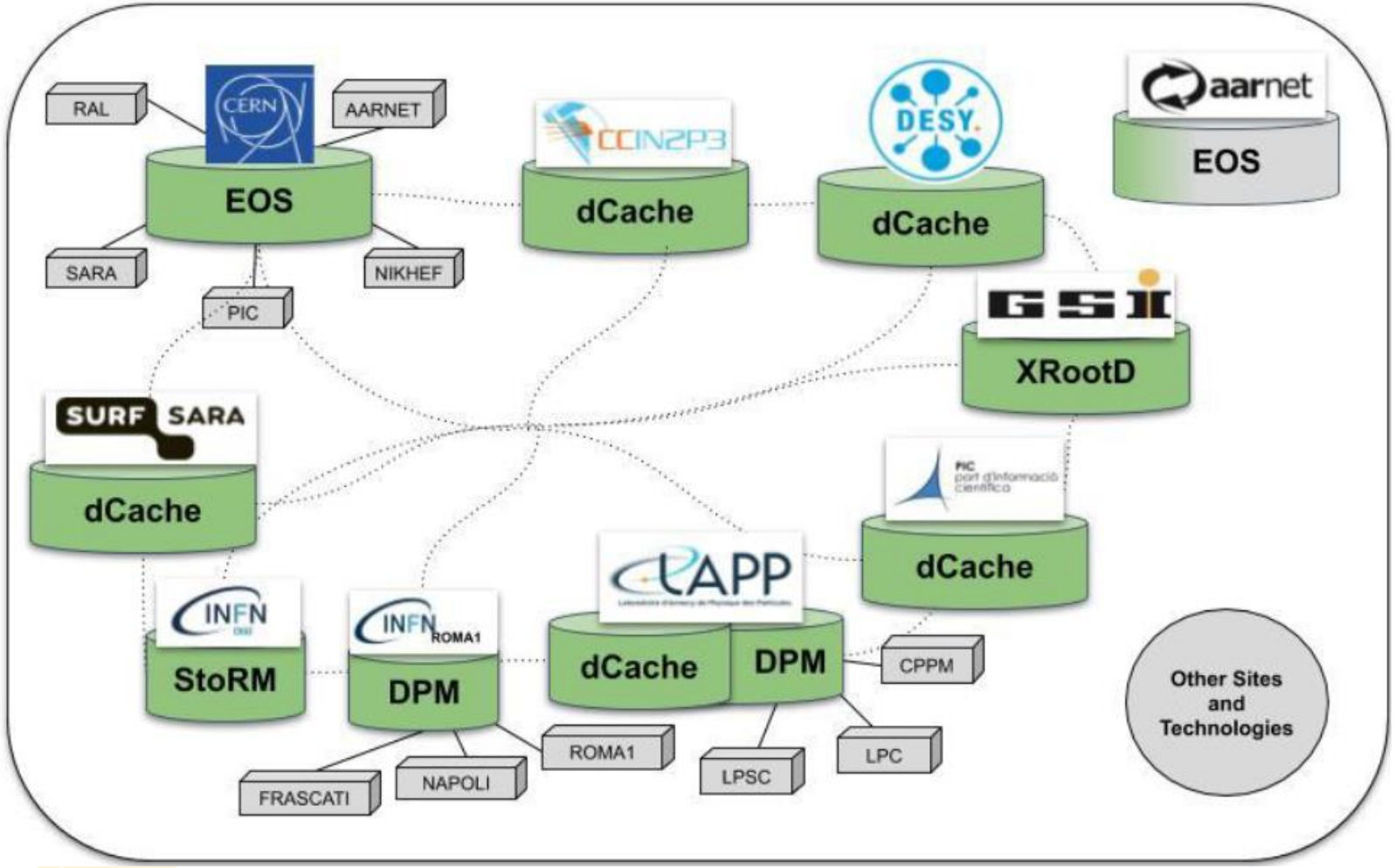
Data Lake



Data Lake



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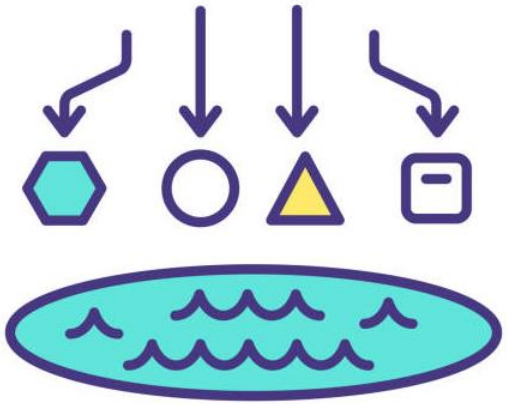
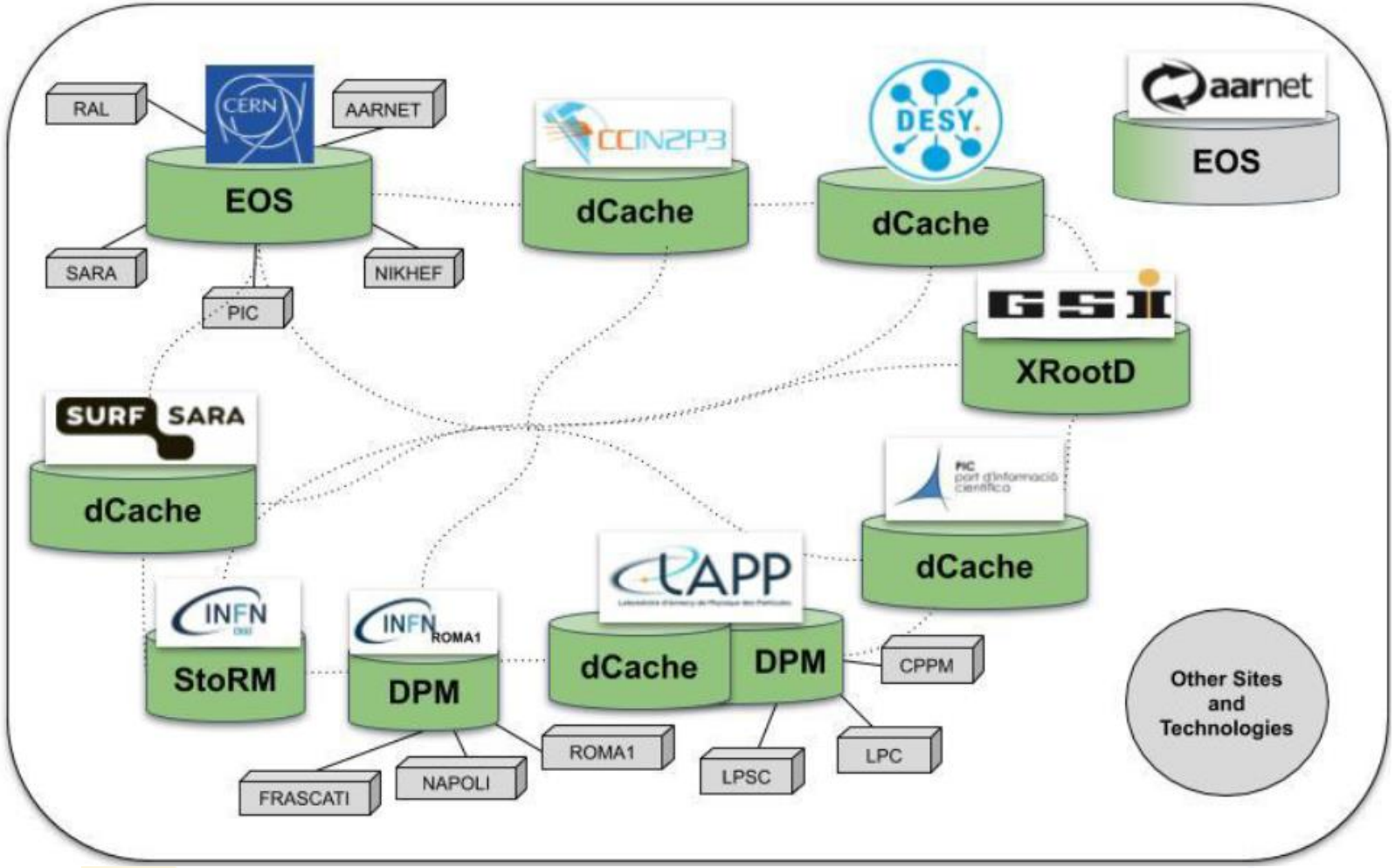
Data Lake



Data Lake



- Data Orchestration
  - Rucio customised to the needs of ESCAPE community

- File Transfer Service → WLCG FTS
  - continuous testing for both FTS and file access libraries

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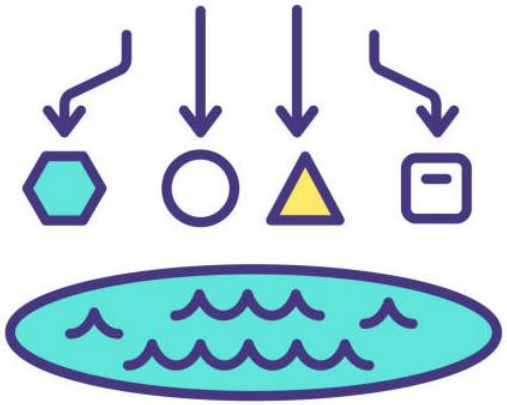
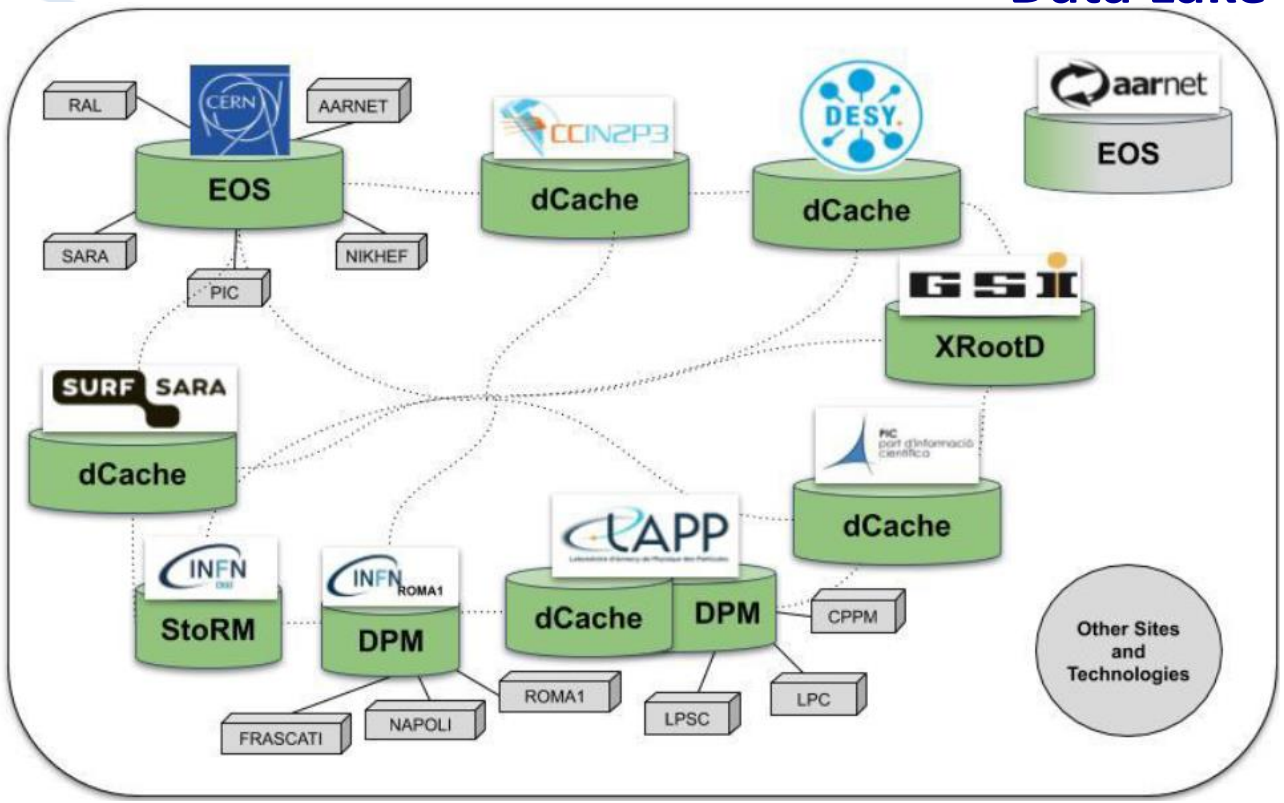
Data Lake



Data Lake



- Data Orchestration
  - Rucio customised to the needs of ESCAPE community

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  - continuous testing for both FTS and file access libraries

For ATLAS experiment:

- 1B+ files, 505 PB of data, 400+ Hz interaction rate
- 120 data centres, 5 HPCs, 600 storage areas
- 500 Petabytes/year transferred & deleted
- 2.5 Exabytes/year uploaded & downloaded

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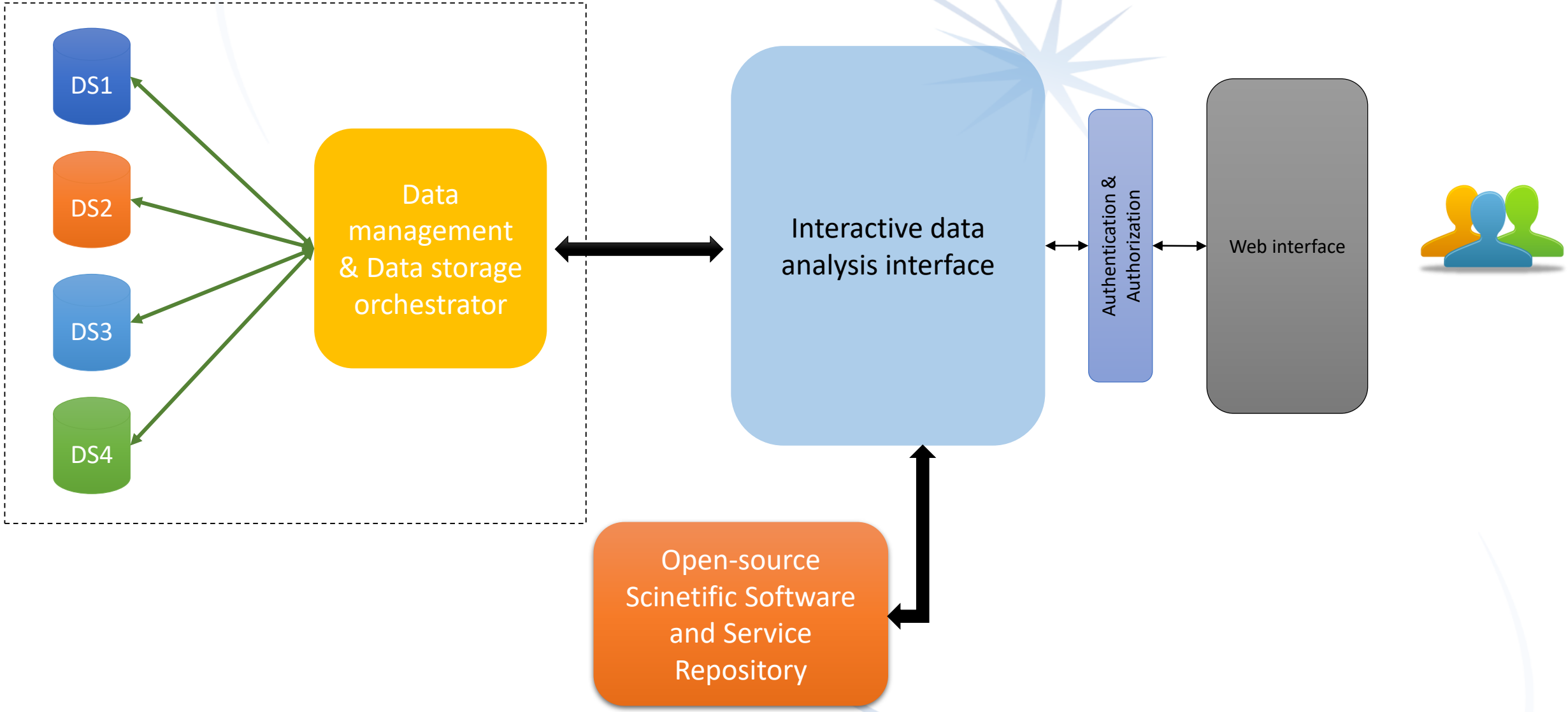
ESCAPE Final Shape



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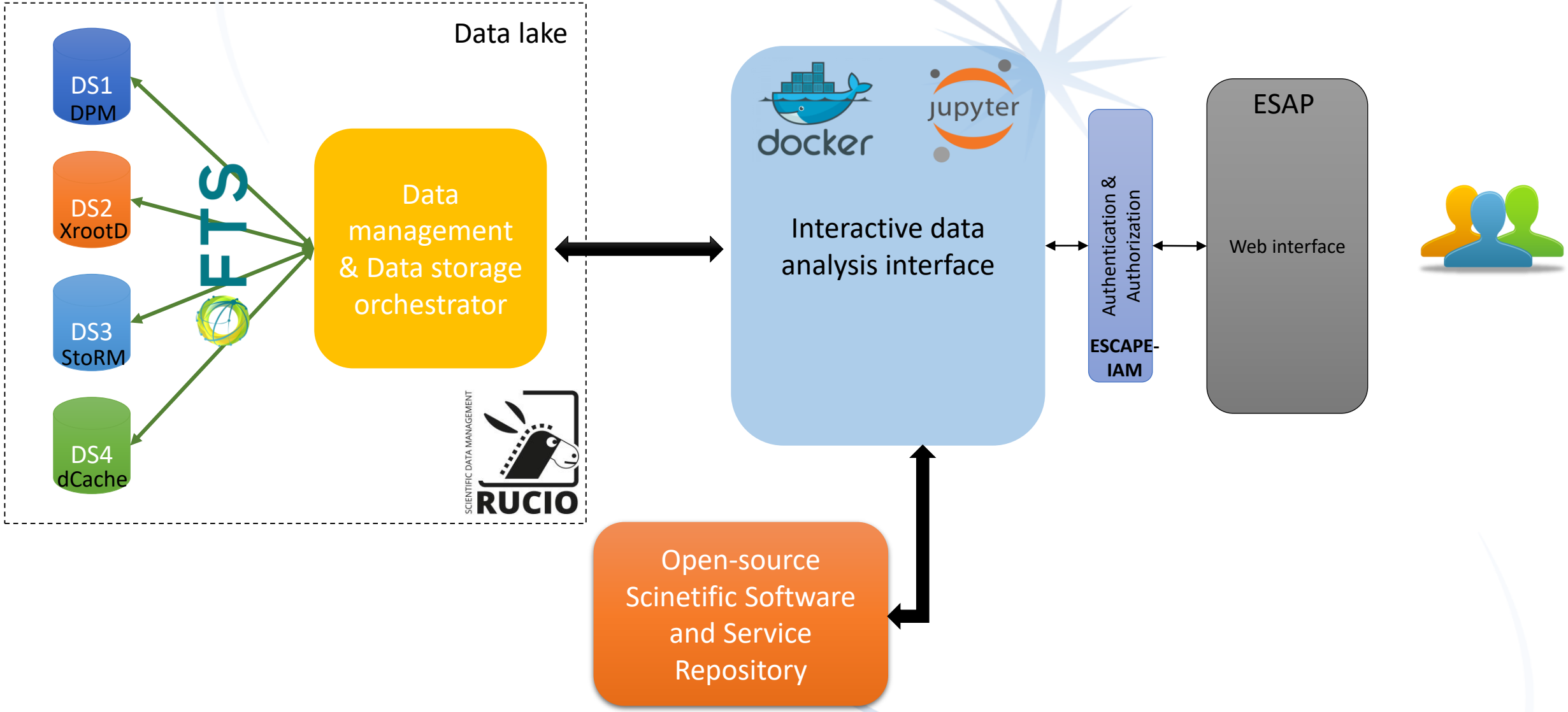
ESCAPE Final Shape



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Data Lake as a Service

- The Data Lake is a place where experiments can ‘dump’ the data
- … and scientists can ‘fish’ data from
- Challenge: making sure the scientists can ‘fish’ easily.

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Data Lake as a Service

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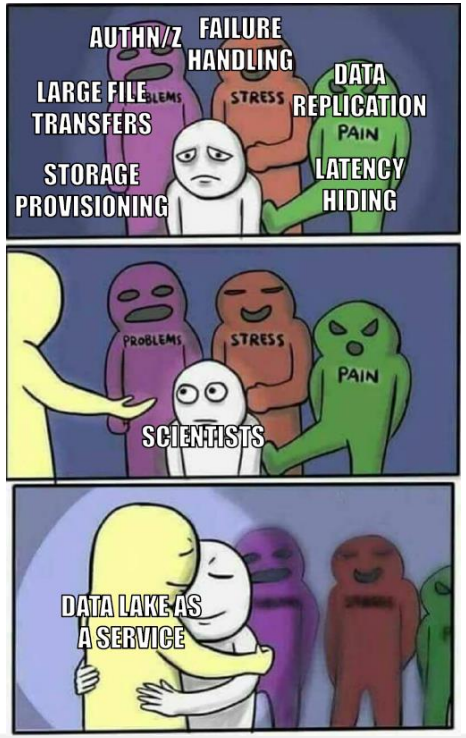
- … and scientists can ‘fish’ data from
- Challenge: making sure the scientists can ‘fish’ easily.

Making ‘data fishing’ easier!

Data Lake as a Service (DLaaS)



- The Data Lake has a lot of moving parts
- The goal of the service is to abstract the complexities of the Data Lake from the scientists.
- This way, scientists can focus their time on doing science instead of data procurement.

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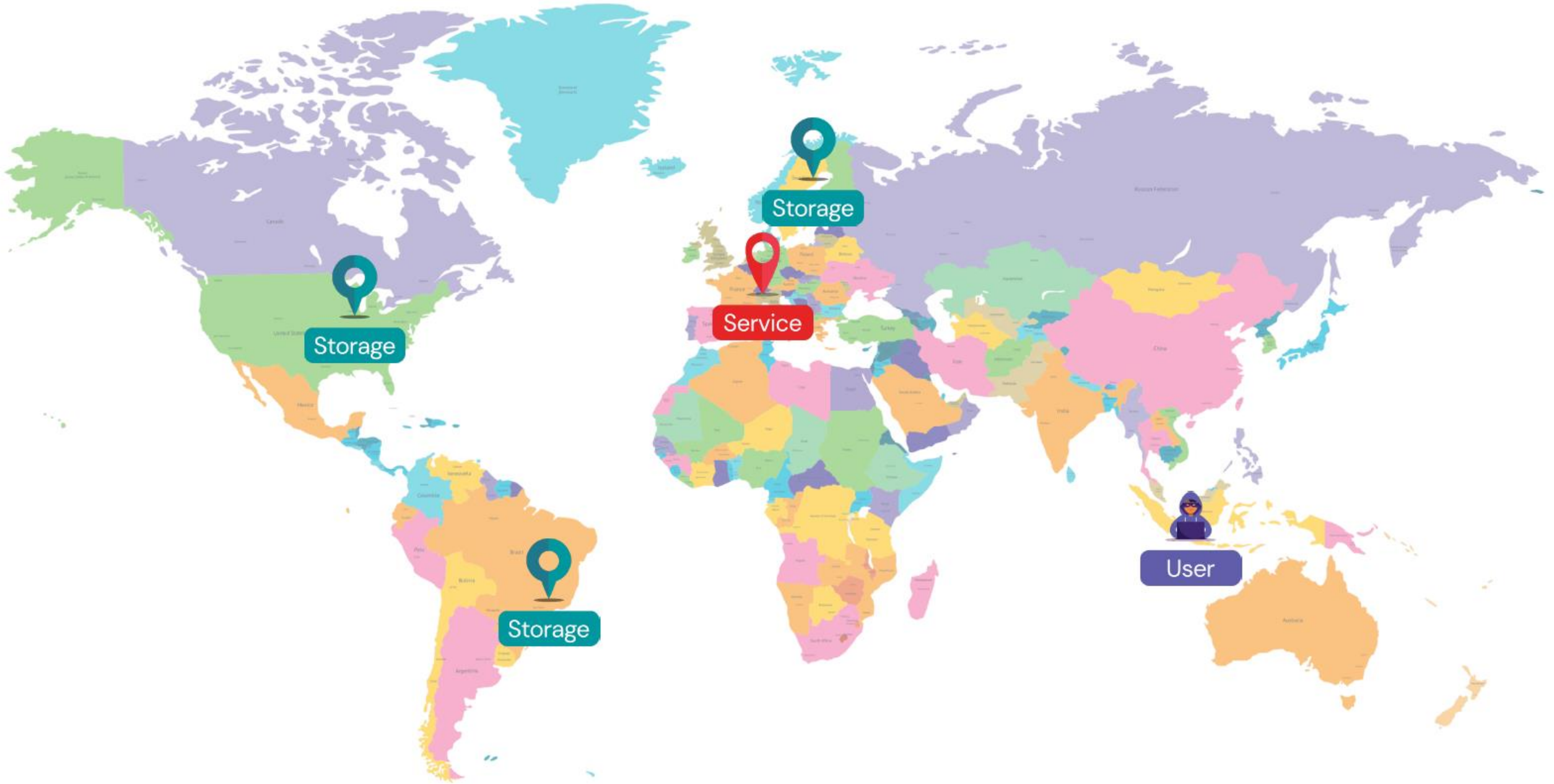
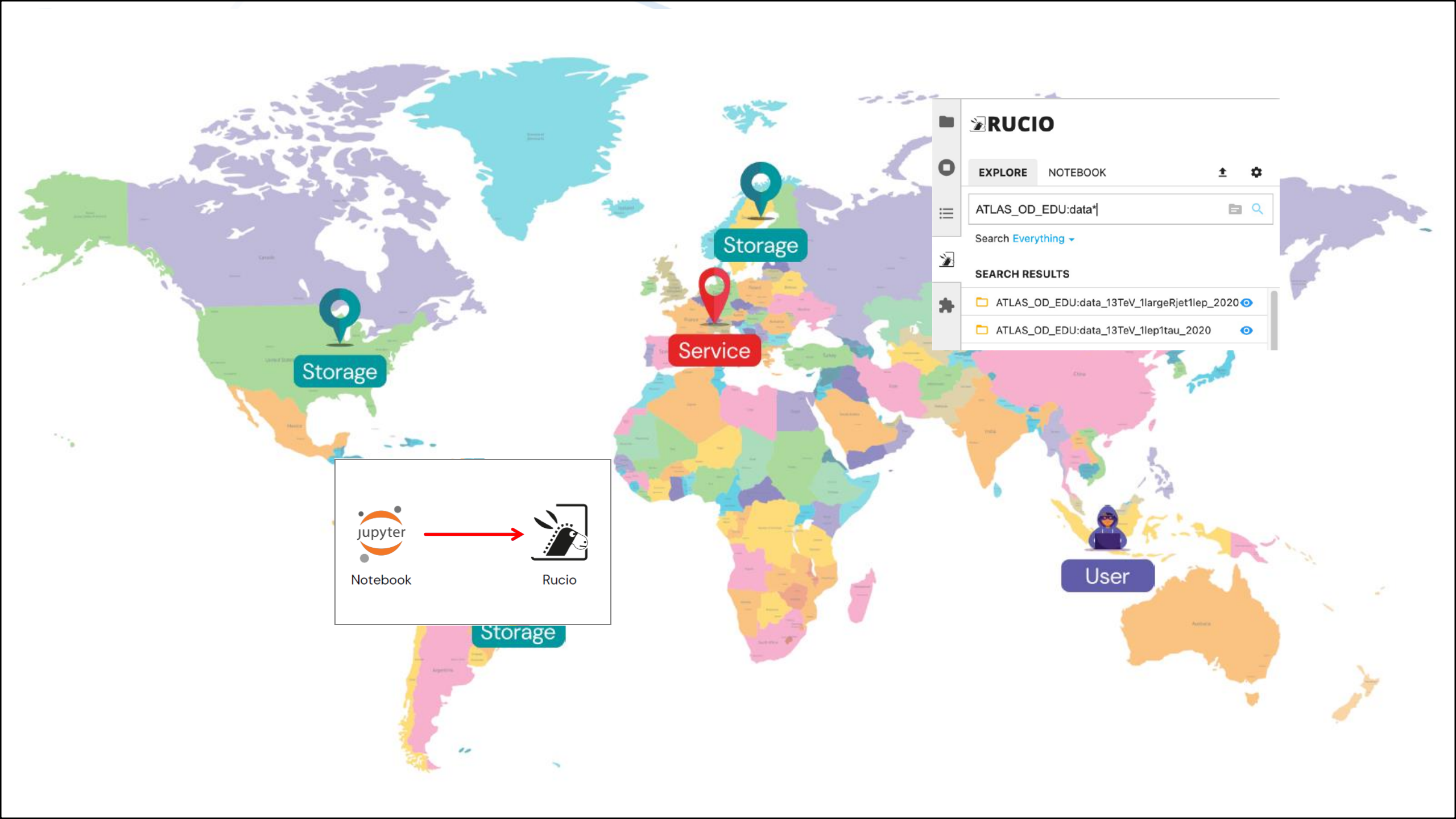

Storage
Storage
Service
Storage
Storage
User


JupyterHub
https://escape-notebook.cern.ch/
jupyterhub
Storage
Storage
Service
Storage
User


RUCIO
EXPLORE
NOTEBOOK
ATLAS_OD_EDU:data*
Search Everything
SEARCH RESULTS
ATLAS_OD_EDU:data_13TeV_1largeRjet1lep_2020
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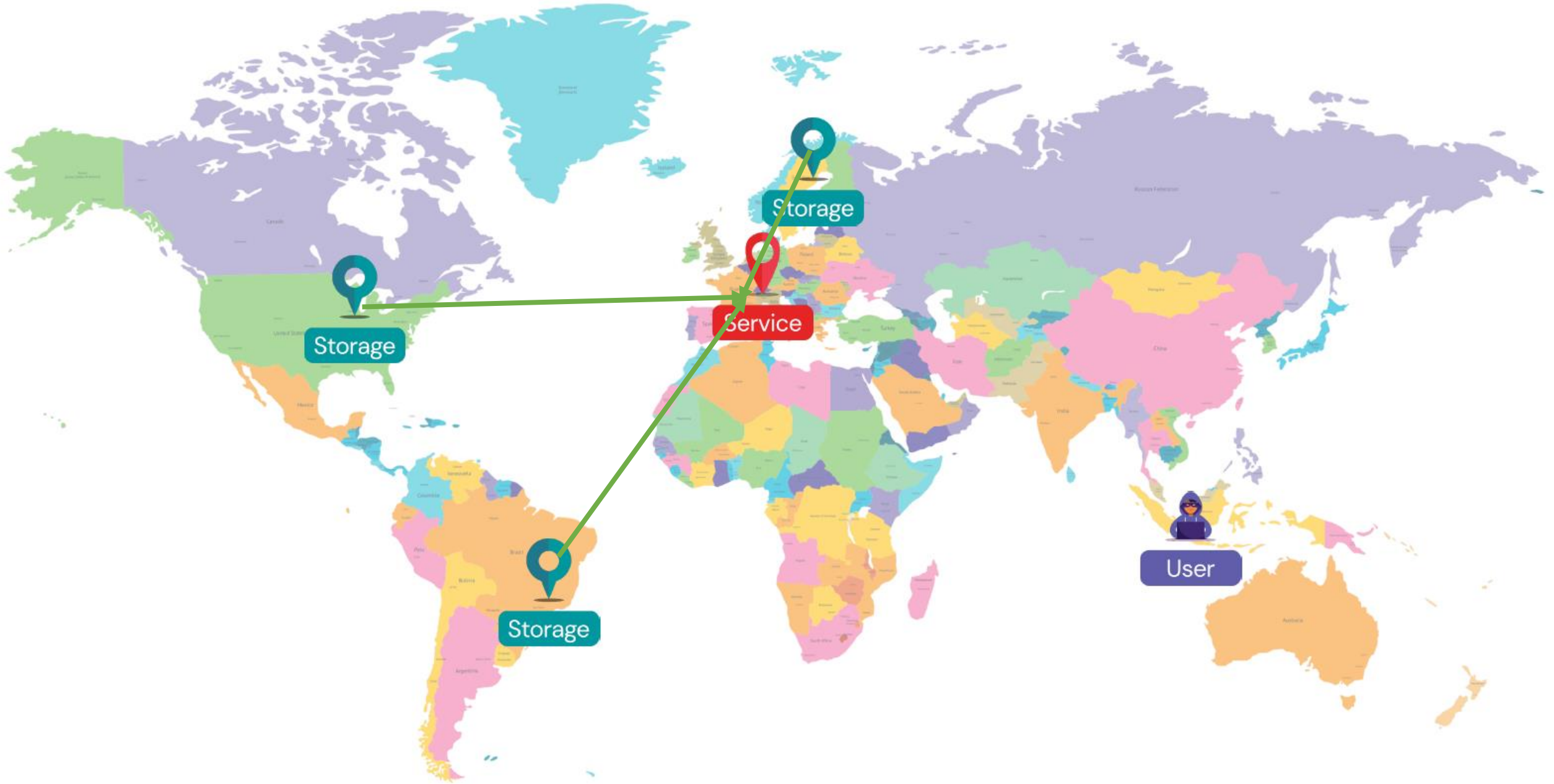
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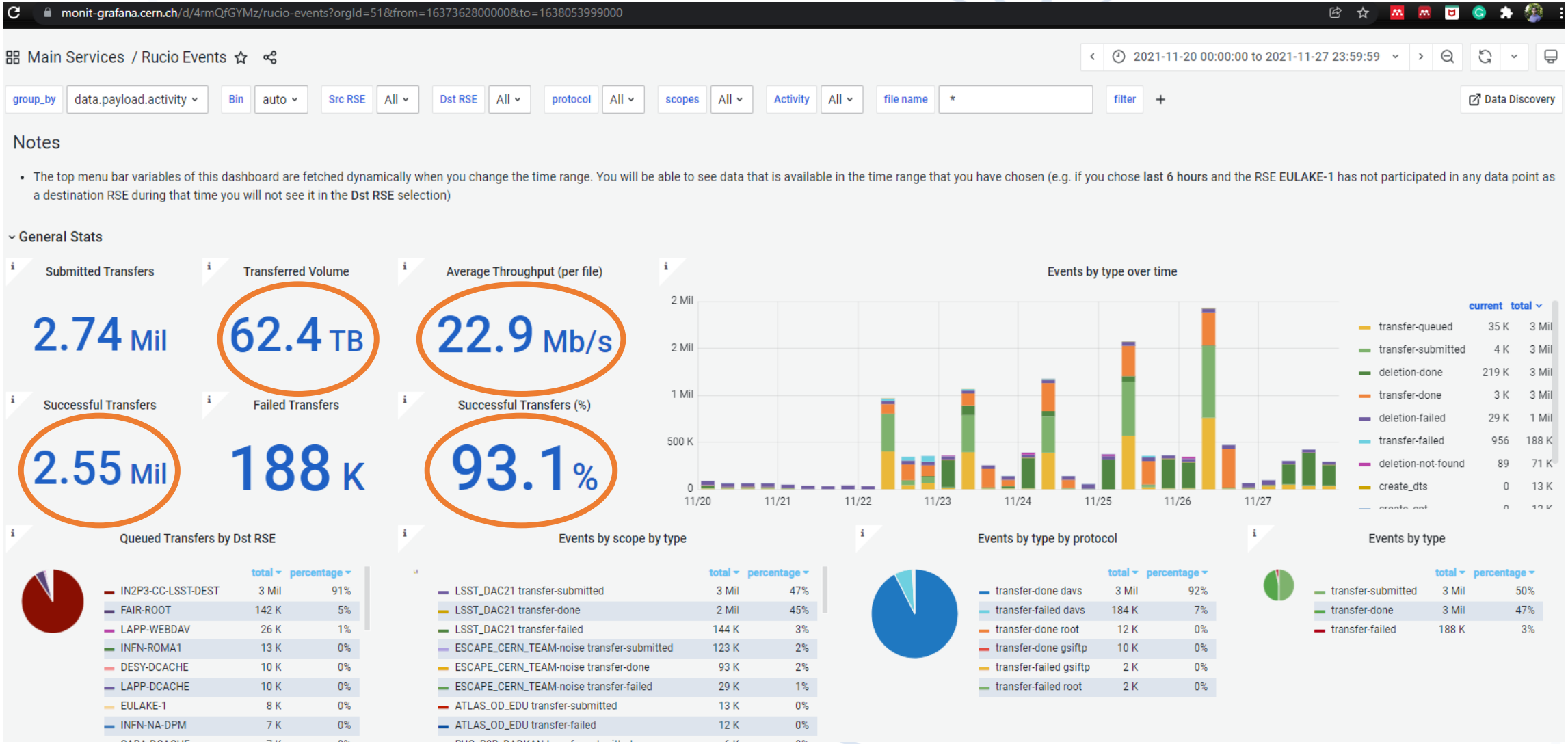
Data Analysis Challenge 2021 (DAC21)



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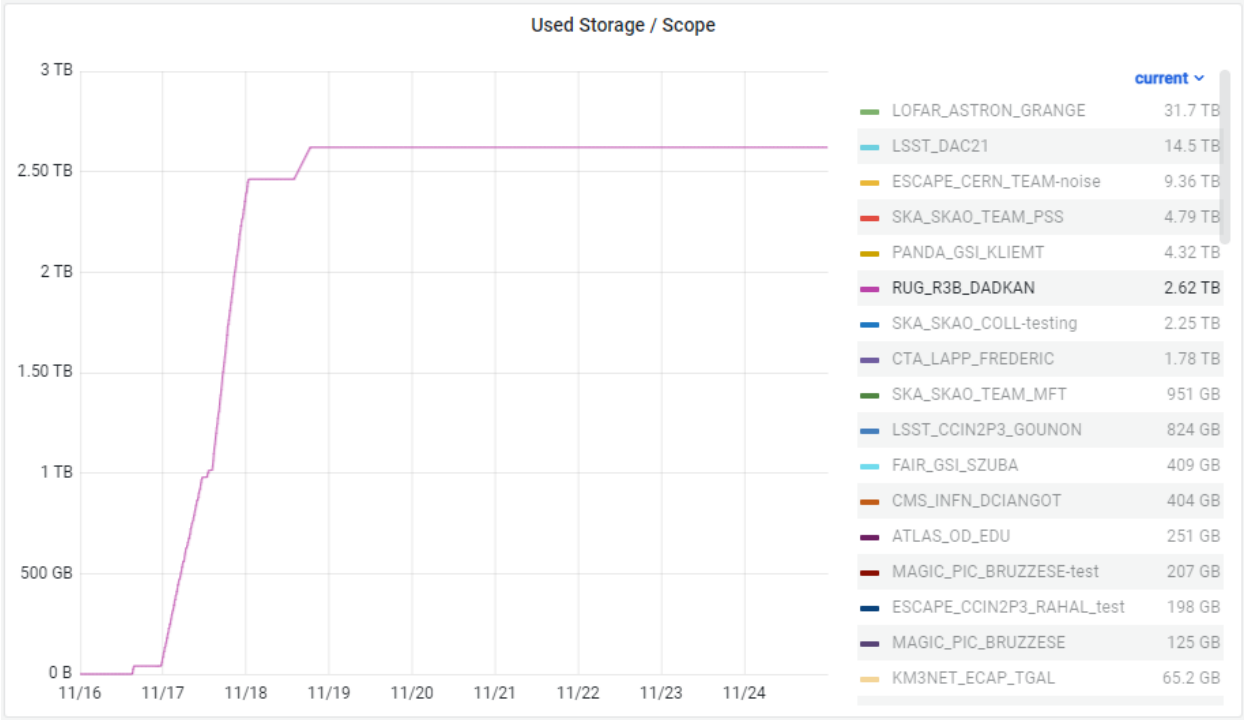

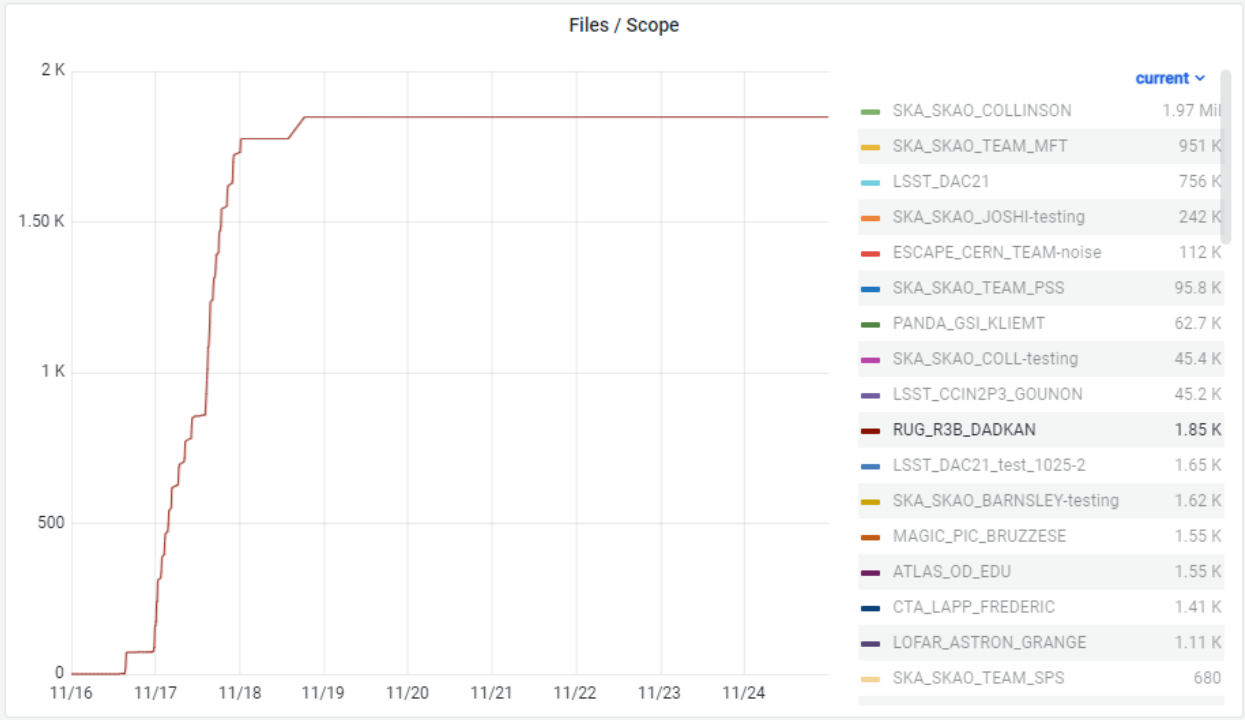

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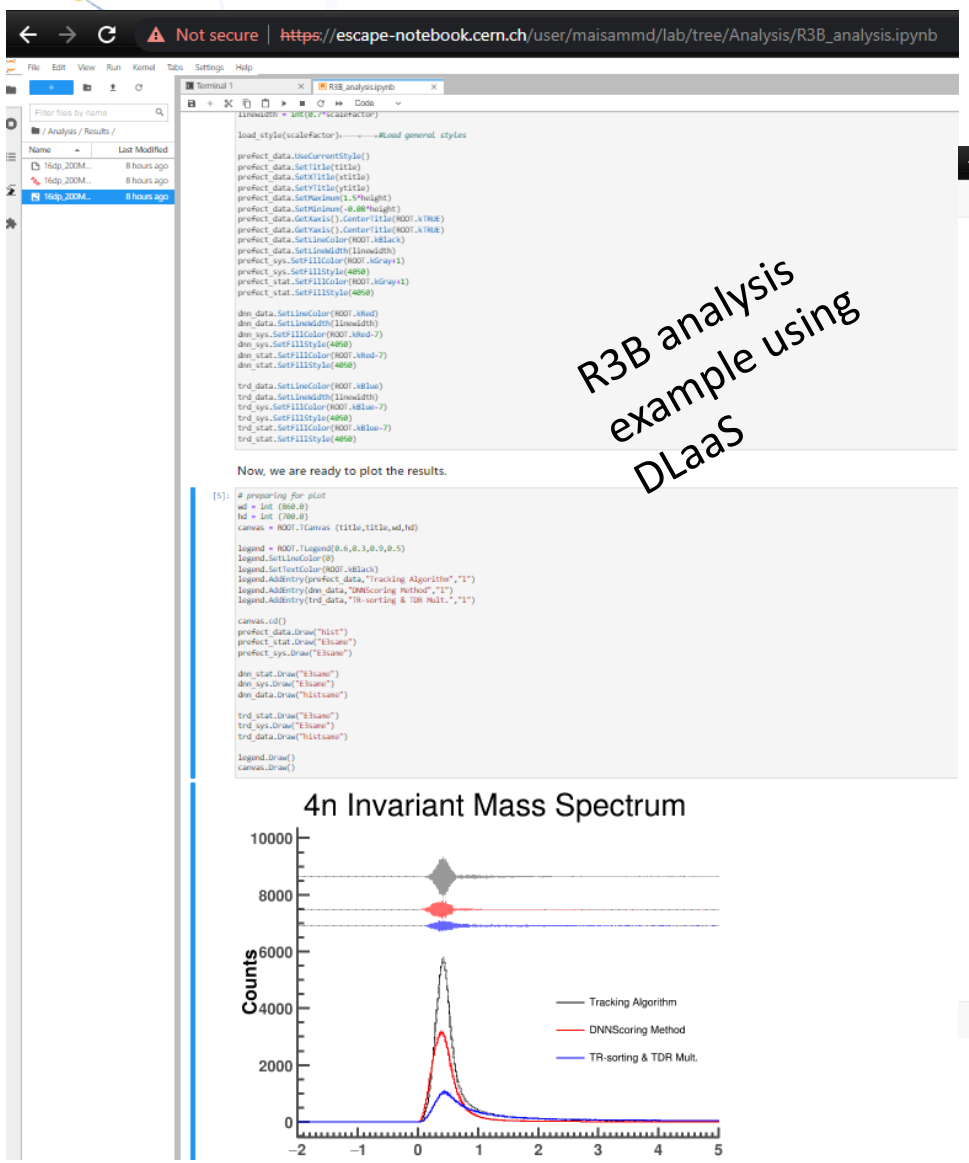
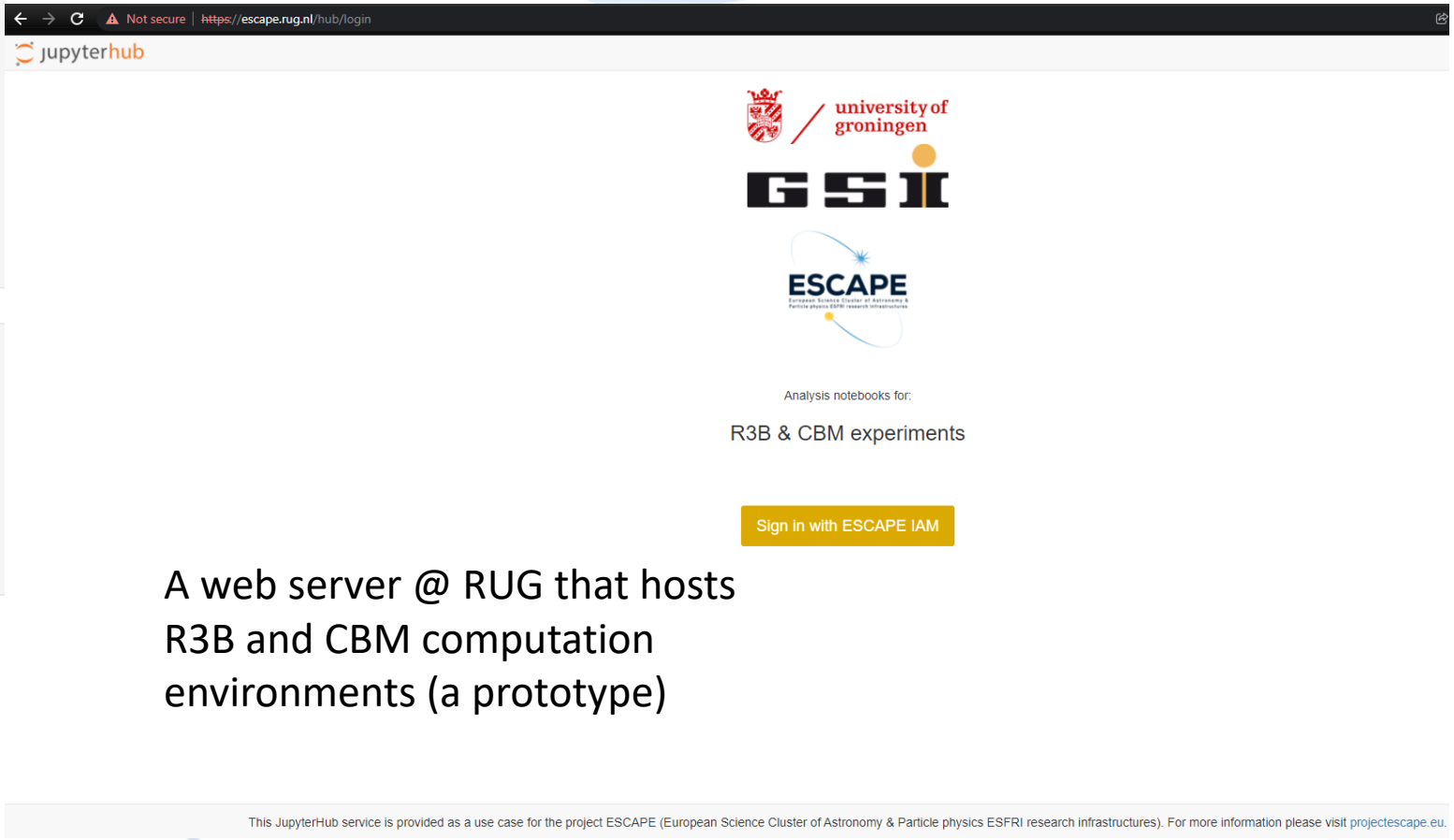
Summary





A web server @ RUG that hosts R3B and CBM computation environments (a prototype)

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Summary

- Issues with the portability & reusability of R3BRoot software stack were resolved using containers
- R3BRoot was Inetegrated with an Interactive analysis interface (Jupyter Lab)
- Deployed as a web application to ensure findability & accessibility of the software and the data
- The ESCAPE Data lake proved that it can be a solution to tackle big data challenges
- Still a lot of effort needs to be made to make data and software FAIR
- Making a sutainable and federated ecosystem for research data under EOSC is still a big challenge but moving forward.

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Thank you!
&
Questions!

'Research is born free and everywhere is in chains'

(apologies to Rousseau)

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Future of ESCAPE & EOSC

- **ESCAPE intends to remain as a collaboration after the end of the current project**

→ Sustained thematic consortium for the sustainability of EOSC

→ Additional thematic RI's are interested in participating

- **Many potential collaborative actions**

→ Data Management at Exascale

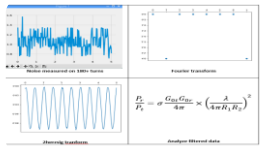
→ Common software challenges

→ Cross-fertilisation of software tools and services

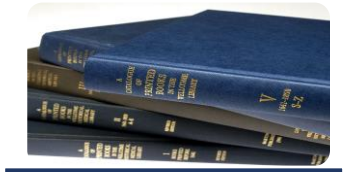
→ Building a platform for multi-messenger astronomy and cross-domain collaborations

→ Connection of data infrastructure to heterogeneous computing

Services for integration of the Exabyte scale data infrastructure supporting Open Science and FAIR data



Interoperable data-analysis platform



Development and sustainability of the services for the software catalogue and workflow

Partnership with EuroHPC/Prace/FENIX to provide the services for integration of Data-Lake with HPC resources

Collaborative scientific environment. Include new ESFRI and SME

Global integration of some of the above with global partners in USA, Australia and Africa

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Future of ESCAPE & EOSC

EOSC-Future

Five thematic Science Clusters (80% of ESFRI RIs)

EOSC FUTURE

INFRAEOSC-07 Projects

EUROPEAN OPEN SCIENCE CLOUD

EuroHPC Joint Undertaking

PRACE PARTNERSHIP FOR ADVANCED COMPUTING IN EUROPE

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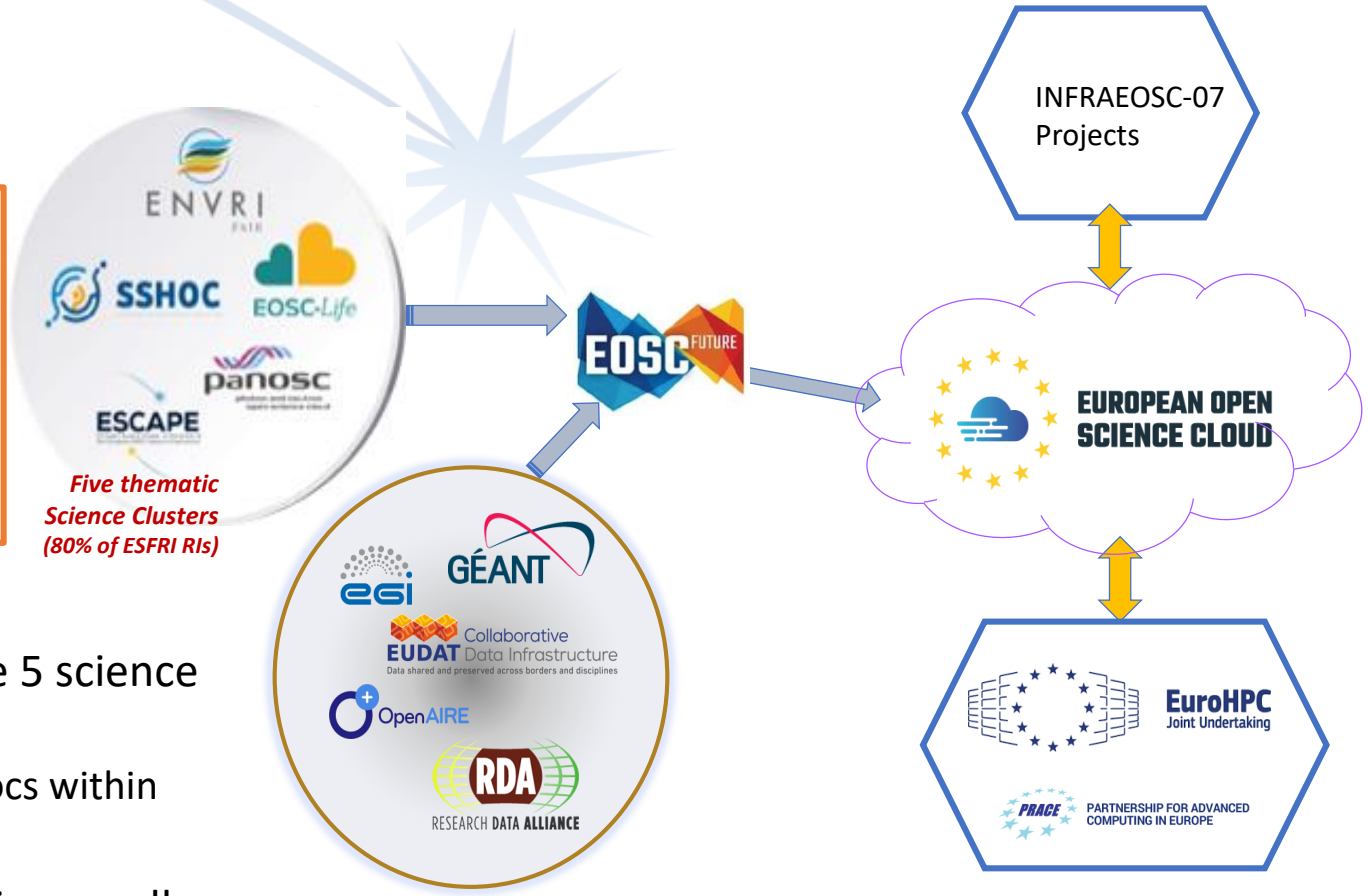
Future of ESCAPE & EOSC

EOSC-Future

- Project – started 1st April;
- Responding to EU H2020 funding call, (INFRAEOSC-03-2020): 30 months, 40 M euros

➢ ***EOSC-Future is a prototype of an integrated EOSC***



- WP6 (T6.3) includes 2 science projects from each of the 5 science clusters
  - Several partners from ESCAPE have funding for 6 post-docs within that to work on the TSP's
- ESCAPE (with other clusters & e-infras) is also involved in overall Technical Coordination of EOSC-Future
  - Specific actions around portal integration, work with HPC community, etc

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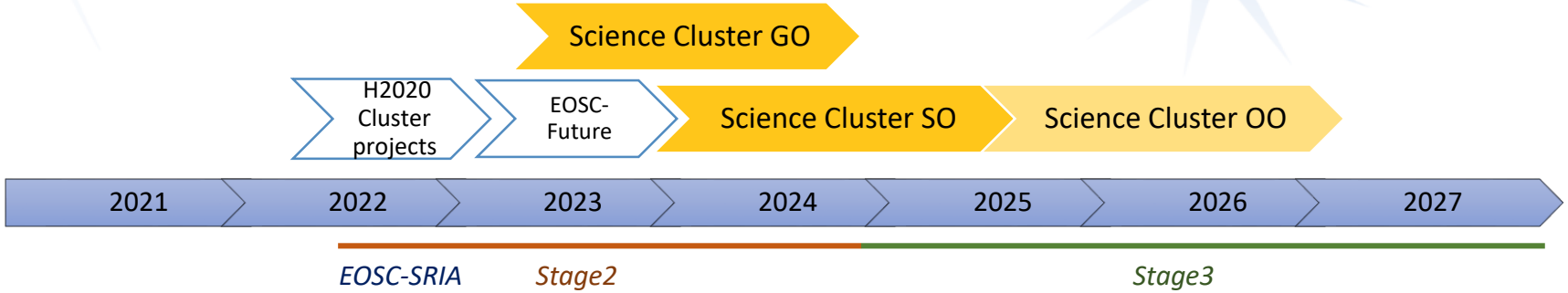
A work plan for the future of the Science Clusters

There is a prompt need and opportunity to support the Science Clusters further (in 2022-2025) within **Horizon Europe framework**



H2020 and potential **Horizon Europe** funded actions (*aligned with the EOSC-SRIA* Stage2 -to- Stage3*)

General Objectives (**GO**):
- consolidation of thematic data infrastructures (cluster VREs, platforms and a "few core services") as parts of a federation.

Specific Objectives (**SO**):
- relevant scientific results from clusters;
- increased number of RIs;
- enhance researchers uptake of OS and widening dimension.

Operational Objectives (**OO**):
- sustainable operation of the deployed cluster as a "platform infrastructure";
- continuous promotion, extension and hosting of inter-domain FAIR Science Projects (new Open Science Objectives).

*Strategic Research and Innovation Agenda

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Recap

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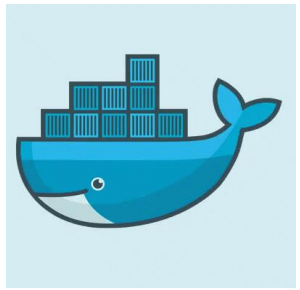
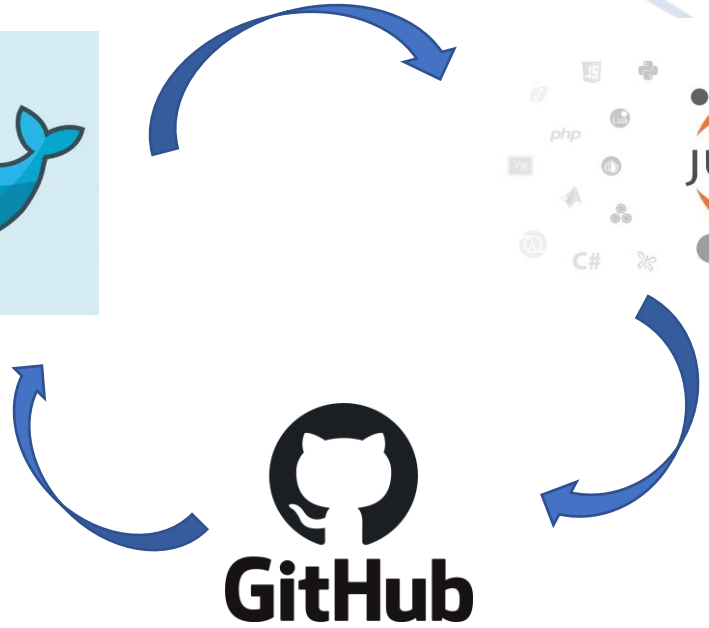


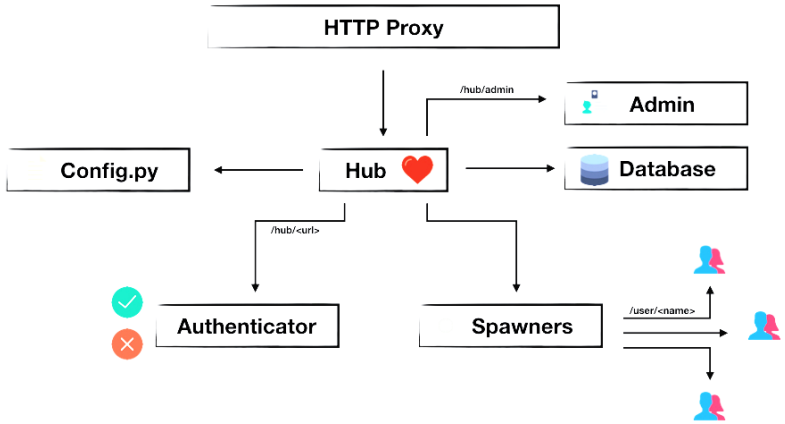


A version control system for software with a free online repository

A **Web IDE** for **live code**, equations, **visualizations** and **narrative text (Jupyter Notebook)**

Brings the power of **notebooks** to **groups of users** & handles users access to **computational environments** and ... **(Jupyter Hub)**

JupyterHub



- Reusability
- Accessibility
- Interoperability
- Portability
- Micro services & Scaling

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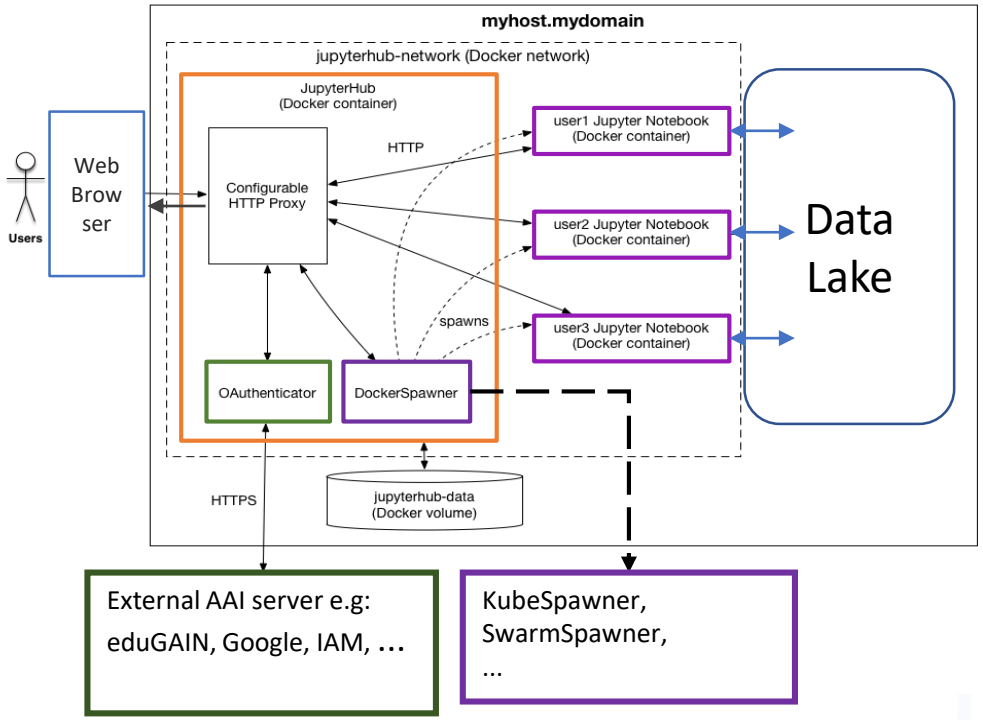
Demo!

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

The prototype of the R3B interactive data analysis (IDA)

- Tested the alpha version on the cloud
- Integrated with an OIDC AuthN/Z (Github)
- Tested connecticity and R/W to the data lake (X509)



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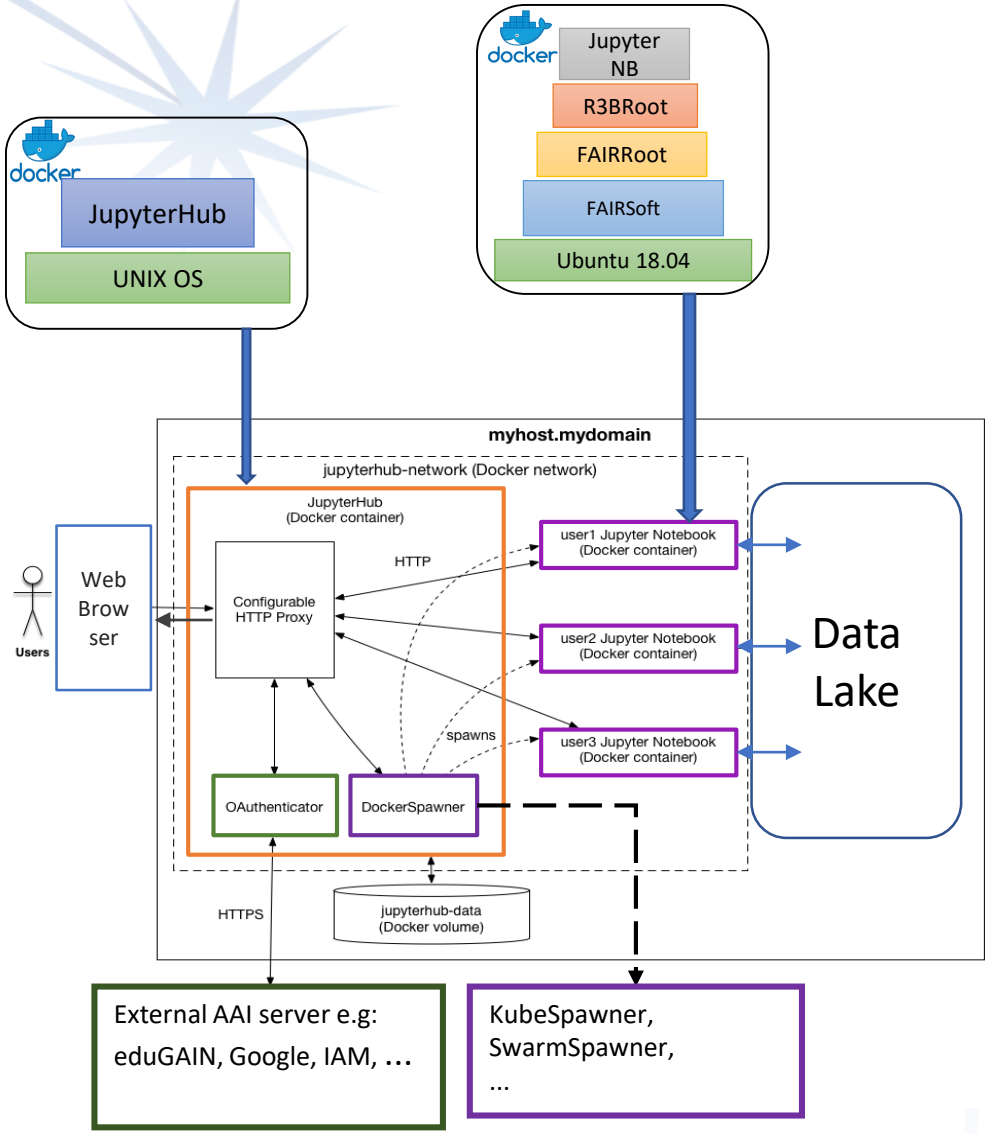

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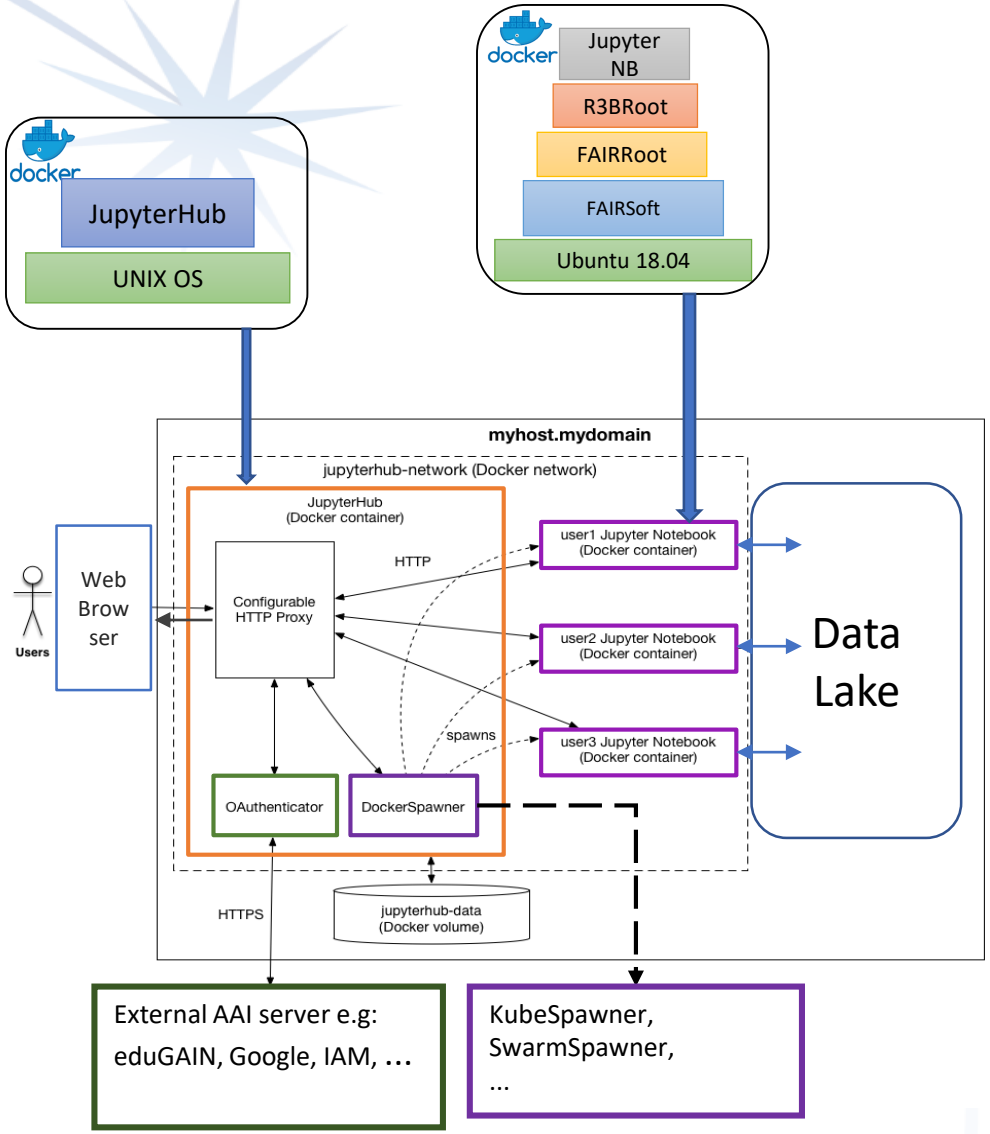
The prototype of the R3B interactive data analysis (IDA)

- Tested the alpha version on the cloud
- Integrated with an OIDC AuthN/Z (Github)
- Tested connecticity and R/W to the data lake (X509)

Things that needed to be improved:

- Not in standard Python environment (CONDA)
- Not ready to be in production (scalability)
- Not integrated with ESCAPE AuthN/Z (IAM)
- Manual settings to access to the Data Lake (DL)



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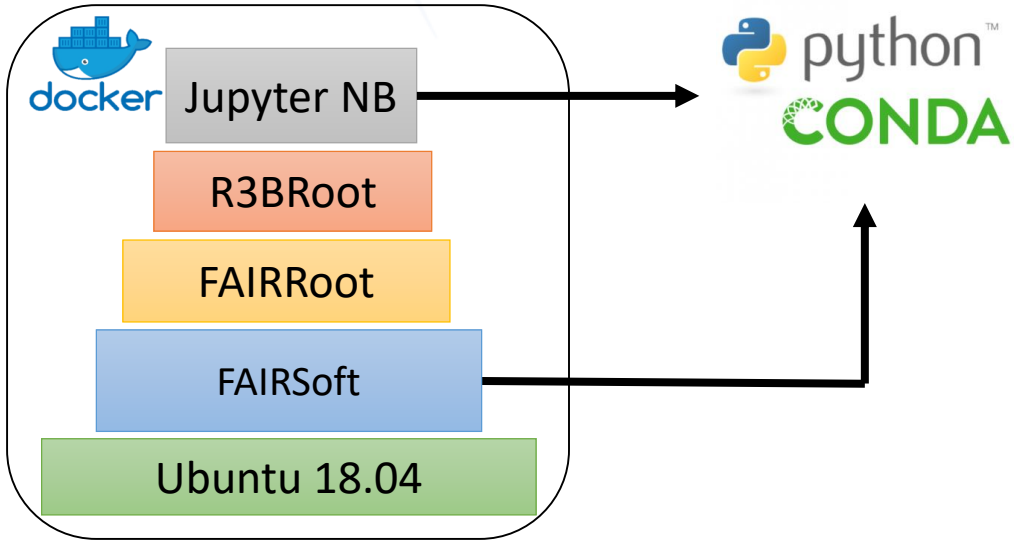
Latest progress

✓ **Standard Python environment**



- New FAIRSoft (some bug are fixed)
- PyRoot and Jupyter NB use the same python version (ensure compatibility)
- Docker images are made for each part (can be used in other FAIR projects)
- Some security issues were resolved (root access limited)

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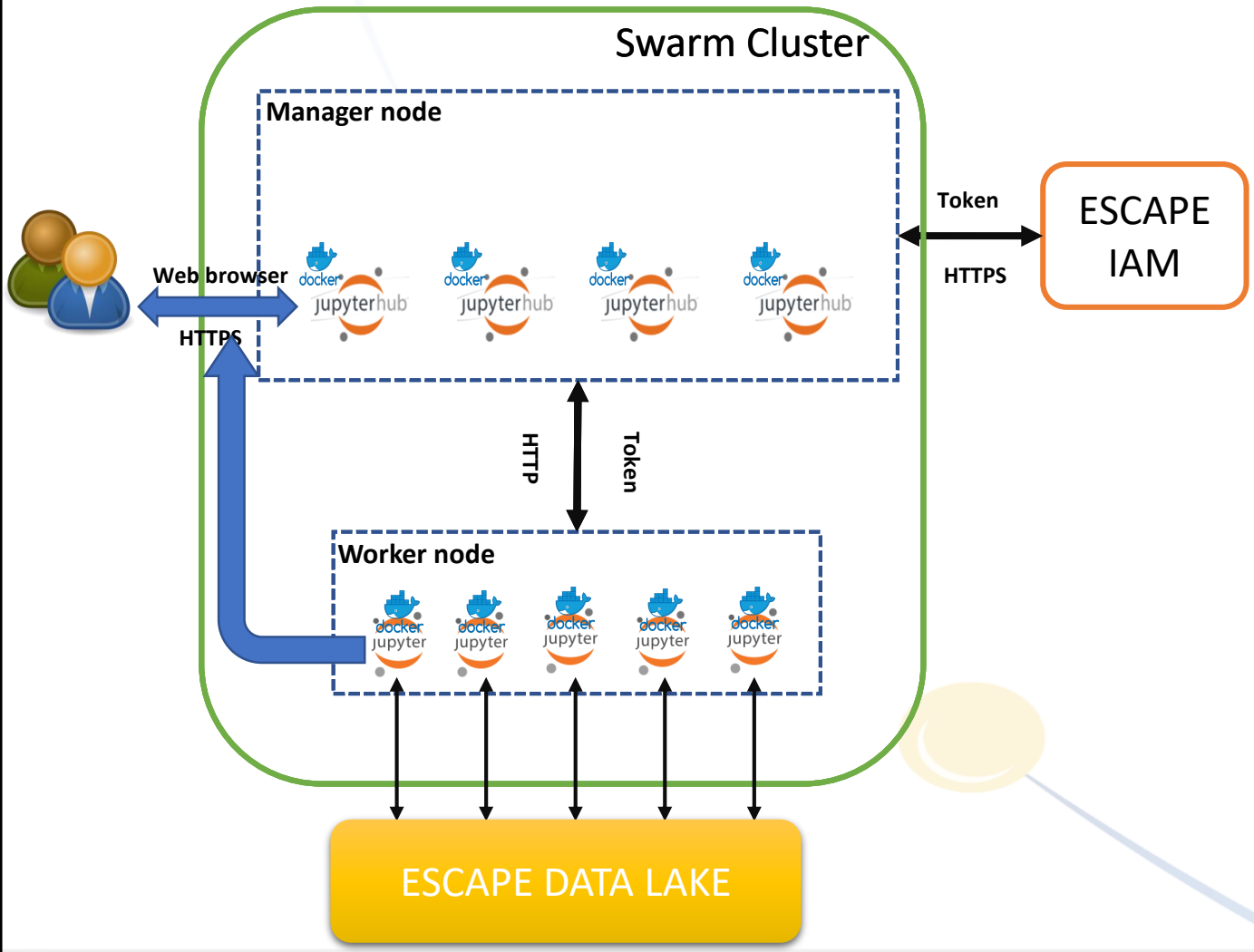
✓ **Ready to be deployed in production (scalability)**



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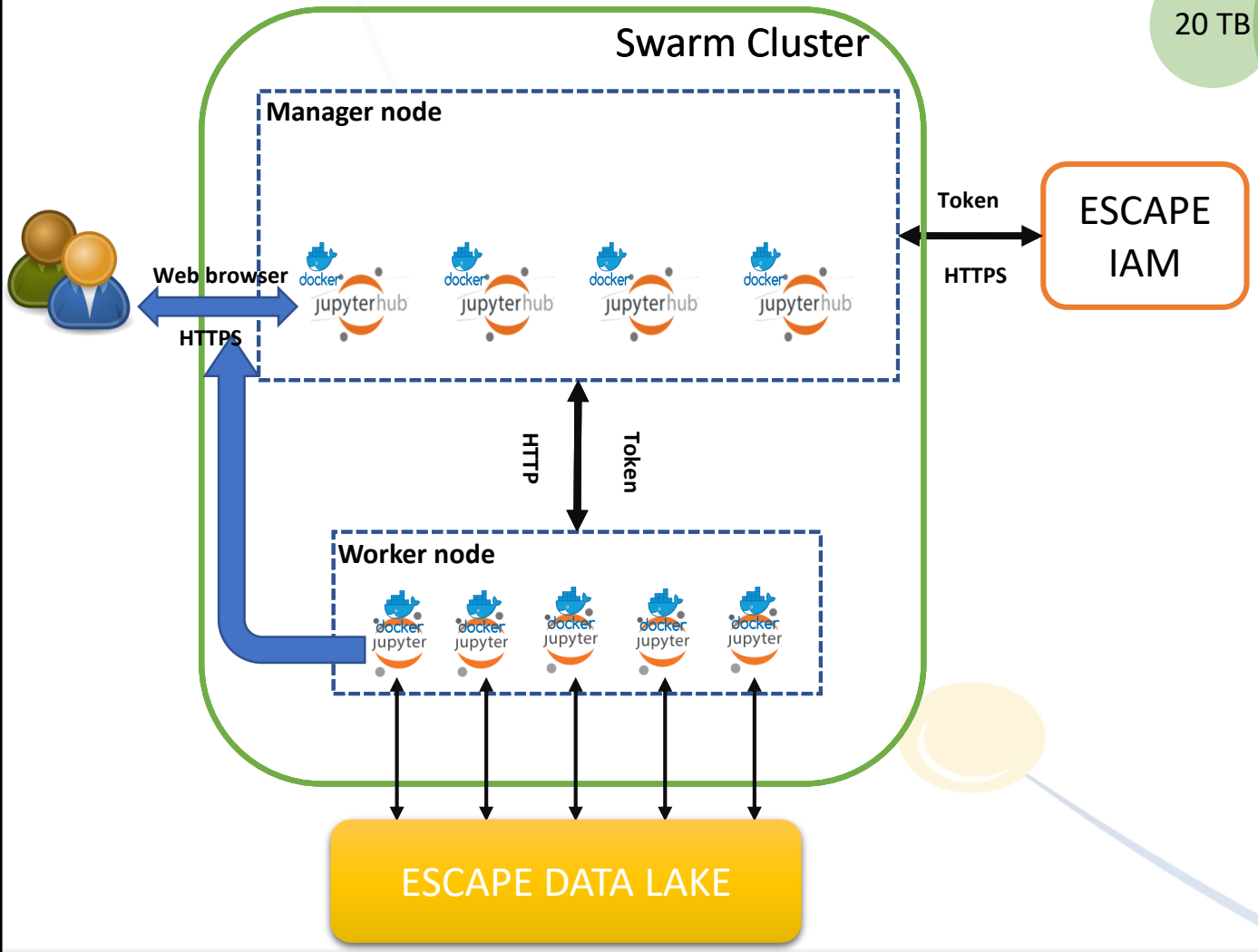
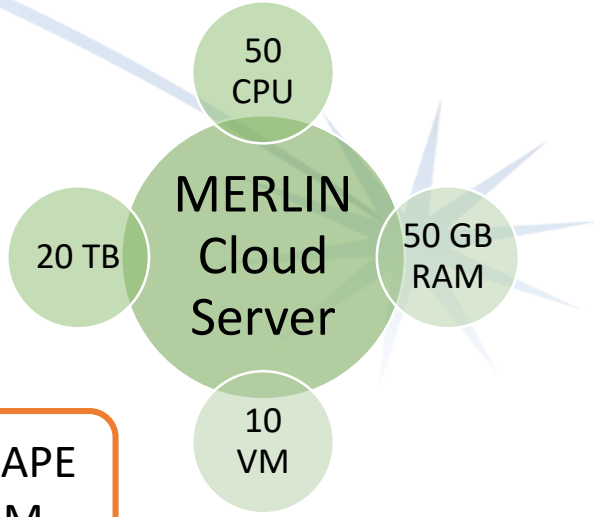
Latest progress

✓ **Ready to be deployed in production (scalability)**





- The JupyterHub works in a different node (higher performance)
- It is scalable
- More security settings were added to the JupyterHub

https://escape.rug.nl

- A token propagation mechanism needs to be added
- Local storage per user needs to be assigned
- End-to-end AuthN/Z needs to be enabled for the data lake

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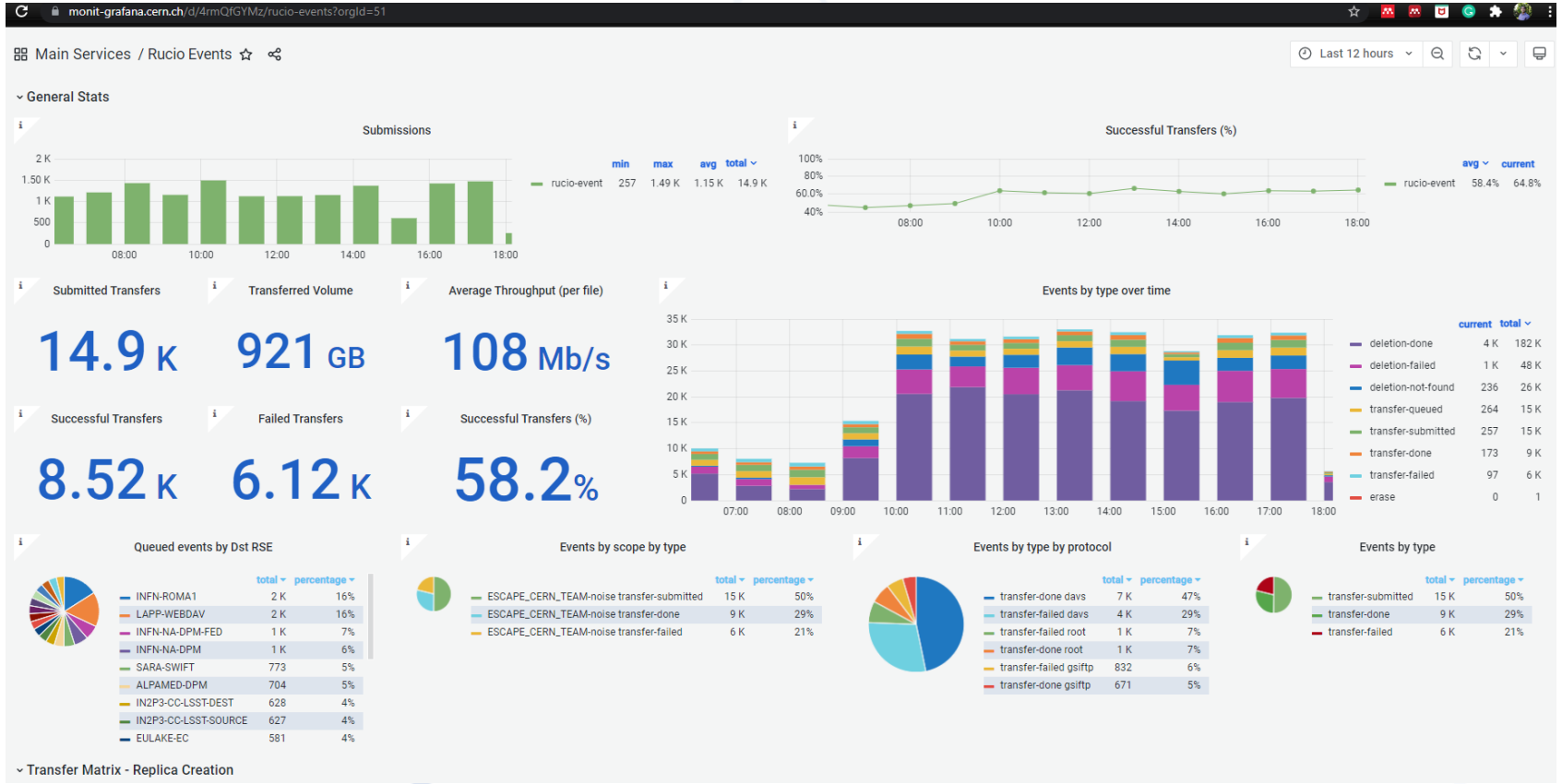
Monitoring of the Data Lake

- Track all the task related to DL
- Show all the informations of data transfering rates
- Health check of RSEs
- ....

https://monit-grafana.cern.ch/



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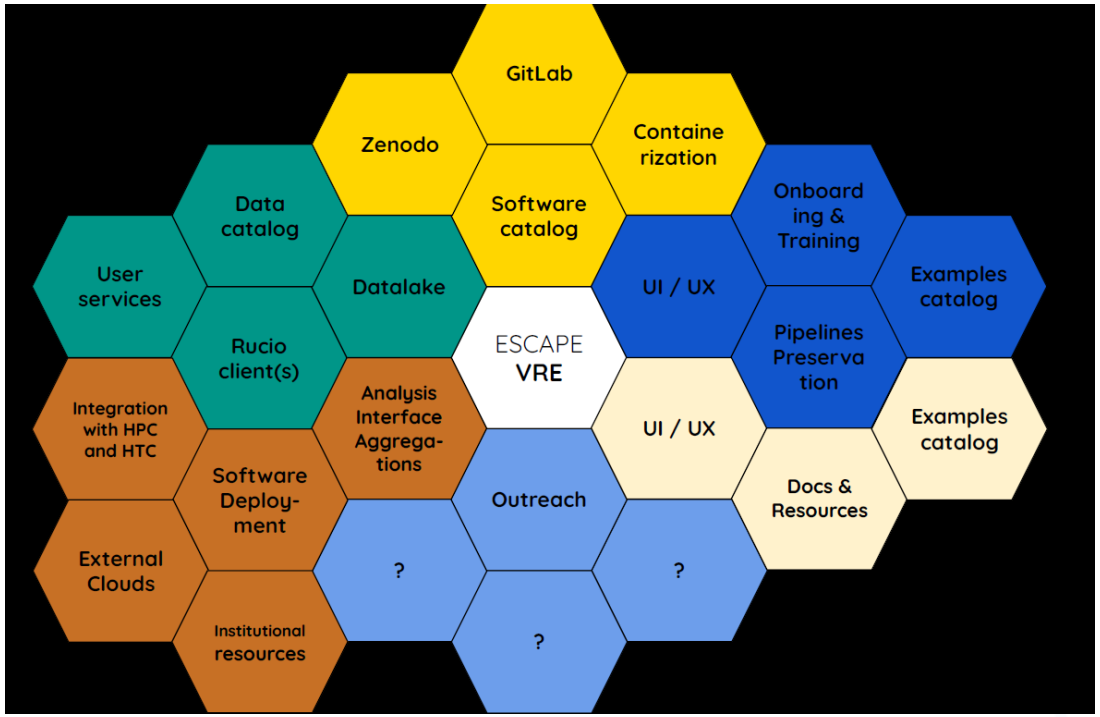
Virtual Research Enviroment (VRE)

https://escape2020.pages.in2p3.fr/virtual-environment/home/

An exercise to imagine how current resources can be aggregated so as to be reachable and use from a single entry point

- Simple User Onboarding
- Good UI/UX as an essential component
- Scalability
- CI/CD by default
- Portability



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DAC21: Data and Analysis Challenge (November 2021):

The aim is to finish the prototype evaluation by the end of the year.

Goals:

- Run production Data Management, Processing and Analysis workloads
  - Data Management: acquisition, injection, replication, lifecycles
  - Data Processing: Production
  - Data processing: User Analysis. Use cases
- Demonstrate Data Lake orchestration layer sustainability after ESCAPE (towards EOSC)
  - Leverage, integrate and use experiment and site's dedicated installations, e.g. RUCIO and FTS.
  - Demonstrate integration and interplay of these several instances in a common Data Lake/storage infrastructure.
- End-to-End AAI
  - Assessment ranging from experiments experts, to advanced users to newcomers and to sporadic web-based access.
  - Token-based Authentication.

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Future of ESCAPE & EOSC

- **ESCAPE intends to remain as a collaboration after the end of the current project**

→ Sustained thematic consortium for the sustainability of EOSC

→ Additional thematic RI's are interested in participating

- **Many potential collaborative actions**

→ Data Management at Exascale

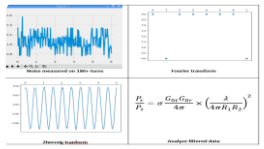
→ Common software challenges

→ Cross-fertilisation of software tools and services

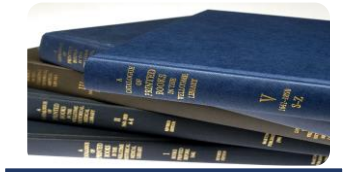
→ Building a platform for multi-messenger astronomy and cross-domain collaborations

→ Connection of data infrastructure to heterogeneous computing

Services for integration of the Exabyte scale data infrastructure supporting Open Science and FAIR data



Interoperable data-analysis platform



Development and sustainability of the services for the software catalogue and workflow

Partnership with EuroHPC/Prace/FENIX to provide the services for integration of Data-Lake with HPC resources

Collaborative scientific environment. Include new ESFRI and SME

Global integration of some of the above with global partners in USA, Australia and Africa

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Future of ESCAPE & EOSC

EOSC-Future

Five thematic Science Clusters (80% of ESFRI RIs)

EOSC FUTURE

INFRAEOSC-07 Projects

EUROPEAN OPEN SCIENCE CLOUD

EuroHPC Joint Undertaking

PRACE PARTNERSHIP FOR ADVANCED COMPUTING IN EUROPE

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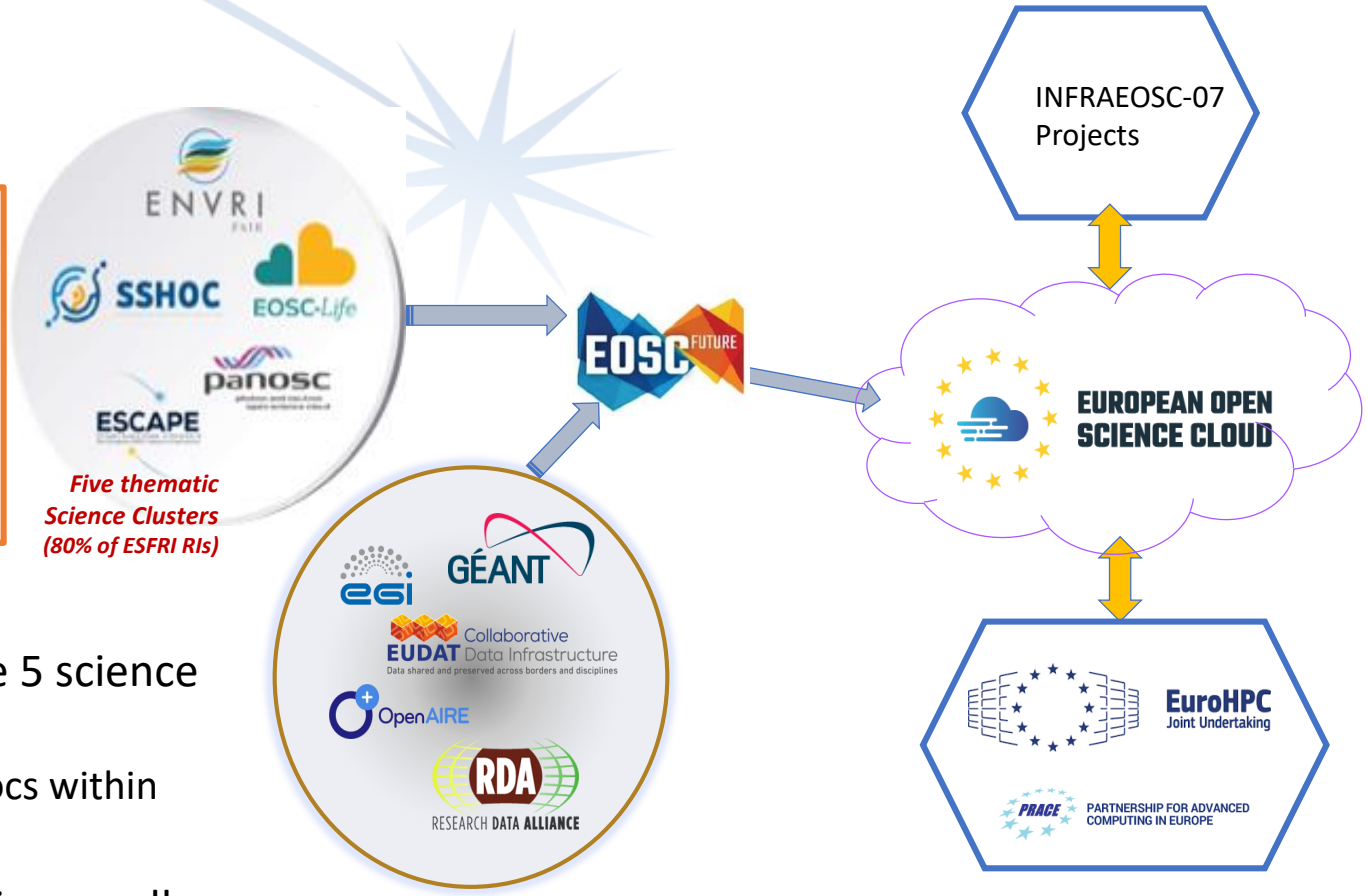
Future of ESCAPE & EOSC

EOSC-Future

- Project – started 1st April;
- Responding to EU H2020 funding call, (INFRAEOSC-03-2020): 30 months, 40 M euros

➢ ***EOSC-Future is a prototype of an integrated EOSC***



- WP6 (T6.3) includes 2 science projects from each of the 5 science clusters
  - Several partners from ESCAPE have funding for 6 post-docs within that to work on the TSP's
- ESCAPE (with other clusters & e-infras) is also involved in overall Technical Coordination of EOSC-Future
  - Specific actions around portal integration, work with HPC community, etc

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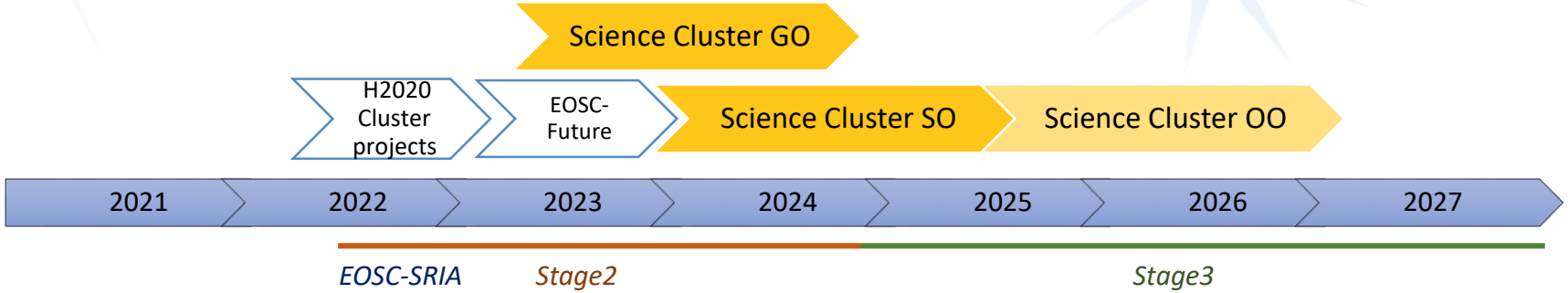
A work plan for the future of the Science Clusters

There is a prompt need and opportunity to support the Science Clusters further (in 2022-2025) within **Horizon Europe framework**



H2020 and potential **Horizon Europe** funded actions (*aligned with the EOSC-SRIA* Stage2 -to- Stage3*)

General Objectives (**GO**):
- consolidation of thematic data infrastructures (cluster VREs, platforms and a "few core services") as parts of a federation.

Specific Objectives (**SO**):
- relevant scientific results from clusters;
- increased number of RIs;
- enhance researchers uptake of OS and widening dimension.

Operational Objectives (**OO**):
- sustainable operation of the deployed cluster as a "platform infrastructure";
- continuous promotion, extension and hosting of inter-domain FAIR Science Projects (new Open Science Objectives).

*Strategic Research and Innovation Agenda

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Next steps

Priority 1

- Finalizing the configuration of DL (FAIR & CERN)
- Testing the Beta version of the JHub service
- Cooperating in the relevant task forces of DAC21 (in harmony with GSI)

Priority 2

- Integration the JHub platform with token based IAM
- Integration with ESAP (ESCAPE Science Analysis Platform)
- Put & test Release Candidate (RC) version of our service in production.

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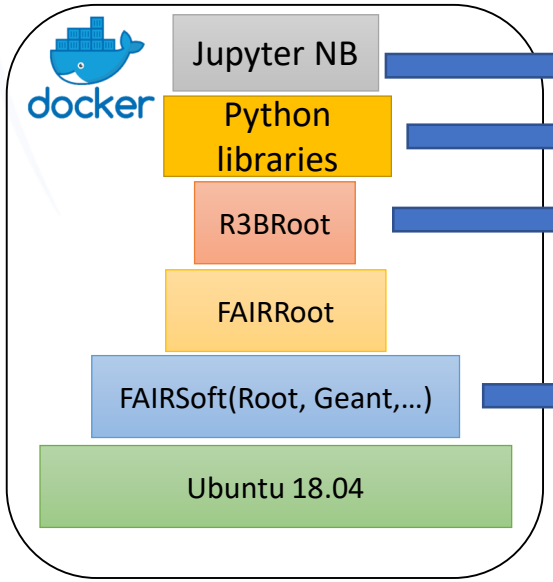
R3B-NeuLAND

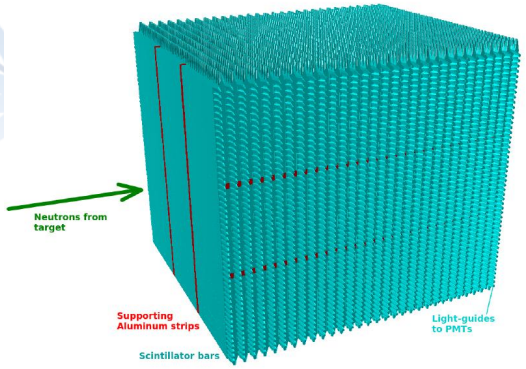


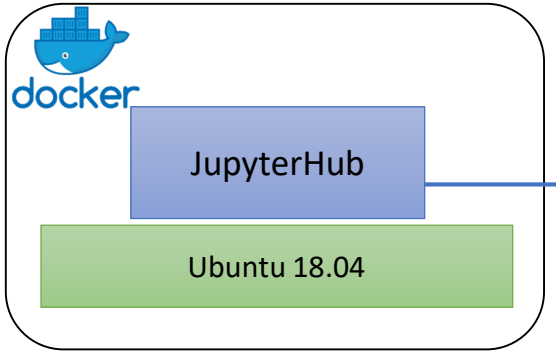
Configured JNB

Numpy, TensorFlow, Keras,...

Made compatible with Docker container needs

Python2 -> Python3





All the necessary configurations for the web server:

- AuthN & AuthZ
- Spawning
- Proxy settings
- ...

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RUCIO for Data management

Findable:

- Globally unique and persistent identifier
- Indexed in a searchable resource

Accessible:

- Retrievable by their identifier using a standardised communications protocol
- Support AuthN/Z if necessary

Interoperable:

- Formal, accessible, shared, and broadly applicable language

Reusable:

- Clear and accessible data usage license
- Associated with detailed provenance

SCIENTIFIC DATA MANAGEMENT

RUCIO

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Next steps

- Finilizing configuration of the data-lake VMs on MERLIN
- Orchestrating all the VMs (Kubernetes maybe!)
- Doing a connection test for data-lake between RUG & GSI
- Configuring RUCIO on JupyterLab
- Test GUI prototype of the R3B-NeuLAND simulation software (Using JupyerLab widgets!).

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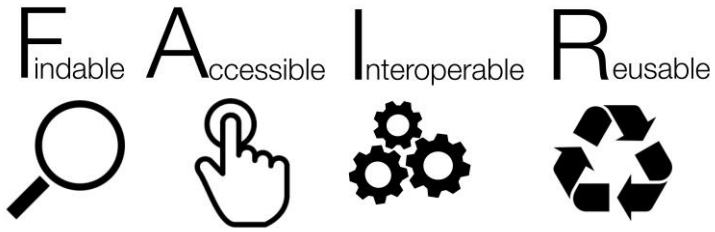
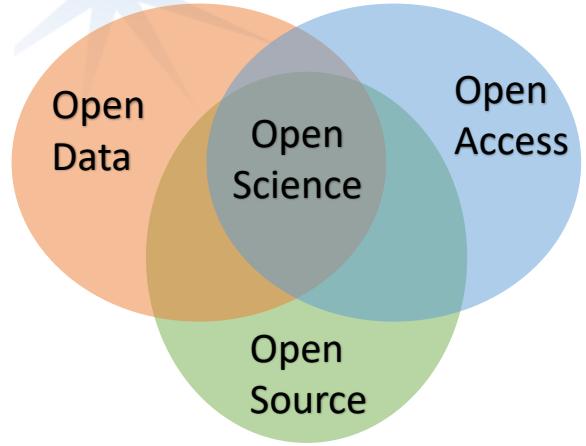
Introduction





1. When scientists share knowledge and resources their results improve people's lives.

2. Scientists need easy access to state-of-the-art infrastructures to test their ideas.

3. Avoiding unnecessary duplication of efforts

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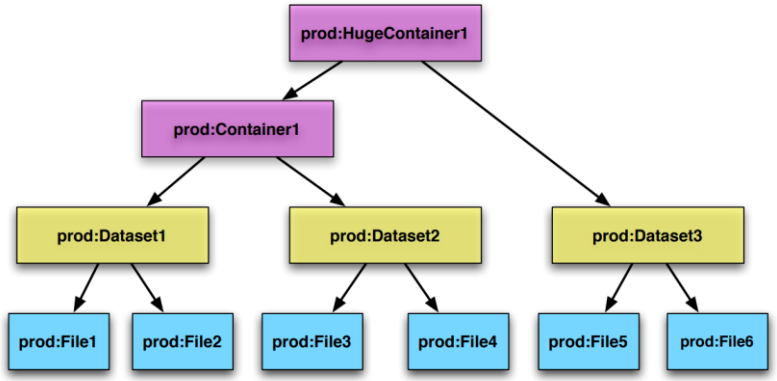
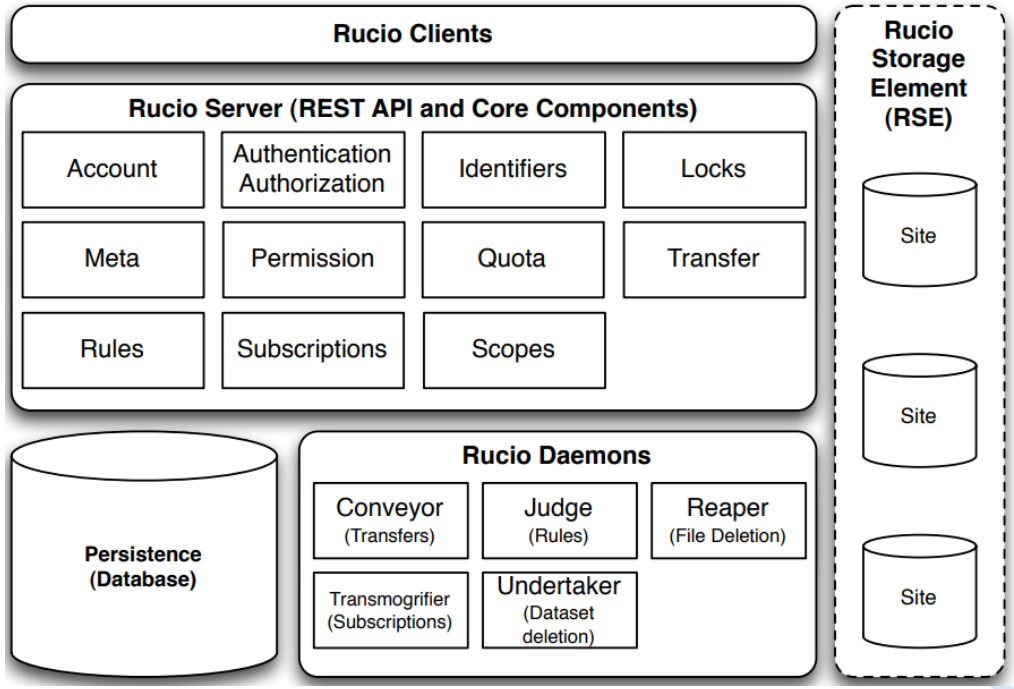
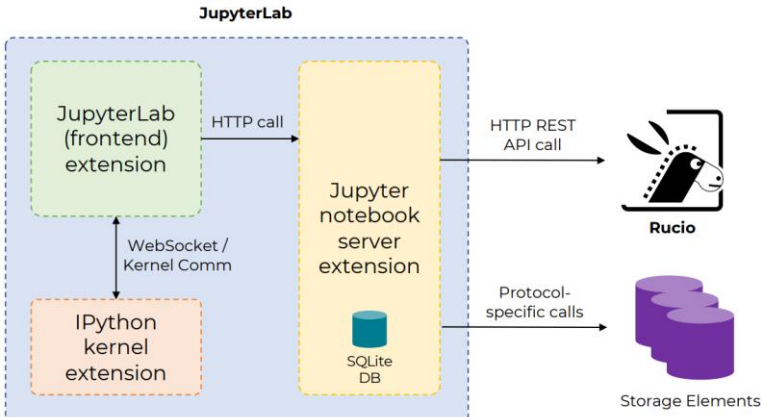
FAIR & Data management





SCIENTIFIC DATA MANAGEMENT

RUCIO



RUCIO Jupyterlab extension

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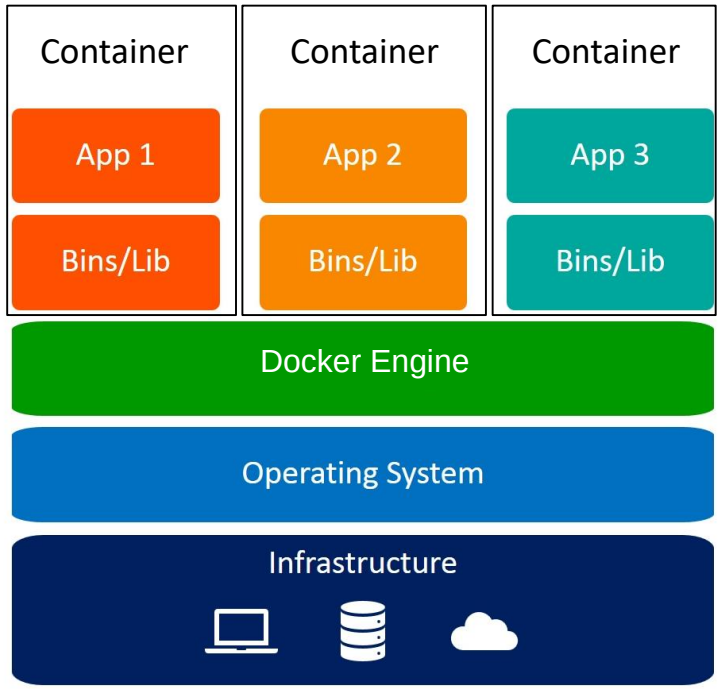
ESCAPE Science Analysis Platform (ESAP)

A standard OS-virtualization platform for **packing up software** and all the **dependencies** to **run applications on different environments**.

Advantages:

- Lighter than VM (Mb << Gb)
- Higher performance (~seconds)
- Less resource utilization
- Portability
- Micro services & Scaling



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ESCAPE Science Analysis Platform (ESAP)

Jupyter Notebook (lab)

The Jupyter Notebook is an open-source **web application** that allows you to **create and share** documents that contain **live code**, **equations**, **visualizations** and **narrative text**.

JupyterHub

JupyterHub brings the power of **notebooks** to **groups of users**. It gives users access to **computational environments** and **resources without** burdening the users with **installation and maintenance tasks.**

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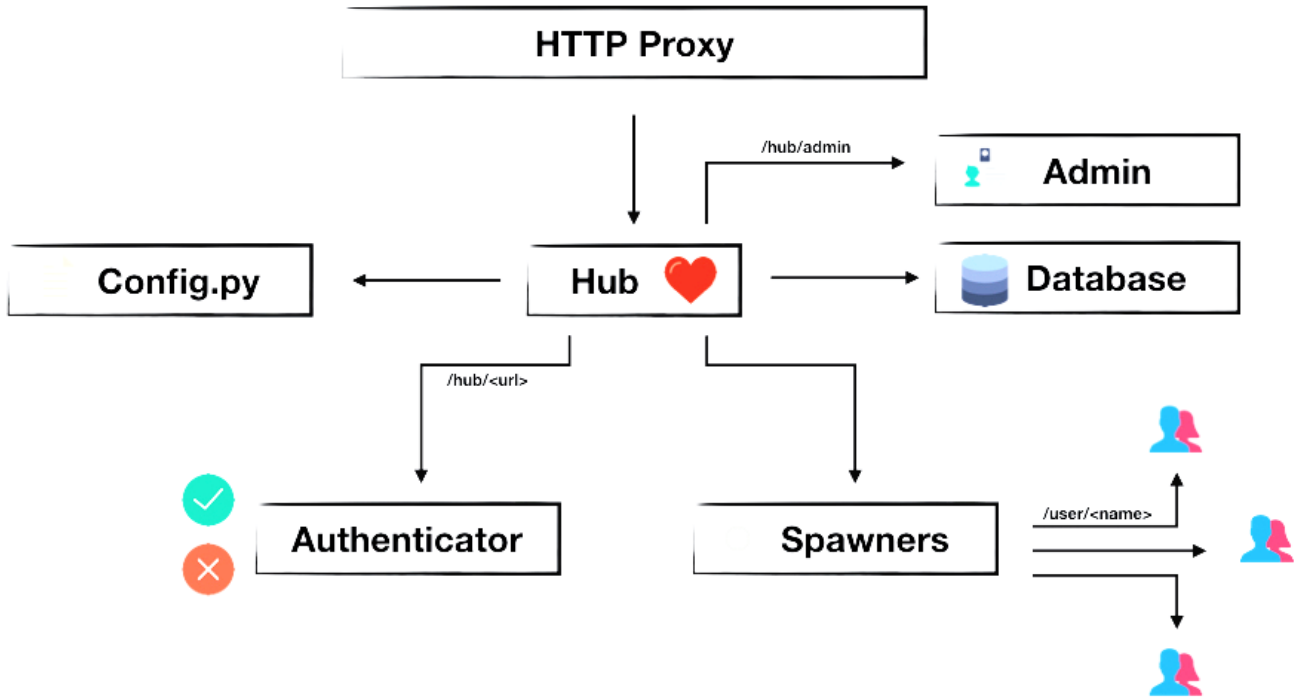
AAI and Spawning

JupyterHub



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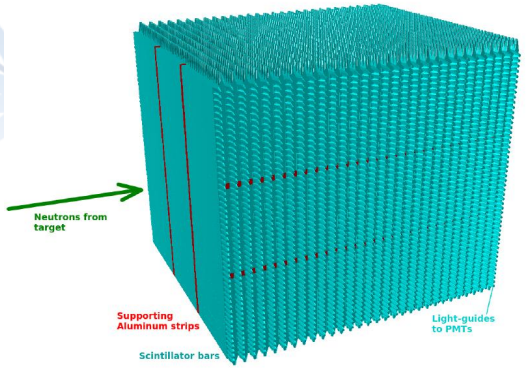
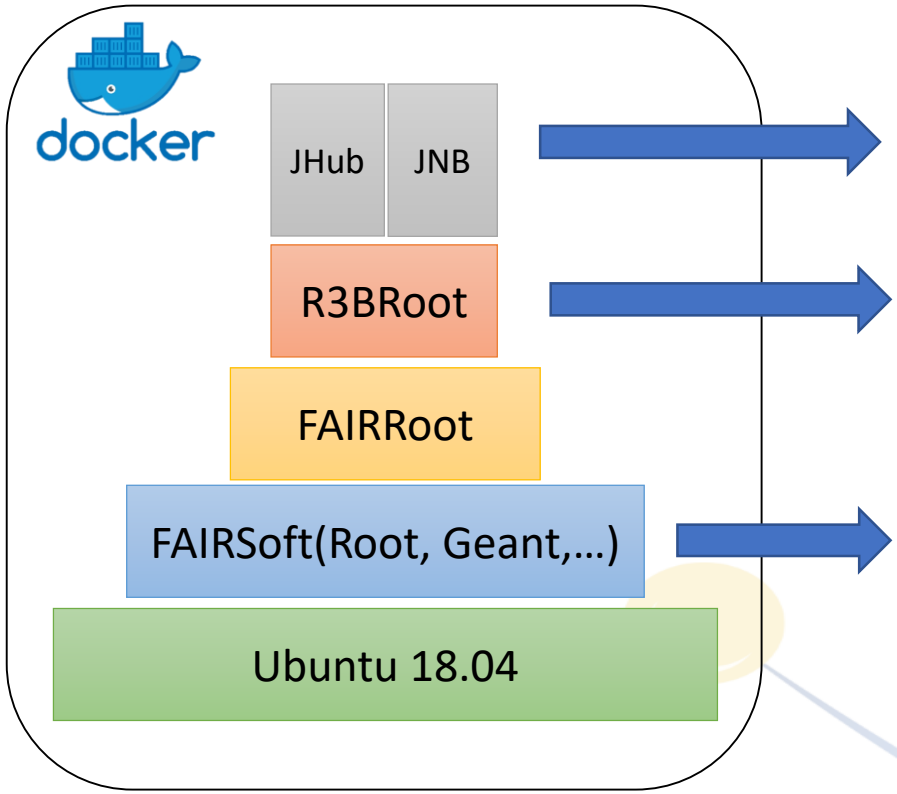
R3B-NeuLAND





Configured JHub and JNB

Made compatible with Docker container needs

Python2 -> Python3

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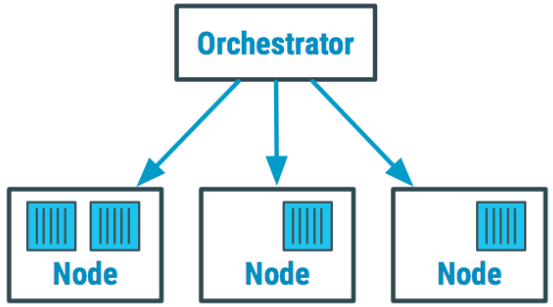
Spawning

Container Orchestration:



docker Compose

Orchestration on a single host

- No autho scaling
- Easy to start cluster
- Lower scalibility
- Limited API
- Suitable for small groups (<a few 100s)

docker SWARM

kubernetes

- Autho scaling
- Difficult to start cluster
- Higher scalibility
- All in All API
- Suitable for very large group

Orchestration on cluster

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Structure of ESCAPE

ESCAPE DIOS | Data Infrastructure for Open Science

ESCAPE OSSR | Open-source Scientific Software and Service Repository

ESCAPE VO | Virtual Observatory

ESCAPE SAP | Science Analysis Platform

ESCAPE CS | Citizen Science

- Distributed data management
- Keeps track of data locations
- Replication
- Metadata management
- Usage Logging
- Access to existing storage elements
- Definition of access control rules/systems

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Structure of ESCAPE

ESCAPE DIOS | Data Infrastructure for Open Science

WP2: **Design, implement, and operate a cloud of data services** for open access and open science supporting FAIR principles at the Exabyte scale.

ESCAPE OSSR | Open-source Scientific Software and Service Repository

WP3: Support for a sustainable **open-access repository** to **share scientific software and services** to the science community.

ESCAPE VO | Virtual Observatory

WP4: **Integrating** distributed infrastructures into one **single virtual astronomy** facility.

ESCAPE SAP | Science Analysis Platform

WP5: A **platform-service gateway** with the capability to **access and analyze data** from multiple collections, access ESFRIs' **software tools**, and bring their own **customized workflows**.

ESCAPE CS | Citizen Science

WP6: **Involving society** in the **scientific discoveries** of the **astronomy** and **subatomic** physics facilities in EOSC.

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Structure of ESCAPE

ESCAPE DIOS | Data Infrastructure for Open Science (WP2: EDIOS)

- Task 2.1 Data Lake infrastructure and federation services.
- Task 2.2 Data Lake orchestration service.
- Task 2.3 Integration with compute services.
- Task 2.4 Networking.
- Task 2.5 Authentication and authorization.

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Structure of ESCAPE

ESCAPE SAP | Science Analysis Platform

(WP5: ESAP)

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Structure of ESCAPE

ESCAPE SAP Science Analysis Platform (WP5: ESAP)

- **Task 5.1: Discovery and Staging**
  - This task will provide users of the **science platform** with the capability to access and combine data from **multiple collections** and stage that data for **subsequent analysis**.
- **Task 5.2: Software deployment and virtualization**
  - This task will incorporate the work on the software repository described in WP3 and focus on tools and services to **support the virtualization of relevant software packages and pipelines.**
- **Task 5.3: Analysis interfaces, work flows and reproducibility**
  - The analysis interface task combines a number of elements to form the **working surface for the user of the EOSC science platform**.
- **Task 5.4: Integration with HPC and HTC infrastructures**
  - Once data for analysis has been located and staged, and workflows have been defined, the next step is to **deploy those workflows on the underlying processing infrastructure**.

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Structure of ESCAPE

ESCAPE SAP Science Analysis Platform (WP5: ESAP)

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ESCAPE Science Analysis Platform (ESAP)

Software deployment & virtualization:

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ESCAPE Science Analysis Platform (ESAP)

Software deployment & virtualization:

Compatibility and portability issues

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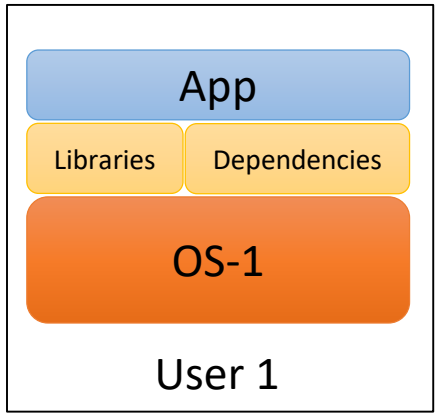
ESCAPE Science Analysis Platform (ESAP)

Software deployment & virtualization:

Compatibility and portability issues



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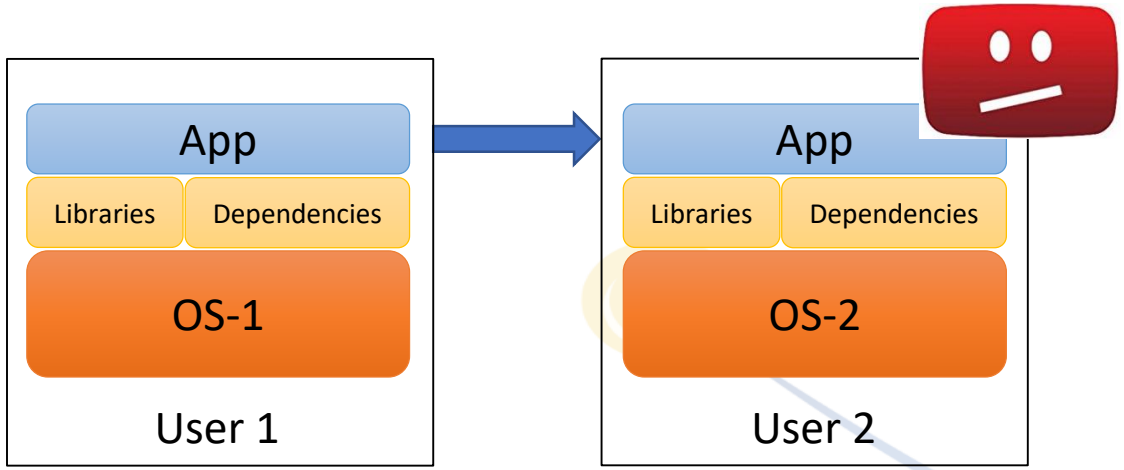
ESCAPE Science Analysis Platform (ESAP)

Software deployment & virtualization:

Compatibility and portability issues



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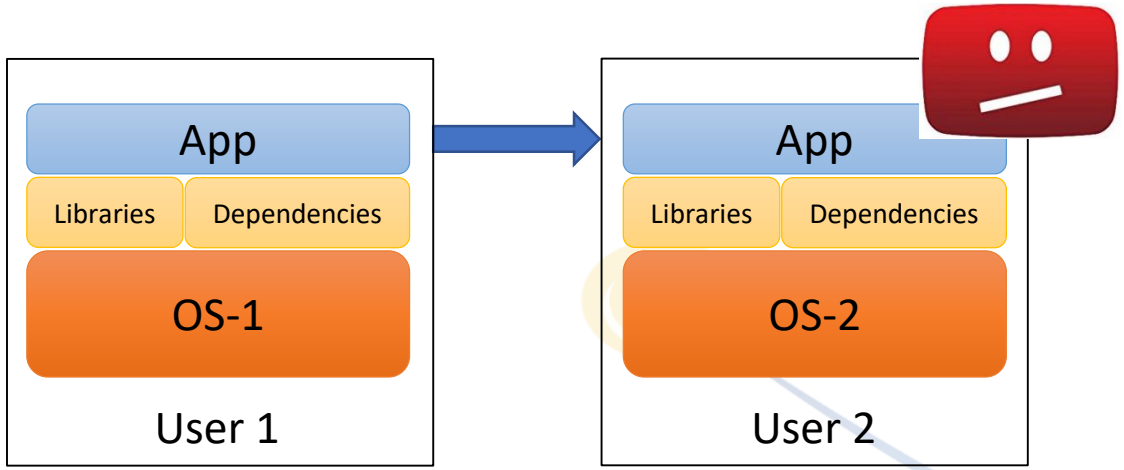
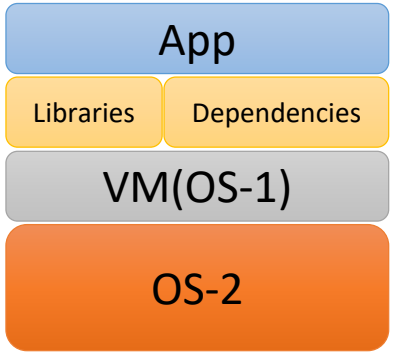
ESCAPE Science Analysis Platform (ESAP)

Software deployment & virtualization:

Compatibility and portability issues



Virtual Machine?!



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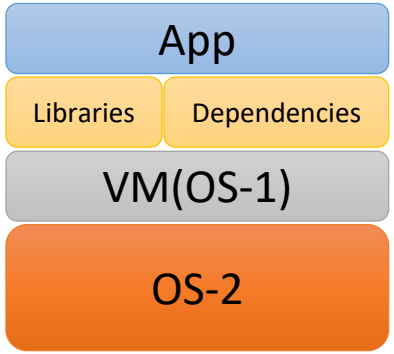
ESCAPE Science Analysis Platform (ESAP)

Software deployment & virtualization:

1. **Compatibility and portability issues**
2. **Configuration is time consuming**
3. **Scaling**
4. **Resource utilization**

Virtual Machine?!



User 2

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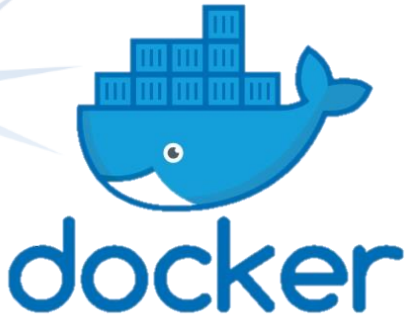
ESCAPE Science Analysis Platform (ESAP)

Software deployment & virtualization:

A standard OS-virtualization platform for **packing up software** and all the **dependencies** to **run applications on different environments**.



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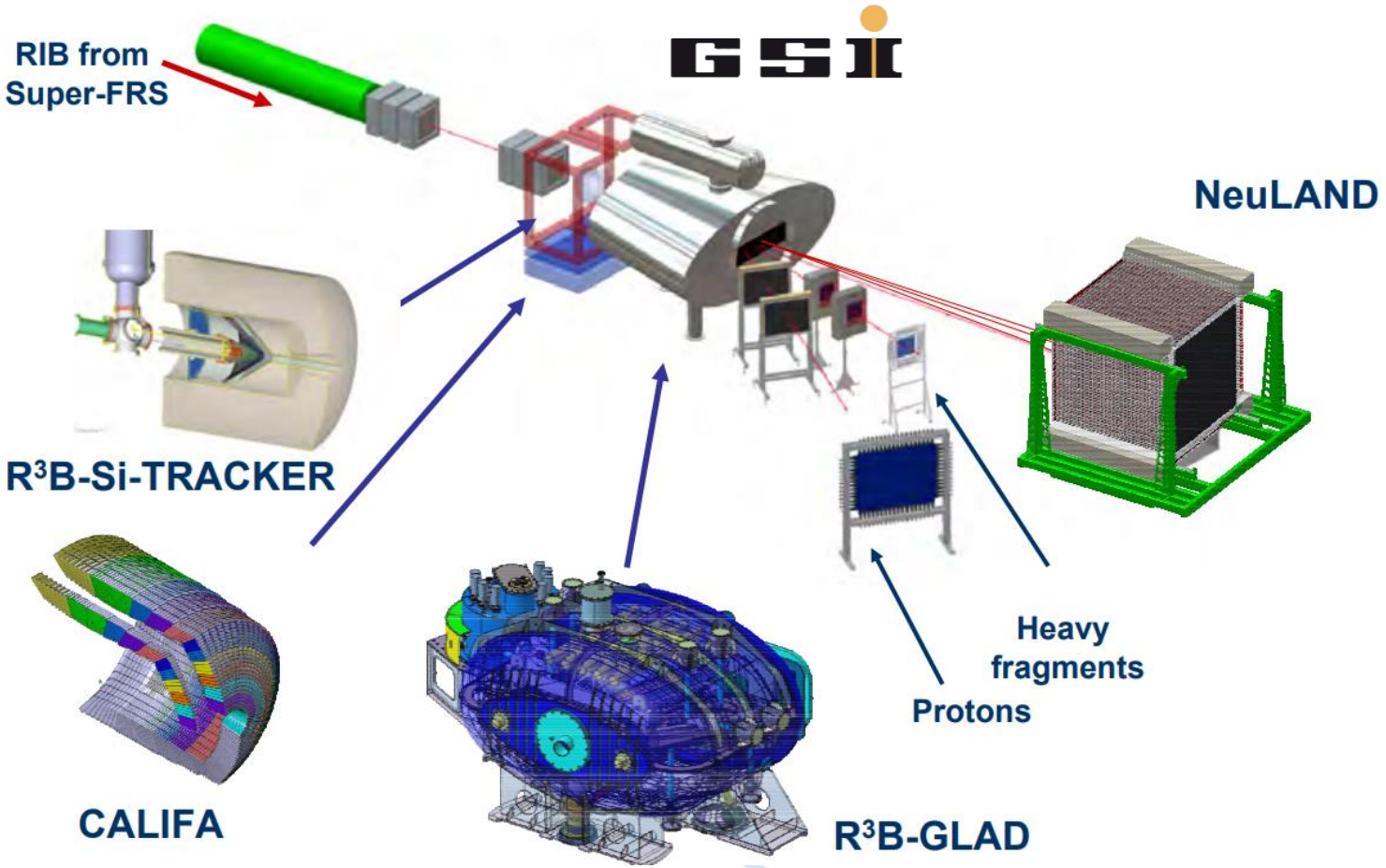
R3B-NeuLAND

R3B (**R**eactions with **R**elativistic **R**adioactive **B**eams)



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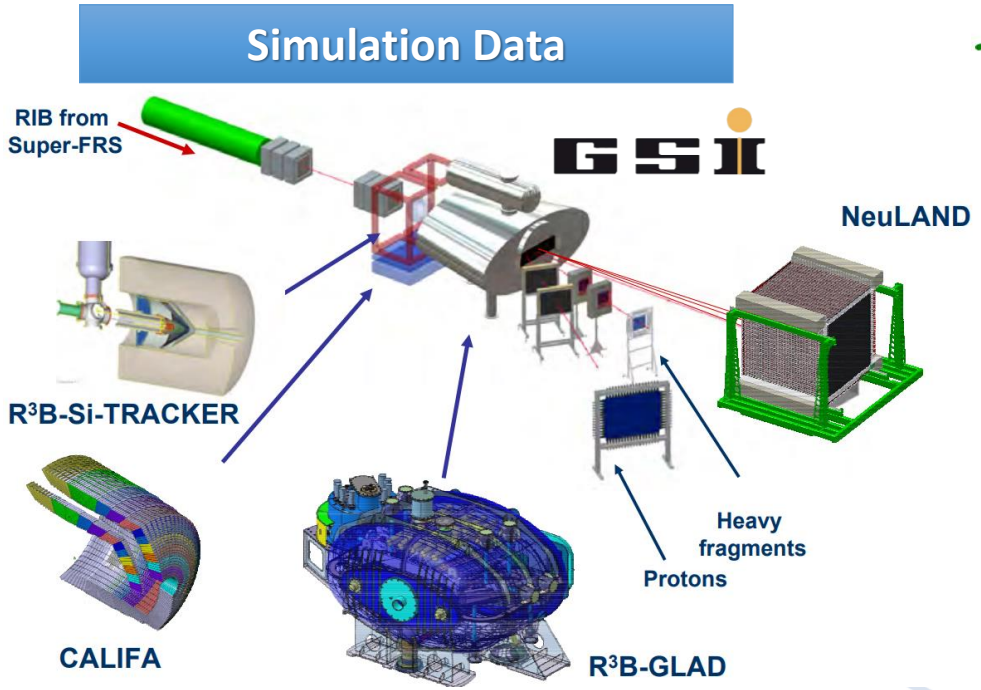
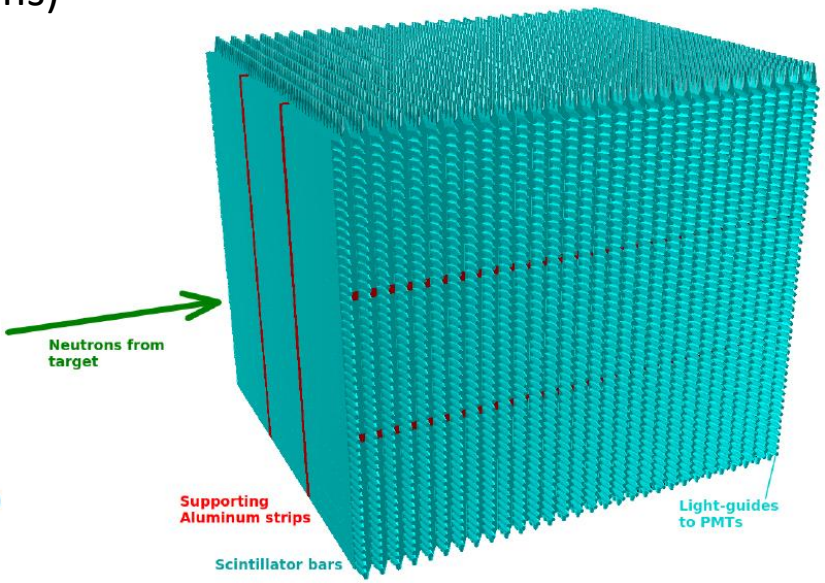
R3B-NeuLAND

R3B (**R**eactions with **R**elativistic **R**adioactive **B**eams)

- Multiplicity determination
- Shower head determination





- 30 doubleplane (dp)
- 100 V-H scintillators/dp
- 2.5*2.5 m^2

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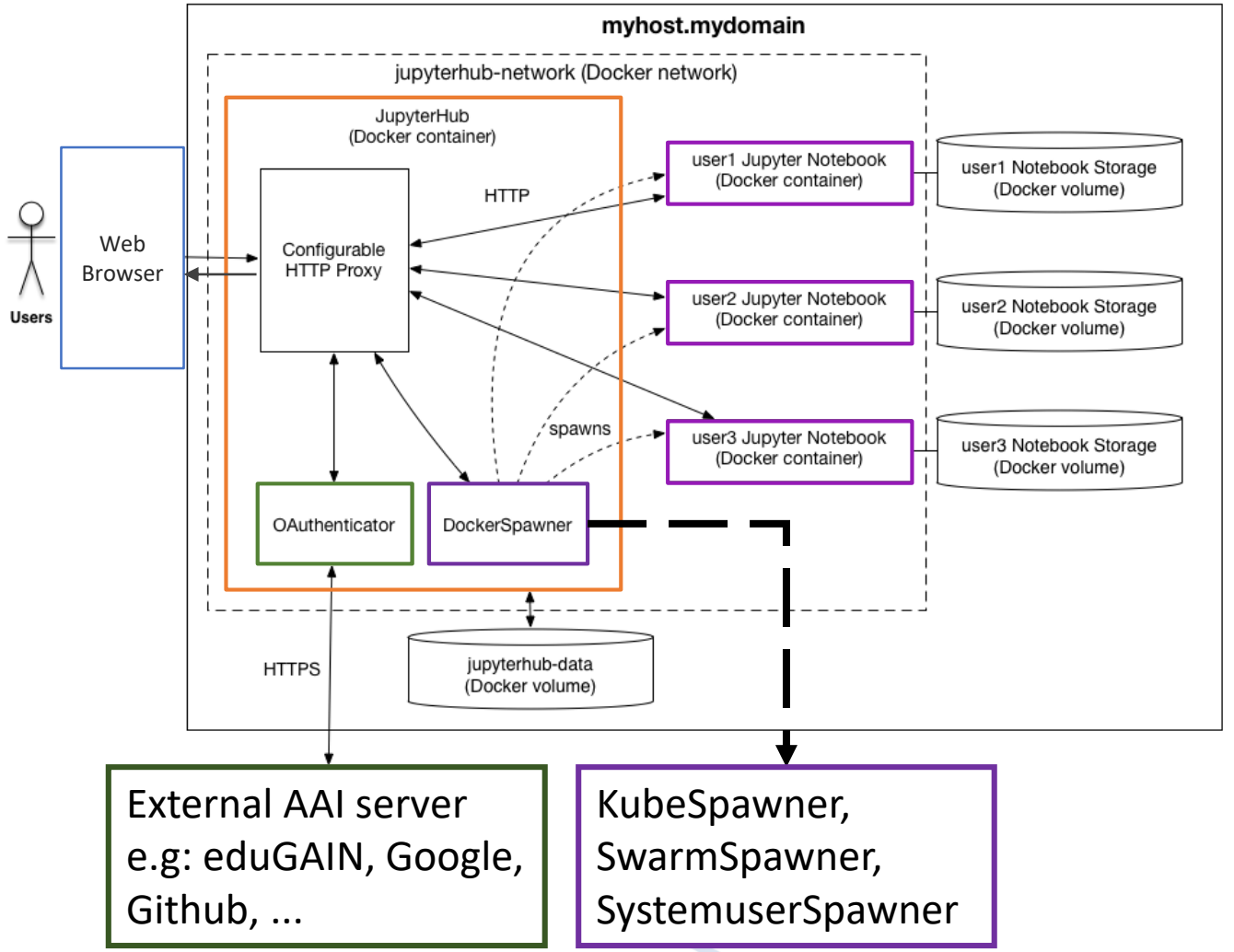
...Recap so far...



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