

Virtual Research Environment

Towards a comprehensive analysis platform

Elena Gazzarrini, Enrique Garcia

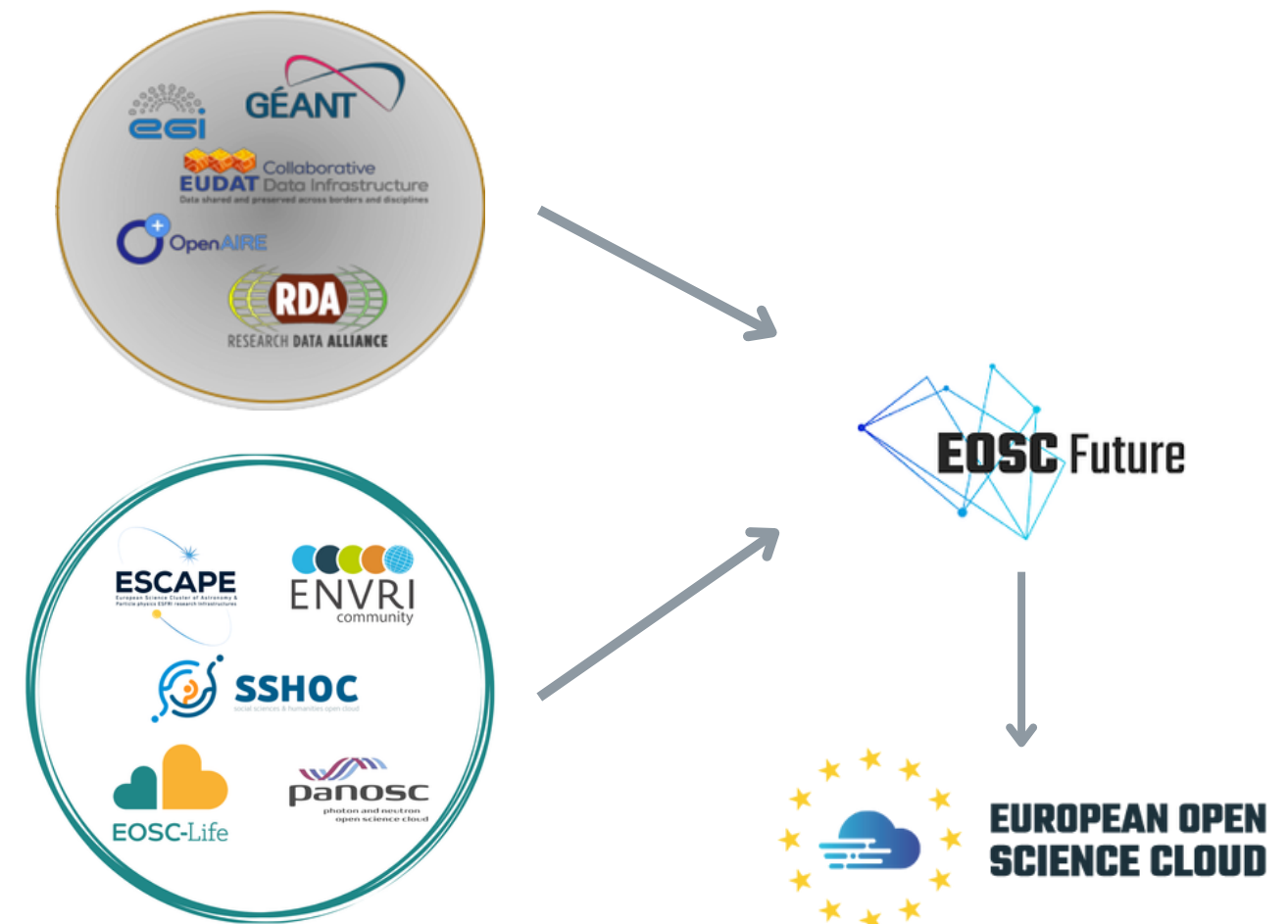


European Union's Horizon 2020 programme Grant Agreement 824064 and 101017536

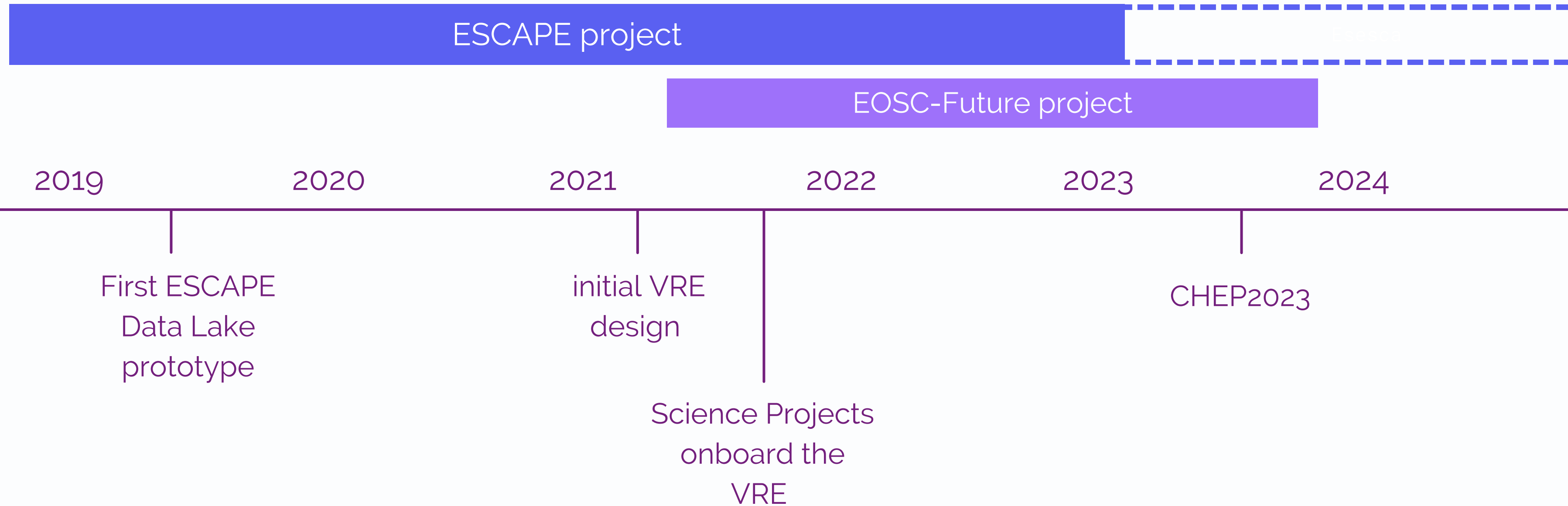
The Virtual Research Environment

The VRE is an **open source** analysis platform where researchers have access to all the digital content needed to **develop, share and reproduce an end-to-end scientific result** in compliance with **FAIR** (findable, accessible, interoperable, reproducible) principles.

(documentation: <https://vre-hub.github.io/>)



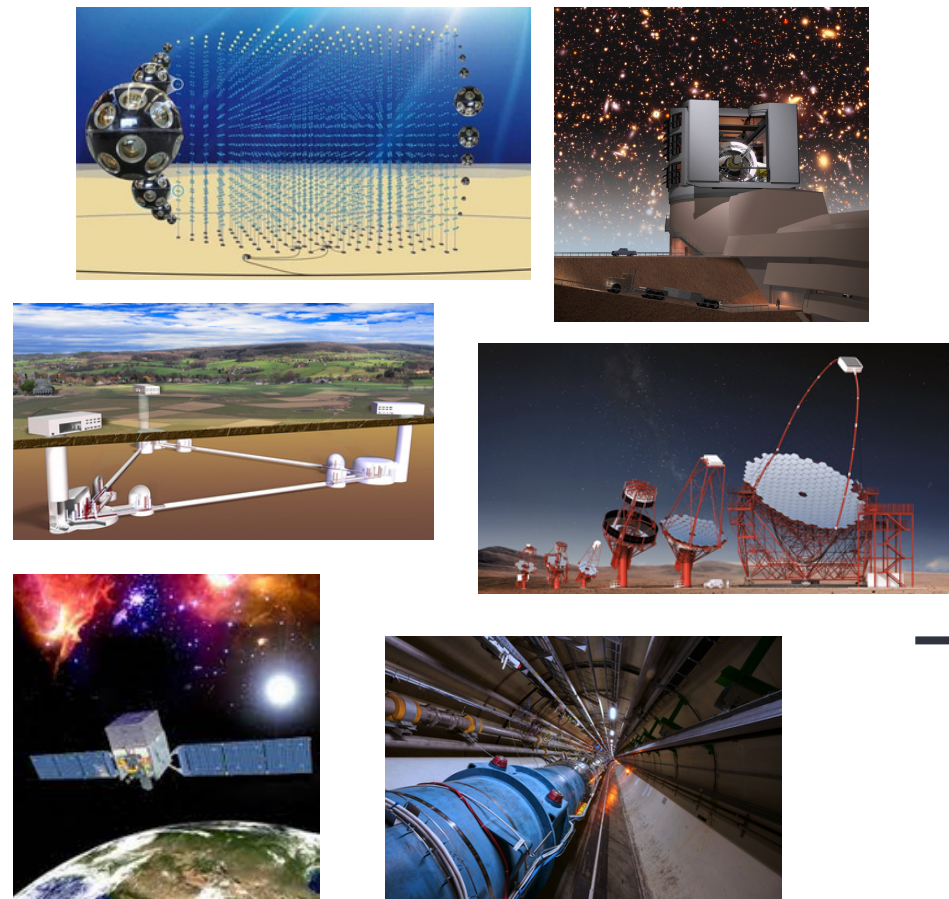
Timeline



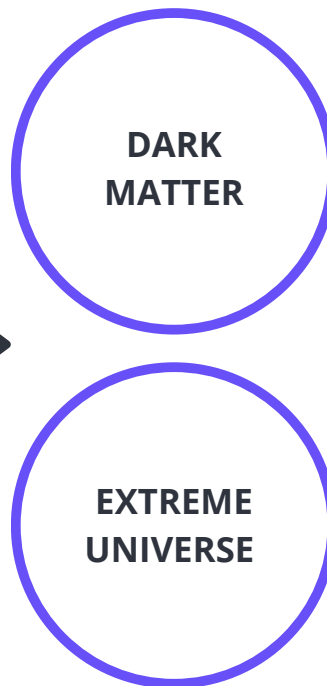
Context: EOSC-Future

EOSC-Future Science Projects demonstrate

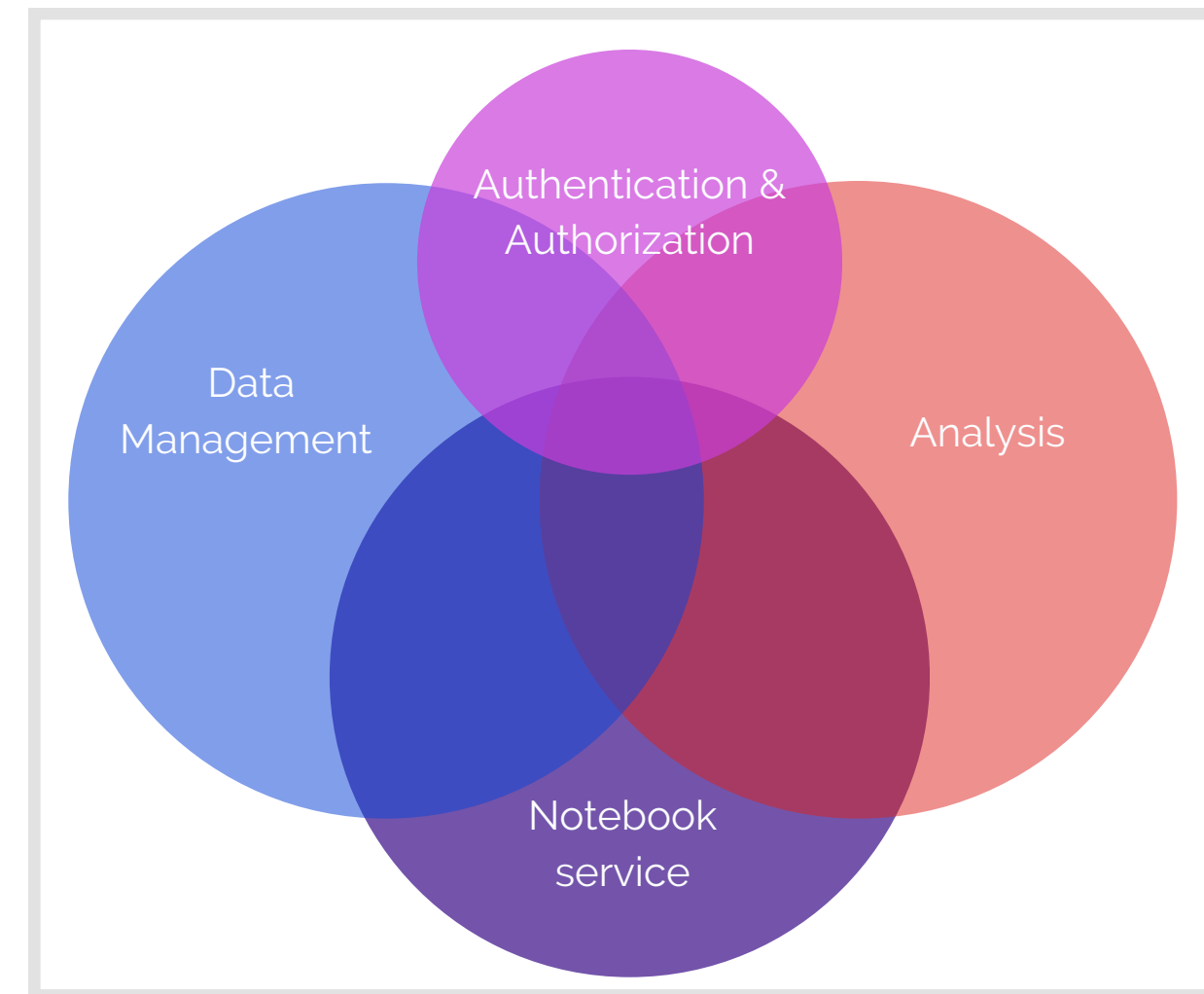
- multi-domain science integration across the **ESCAPE** project
- unification of services under **one Proof of Concept (PoC) analysis platform, the VRE**
- **interdisciplinary open science** example from bottom-up effort as a science driver for other communities



- Neutrino Observations
- High Energy Astronomy
- Low Frequency Telescopes
- Particle Physics
- Gravitational Waves

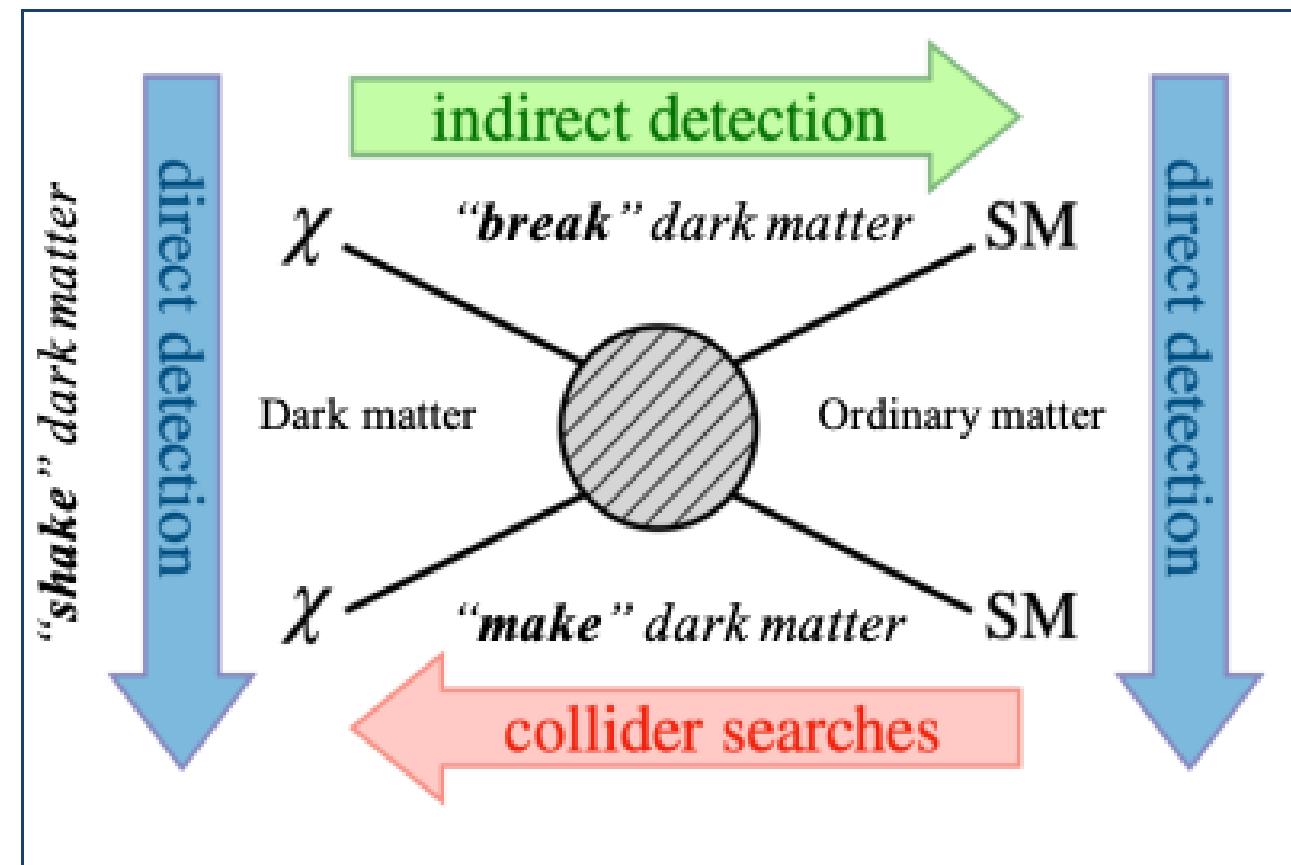


VRE



Dark Matter: Complementary Approach

Focus: Looking for **W**eakly **I**nteracting **M**assive **P**articles (**WIMPs**)



A joint discovery of the nature of dark matter requires different experiments and inputs

Experiments have **different** data sizes, workflows, data, and result sharing policies

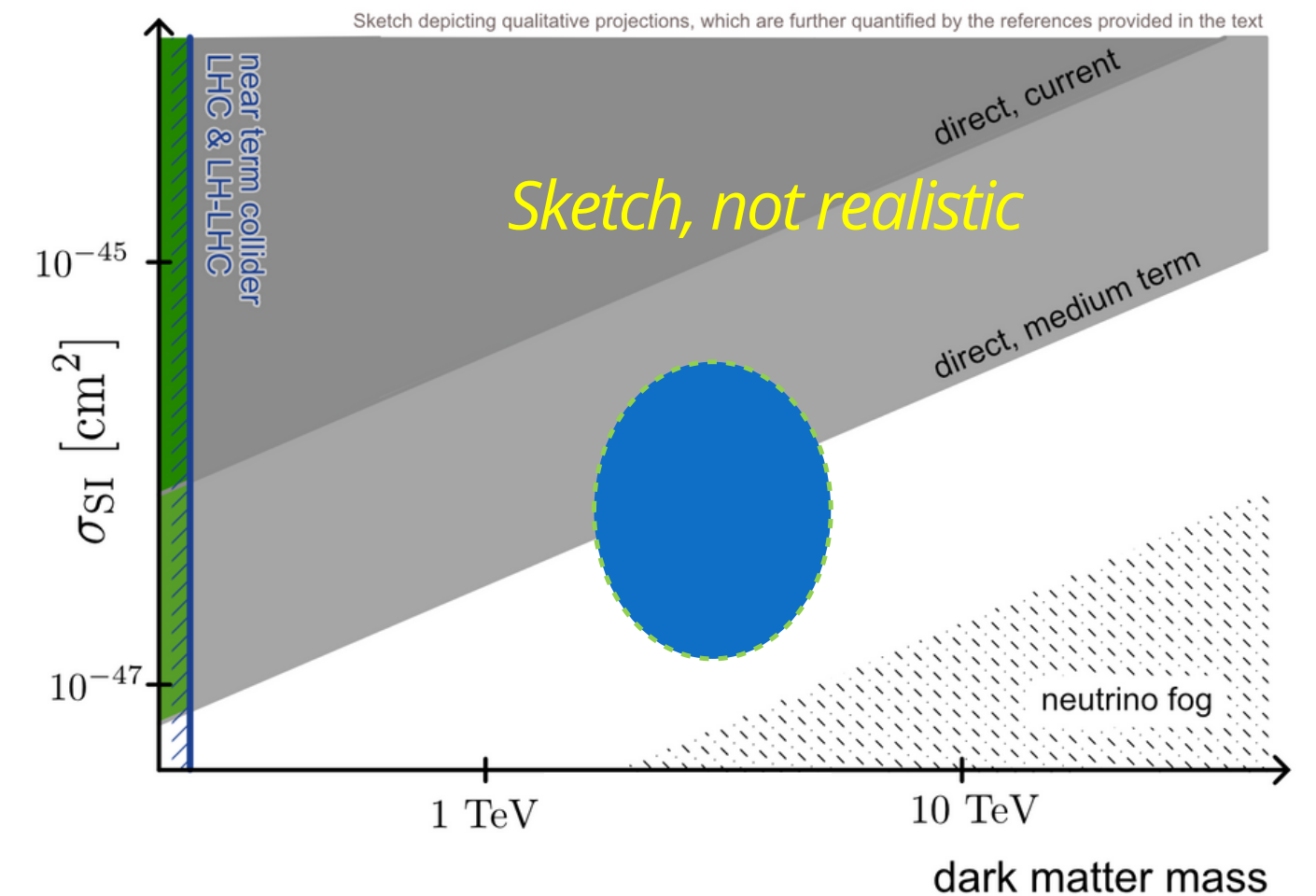
Example of a **discovery scenario**

Late 2020s **Direct detection** experiment sees a hint of a signal, with characteristics compatible with WIMP DM

Mid 2030s

2040s

Inspired by:
 Dark Matter Complementarity (Snowmass report), arXiv:2210.01770
 T. Slatyer's "Paths to discovery" talk at Snowmass 2022



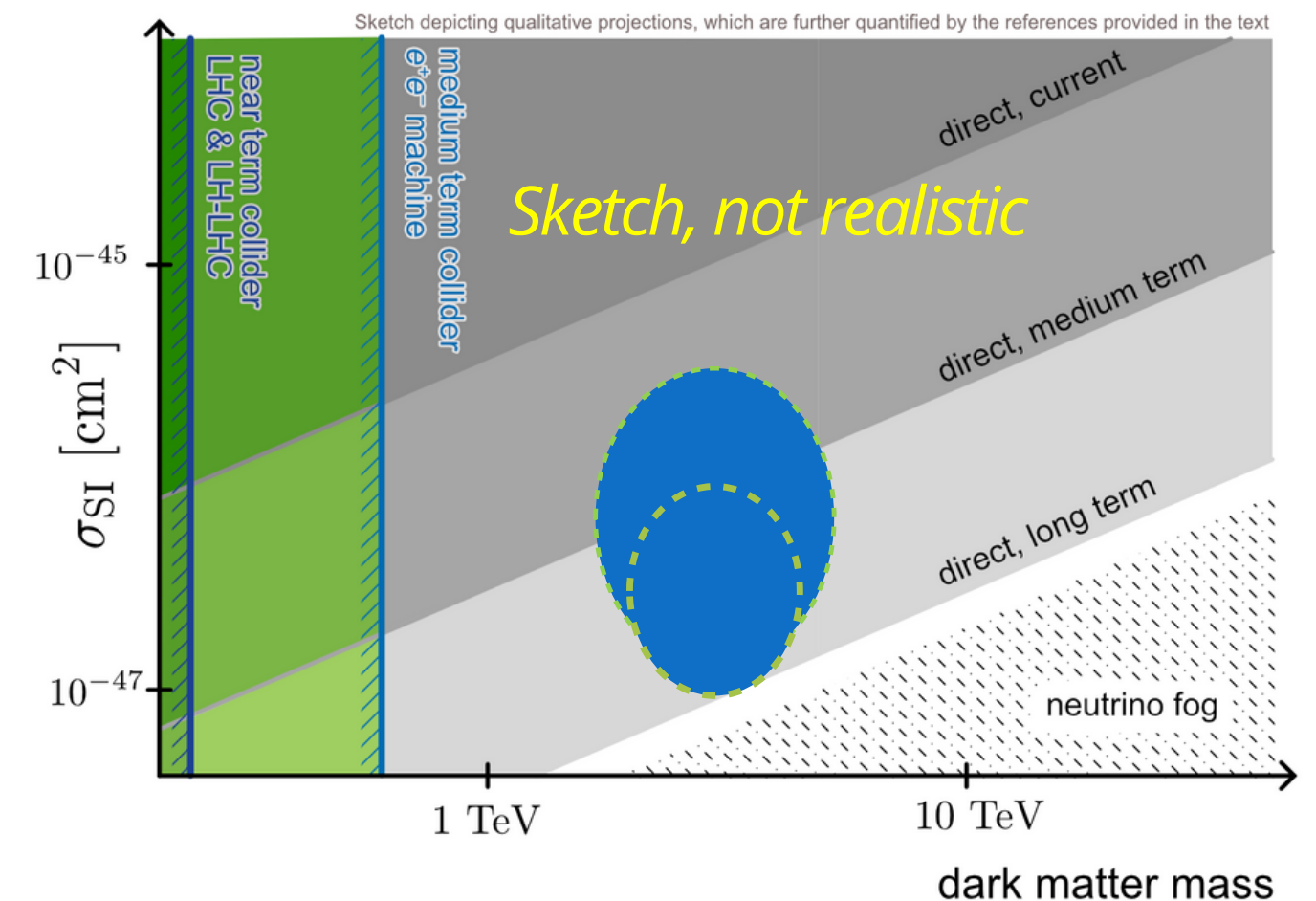
Example of a **discovery scenario**

Late 2020s **Direct detection** experiment sees a hint of a signal, with characteristics compatible with WIMP DM

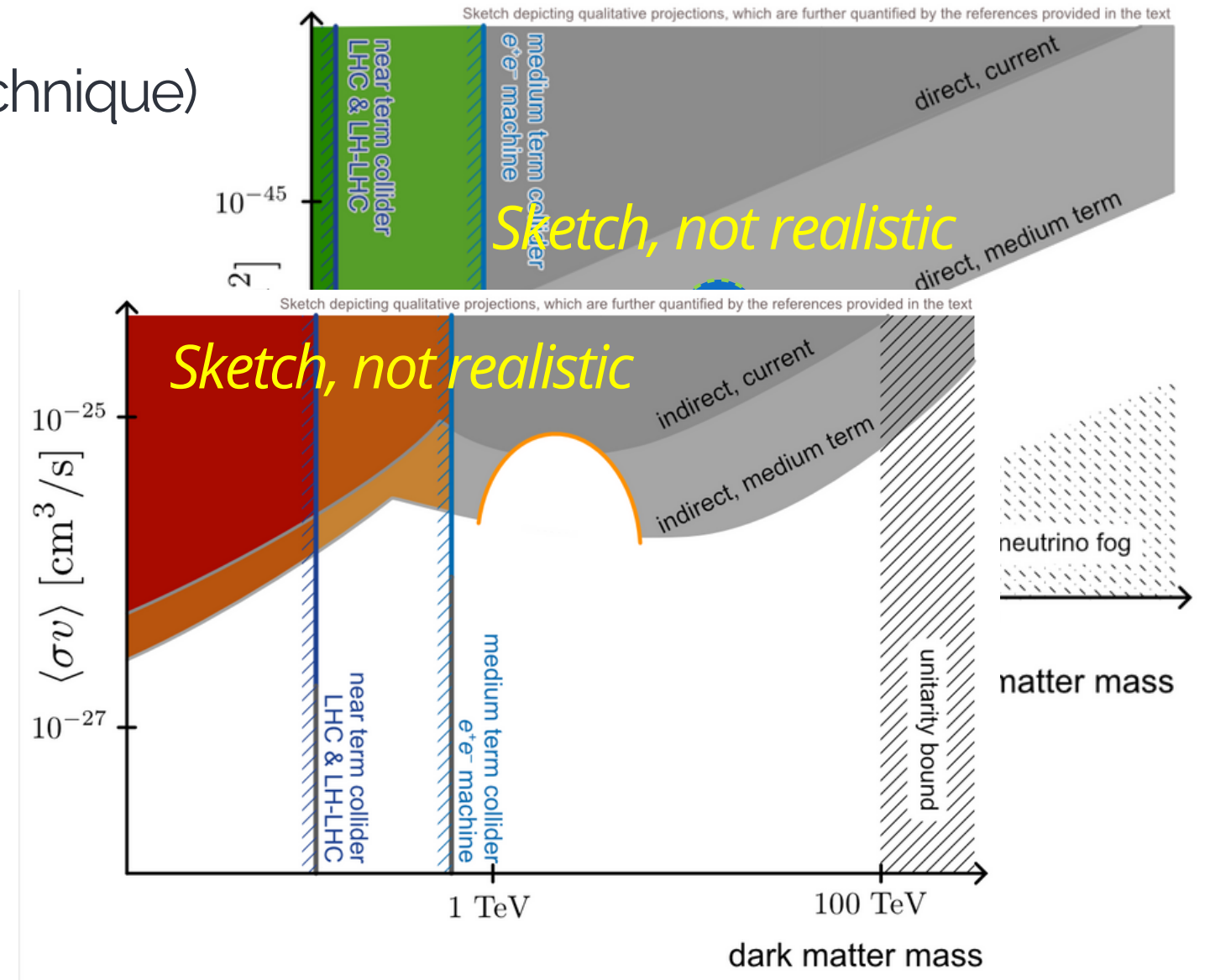
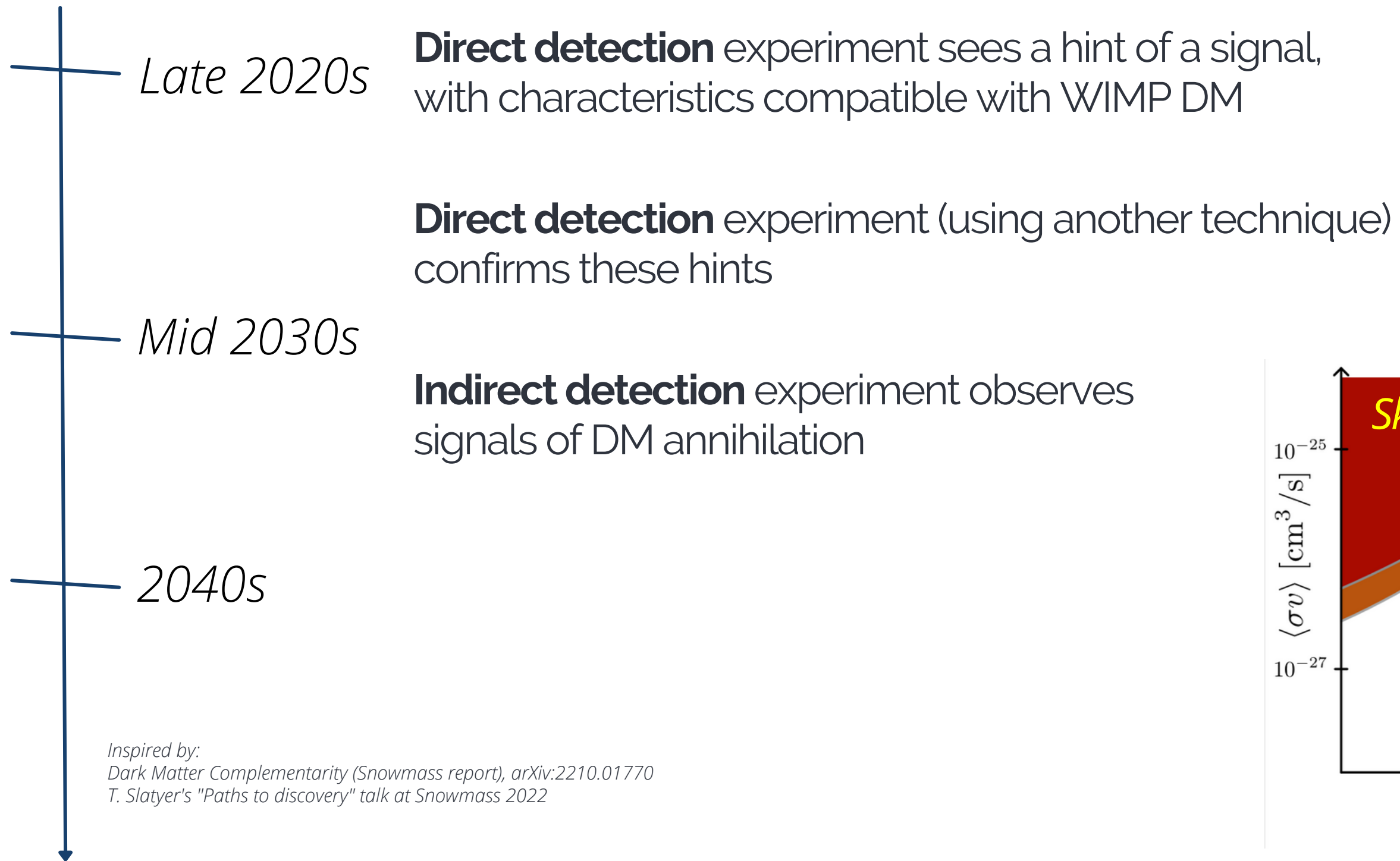
Mid 2030s **Direct detection** experiment (using another technique) confirms these hints

2040s

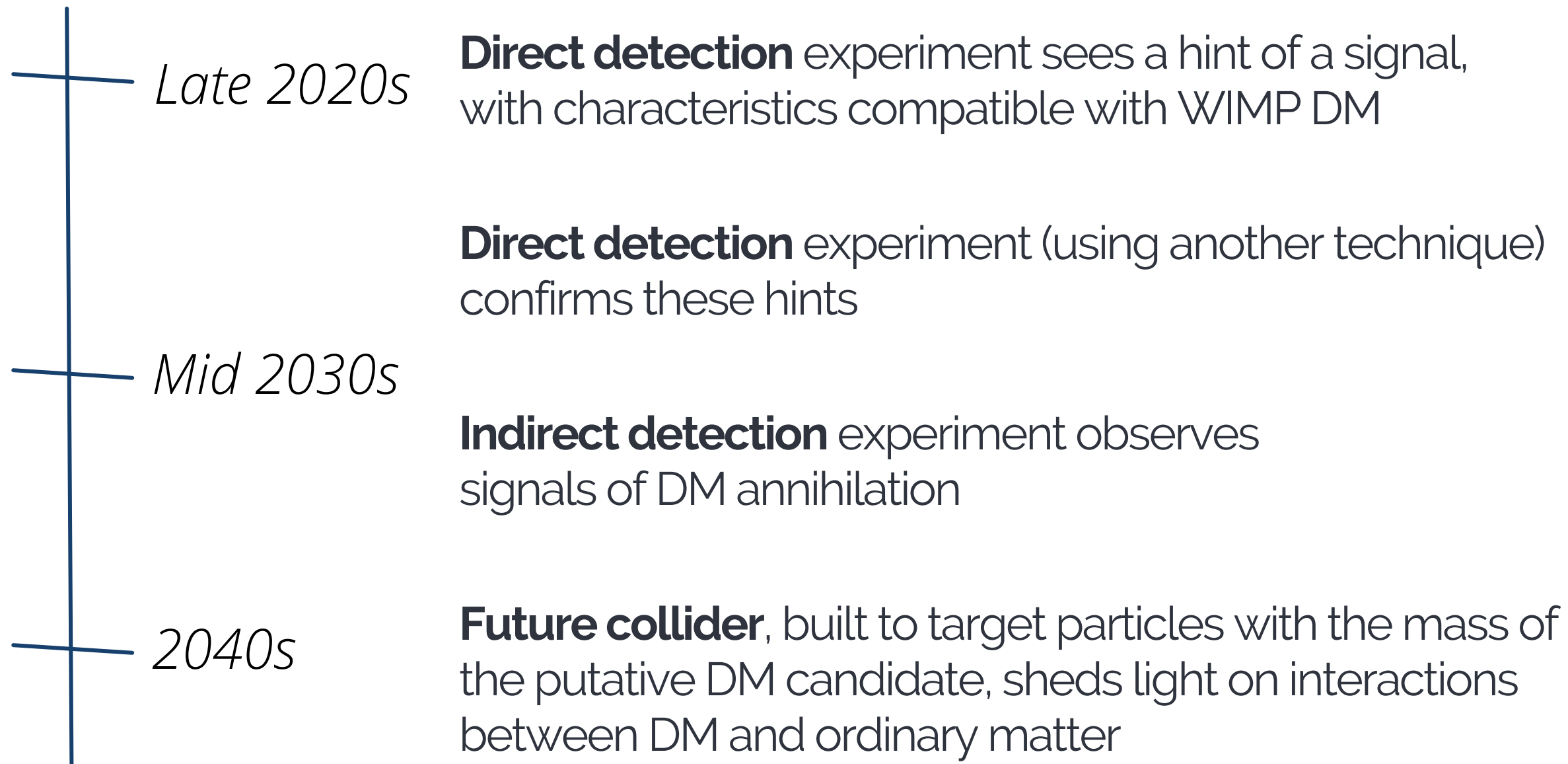
Inspired by:
 Dark Matter Complementarity (Snowmass report), arXiv:2210.01770
 T. Slatyer's "Paths to discovery" talk at Snowmass 2022



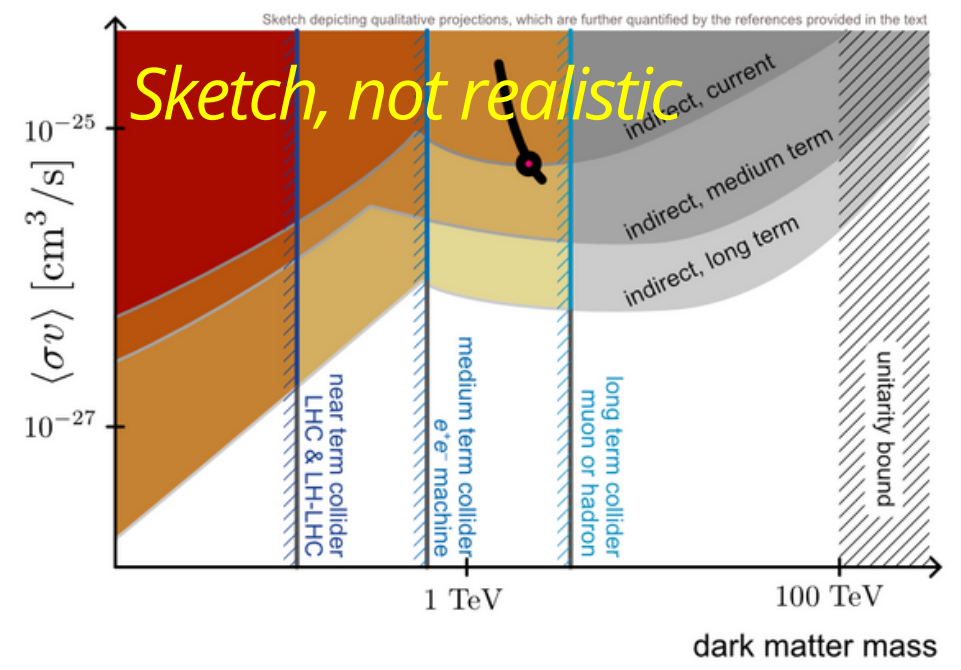
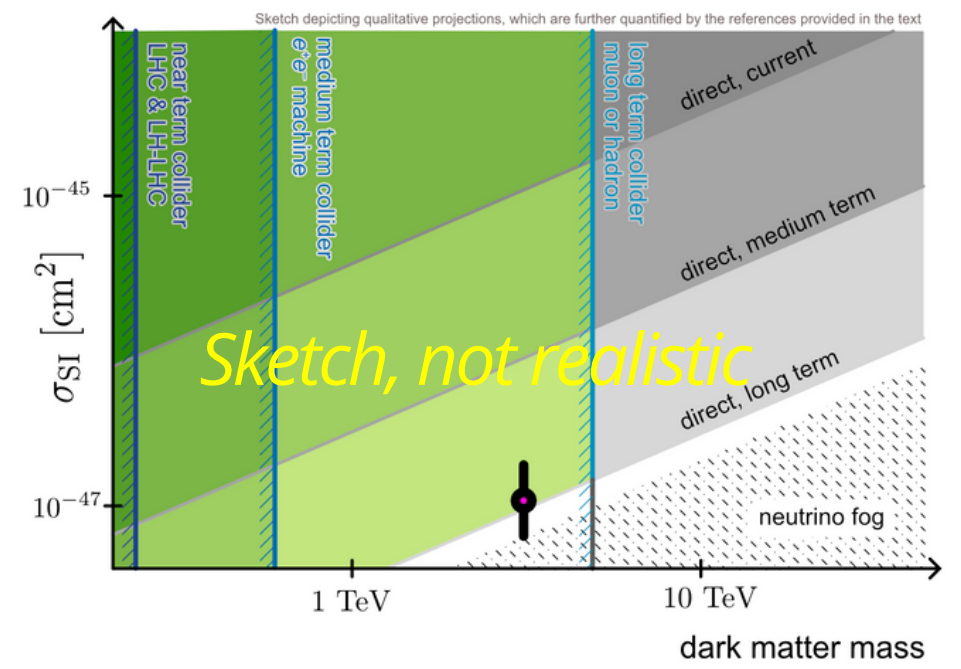
Example of a **discovery scenario**



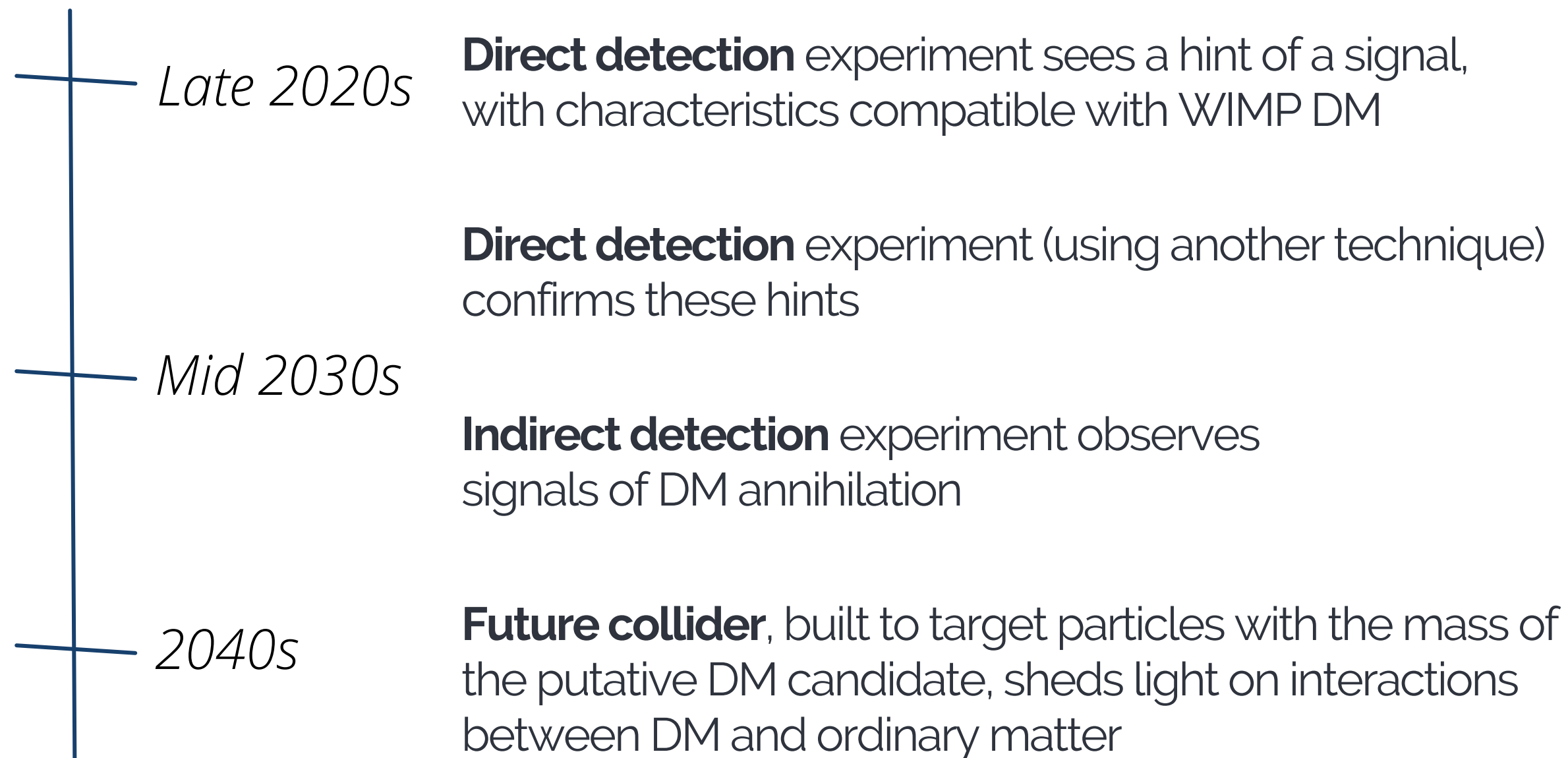
Example of a **discovery scenario**



Inspired by:
 Dark Matter Complementarity (Snowmass report), arXiv:2210.01770
 T. Slatyer's "Paths to discovery" talk at Snowmass 2022



Example of a **discovery scenario**



Such a scenario requires **interoperable** and **reproducible** analyses

- **comparison** and **combination** of results from different experiments
- **end-to-end workflows** available for cross-checks



with the **Dark Matter Science Project**, we build a **prototype** that fulfils these requirements

Inspired by:

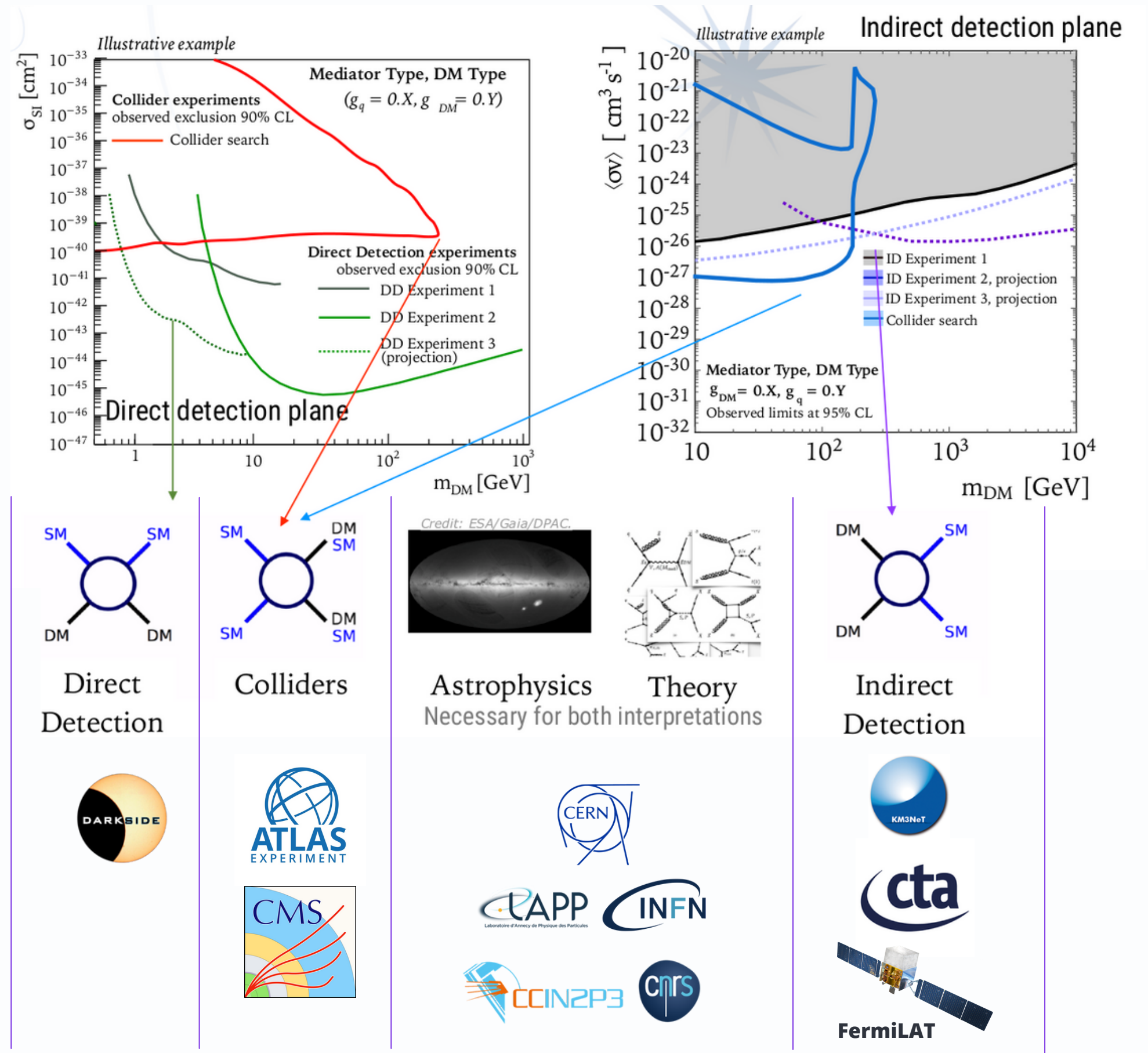
Dark Matter Complementarity (Snowmass report), arXiv:2210.01770

T. Slatyer's "Paths to discovery" talk at Snowmass 2022

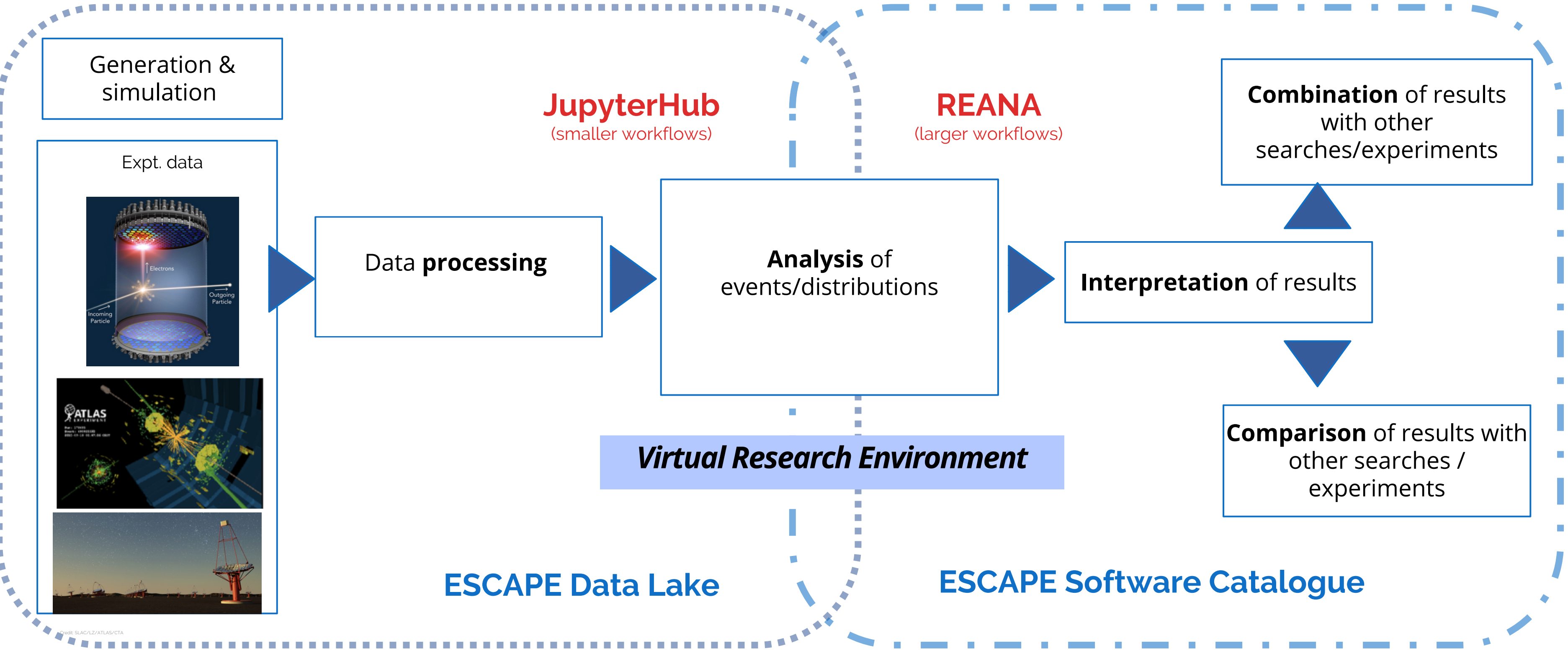


Science outputs of the Dark Matter SP

- Individual results and publications
- Plots highlighting complementarity of different experimental efforts
- Data and software objects + pipelines
- Data on the Data Lake, and software on the ESCAPE Software Catalogue
- Pipelines accessible via VRE
- **Combination of experimental results**



Analysis Workflows for the DM Science Project

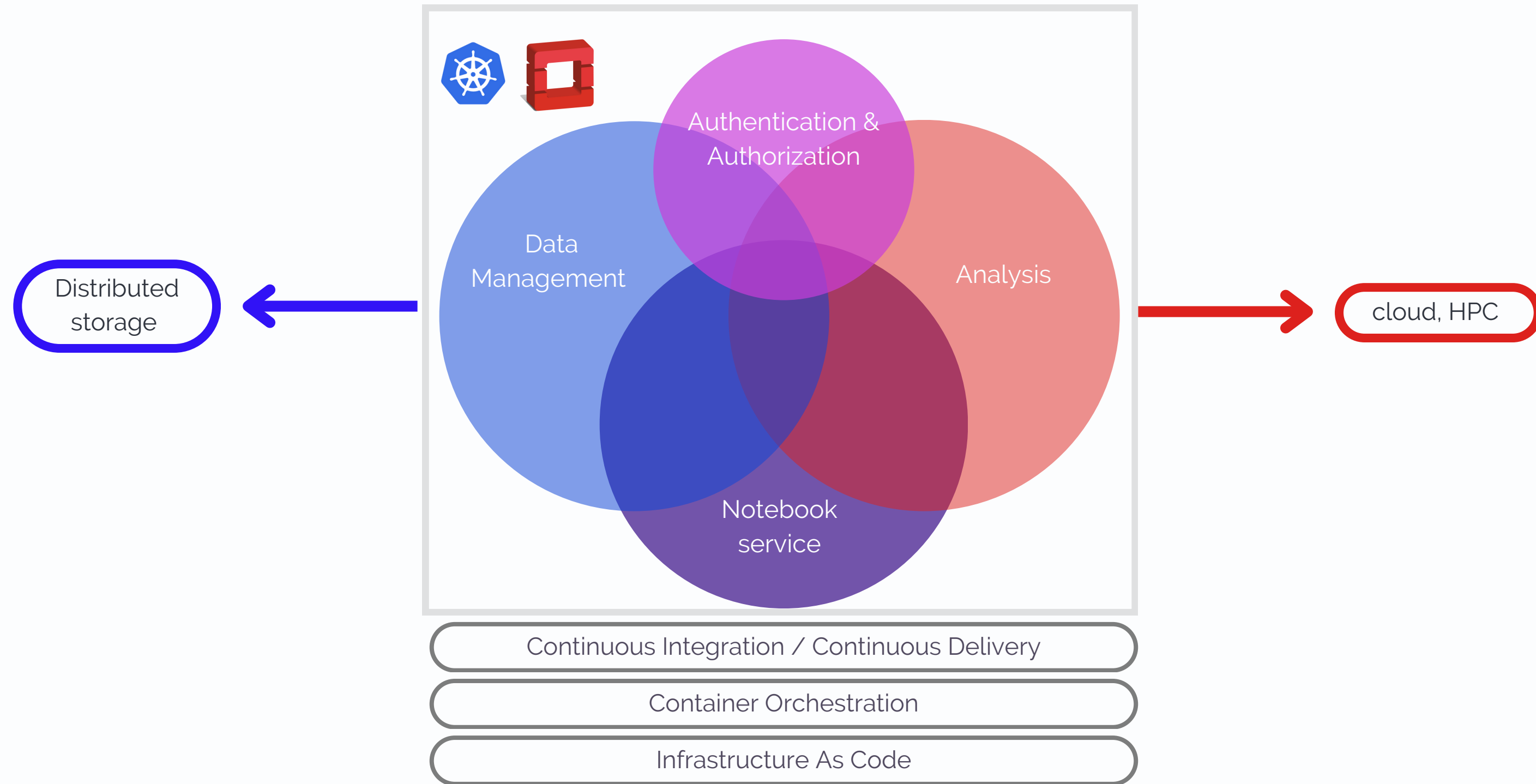


Data sharing and data processing

Data analysis, preservation and interpretation

Credit: SLAC/LZ/ATLAS/CTA

The VRE building blocks

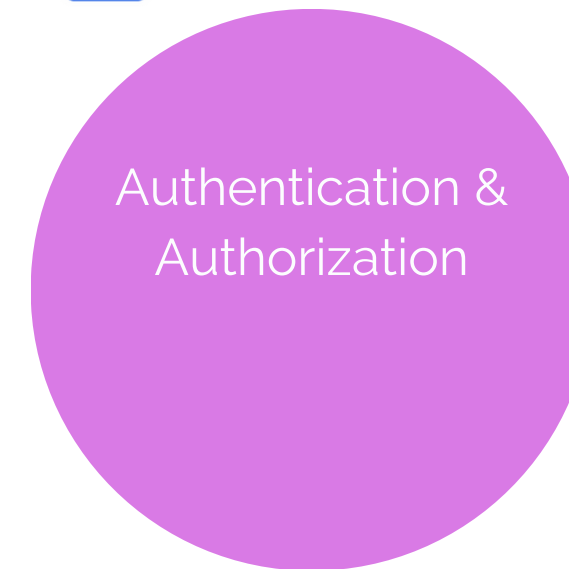


Authentication & Authorisation

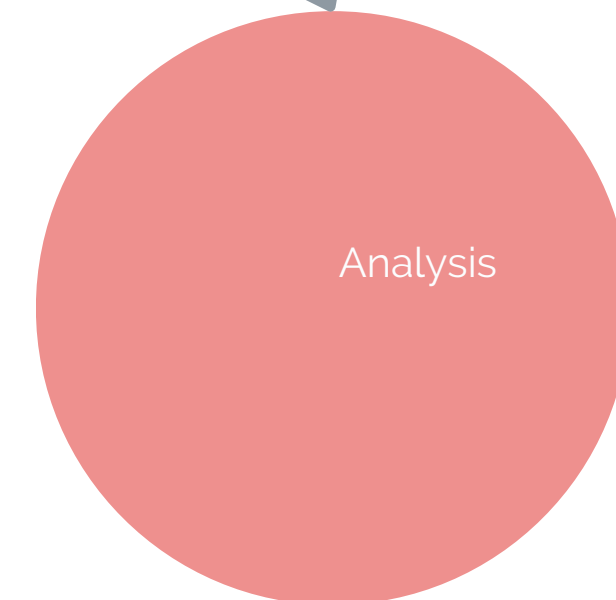
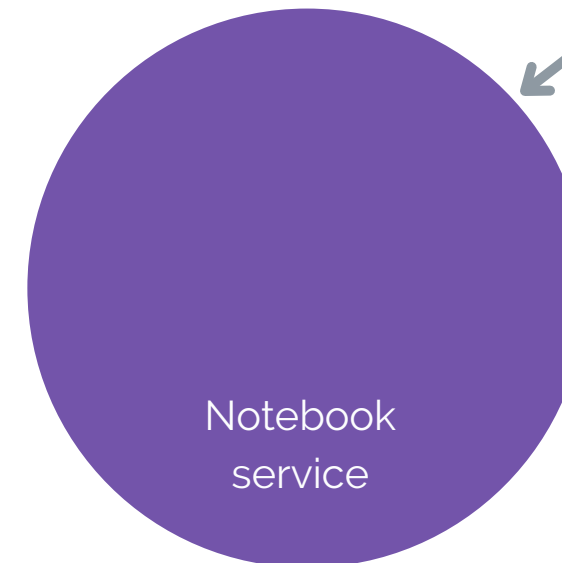


INDIGO Identity and Access Management (IAM) - adopted by WLCG for token

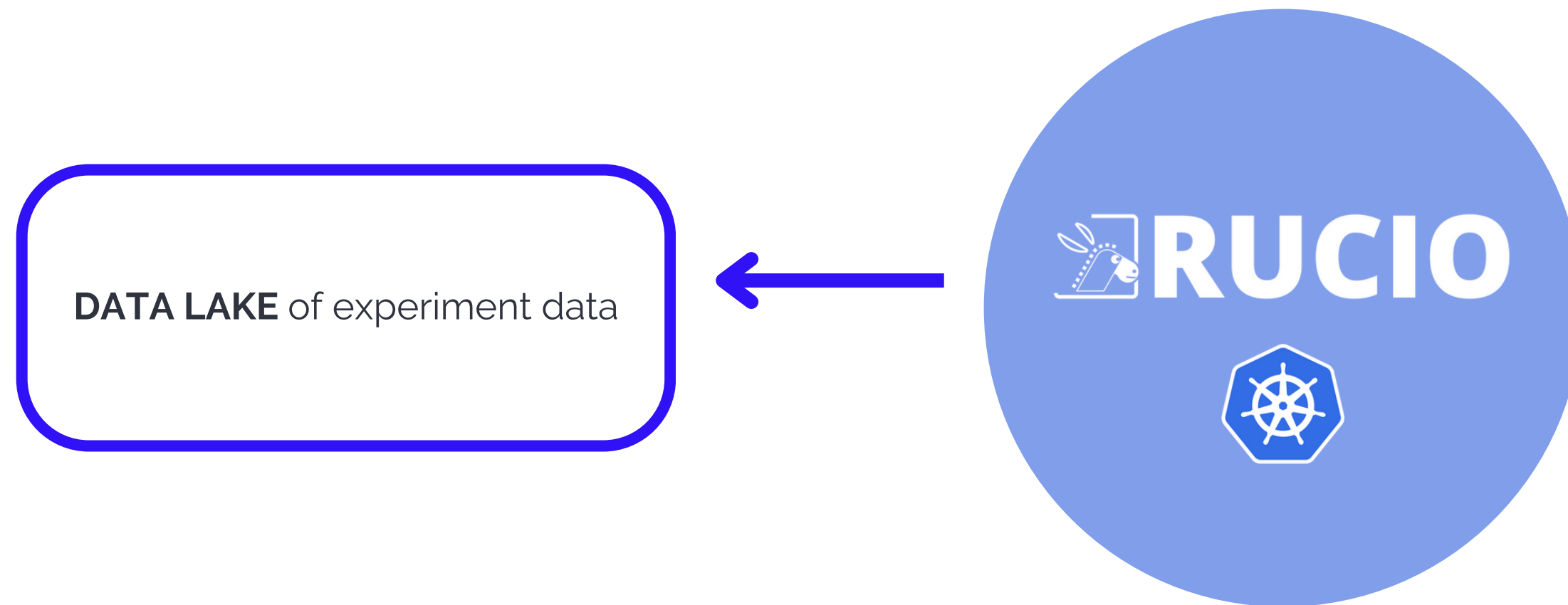
- OIDC tokens
- X.509 certificates / one VO for all the experiments



subject mapping cronjob



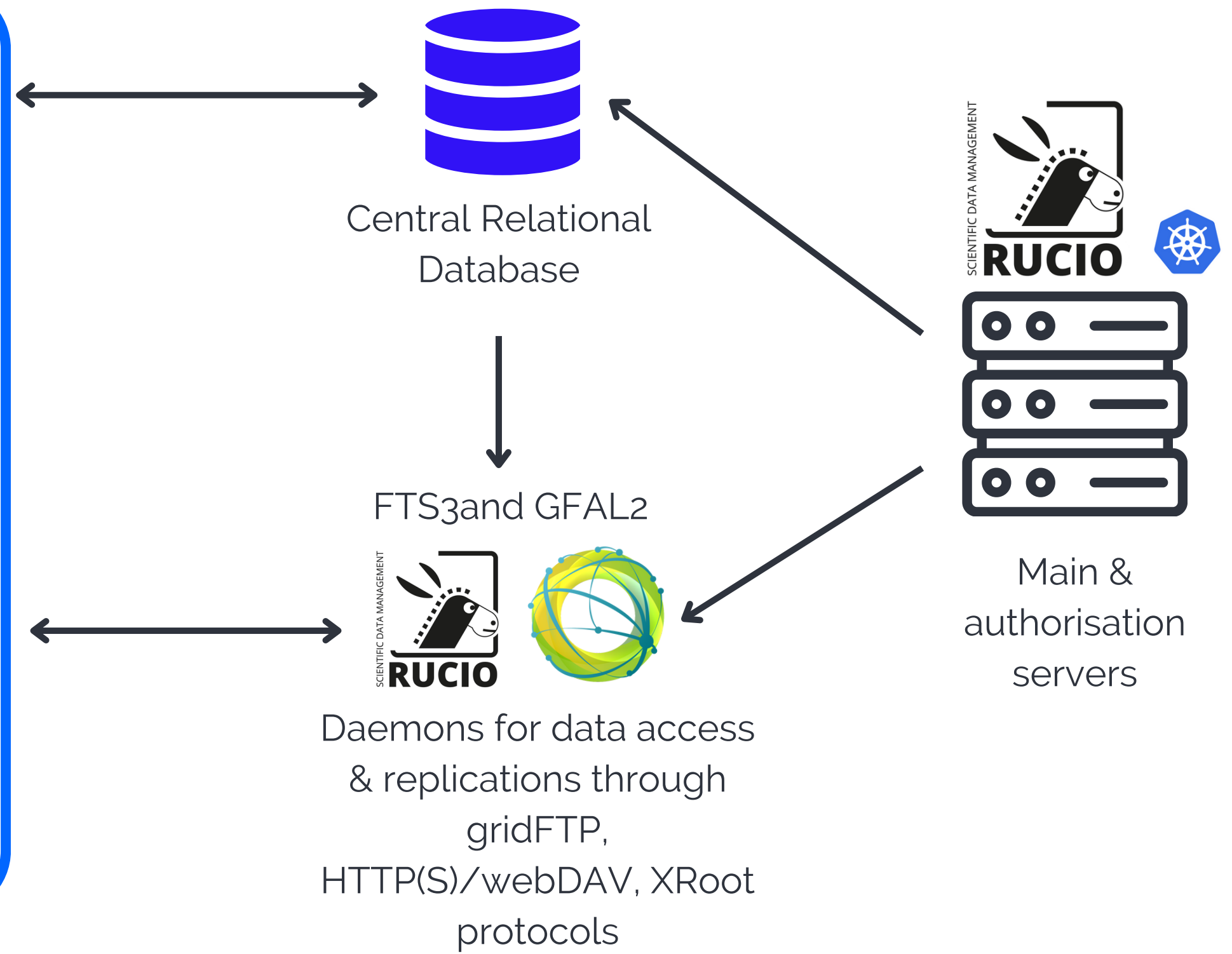
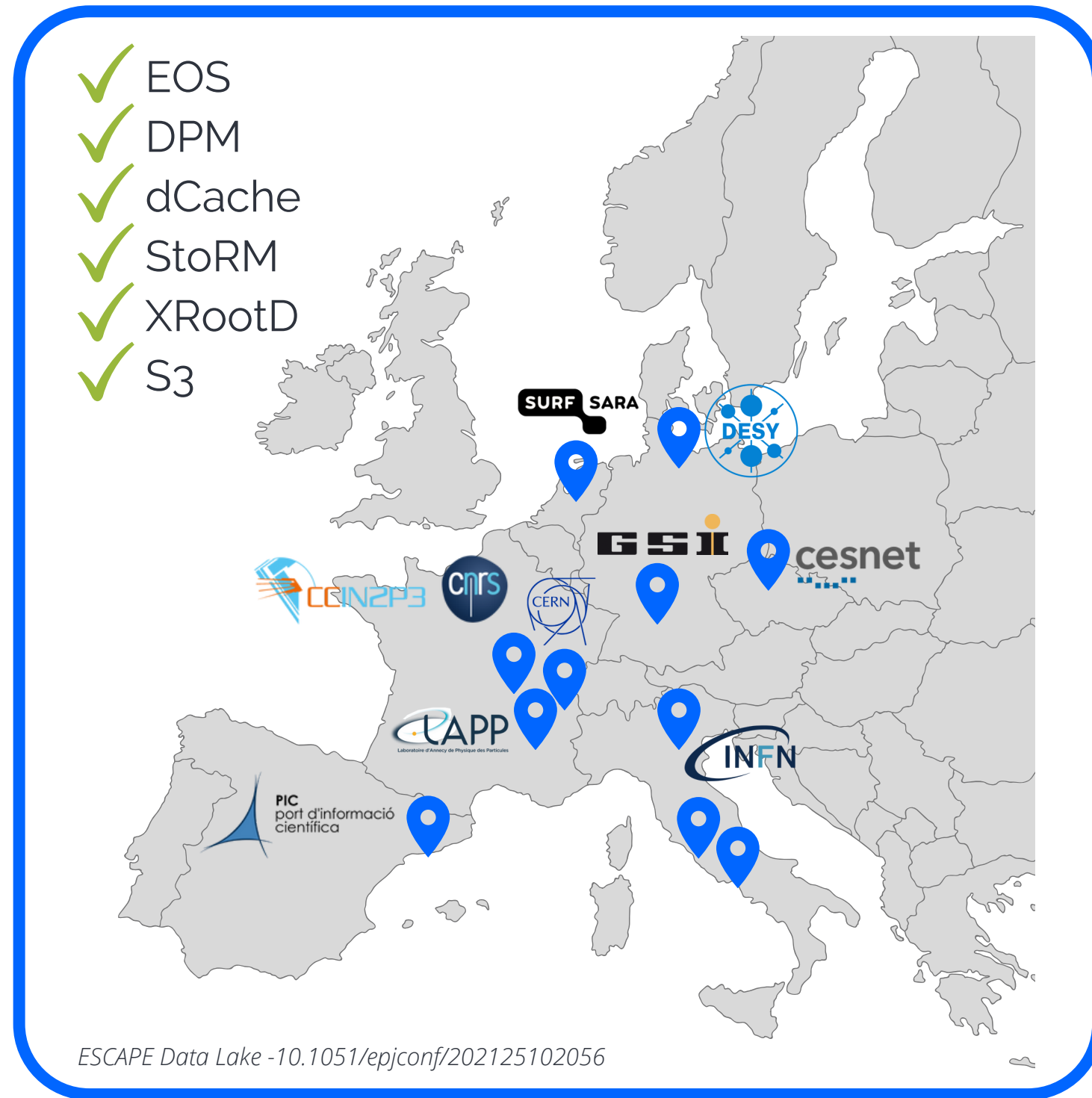
Data Management



Inherited from the ESCAPE WP2 data management group at CERN -> evolved into a GitHub hosted, k8s managed Openstack cluster maintained to comply with latest Rucio software developments.

Rucio instance

Data Lake



Notebook Service

<https://jhub-vre.cern.ch/>



interface to run preliminary analysis



containerised environments on public repositories



EOS accessible from all images jhub nodes



CERN Virtual Machine FS (CVMFS) installed and accessible from all images



client libraries and software installed to interact with underlying services



CephFS volumes provided as shared, temporary storage solution



Rucio VRE instance access

Server Options

- Minimal environment**
Based on jupyter/scipy-notebook (active reana-client)
- ROOT environment**
ROOT v6.26.10, a C++ kernel is implemented too - DASK testing
- Minimal environment - python 3.9.13**
Contains a REANA client
- Virtual Observatory environment**
Contains Jupyter Notebooks examples with the basic usage of the IVOA tools
- Indirect Dark Matter Detection Environment**
Contains a GCC compiler and the MLFermiLATDwarfs and fermitools libraries - not fermipy (bugged)
- Common gamma analysis tools**
Contains a GCC compiler and astropy, sherpa, agnpy, gammapy libraries
- Wavelet Detection Filter (WDF) project environment**
Contains the full WDF env
- Compact stars Science Project environment**
Contains the matchmaker library
- KM3NeT Science Project environment**
Contains the common gamma analysis tools and the km3io, km3pipe and km3irf libraries
- KM3NeT & CTA combined analyses**
Compatible environment with gammapy and the km3io, km3pipe and km3irf libraries (env testing)
- SKA SDC1**
SKA environment profile for SDC
- LOFAR environment**
Based on the prefactor container. Can be used to image LOFAR data
- ESAP shopping basked environment**
Using the ESAP shopping basket library.
- ESAP shopping basked environment (with astropy)**
ESAP shopping basket and astropy, e.g. to download and plot images from the virtual observatory

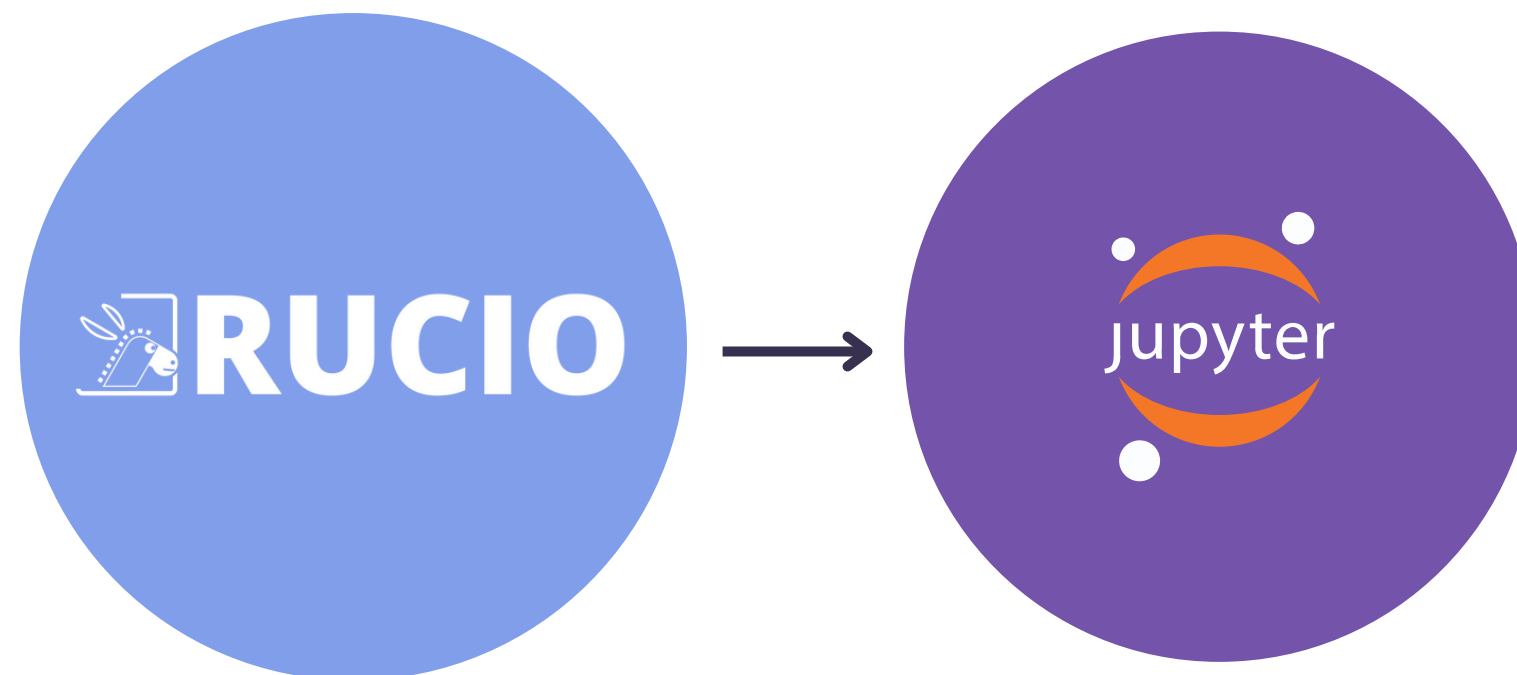
Start



Data into the notebook

The **Jupyterhub Rucio extension** hides the complexity of the Data Lake and allows users to

- browse experiments' data catalogue
- authenticate with OIDC tokens to the Rucio infrastructure
- replicate data into the notebook
- import the data into the notebook by assigning a parameter to it
- run preliminary analysis to prototype code



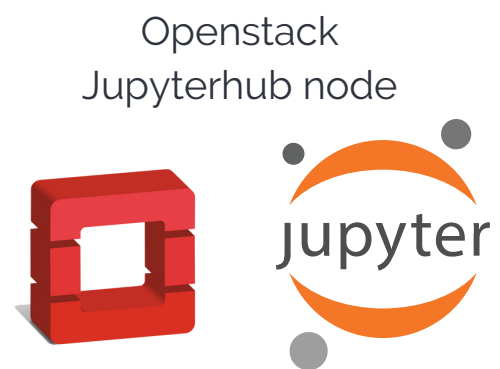
A screenshot of the Jupyter RUCIO extension interface. The interface shows a menu bar with "File", "Edit", "View", "Run", "Kernel", "Tabs", and "Settings". Below the menu bar, there is a "RUCIO" header with a search icon. The main area is divided into "EXPLORE" and "NOTEBOOK" tabs. A search bar contains the text "ATLAS_LAPP_SP:*". Below the search bar, there is a "SEARCH RESULTS" section with a list of folders: "ATLAS_LAPP_SP:DM-dilepton-14TeV-2018", "ATLAS_LAPP_SP:DM.LeptonResonance.Data...", "ATLAS_LAPP_SP:DMsummary.dilepton.14TeV...", "ATLAS_LAPP_SP:DMsummary.dileptonReinter...", and "ATLAS_LAPP_SP:jared_little". A green checkmark and the text "All files available" are shown at the bottom of the search results. A red circle highlights the search icon in the left sidebar.

Data into the notebook

Data gets replicated through Rucio daemons from any storage element to an EOS storage element of half a Petabyte FUSE mounted on the Jupyterhub node.

The computation is limited to the CPU capacity of the node.

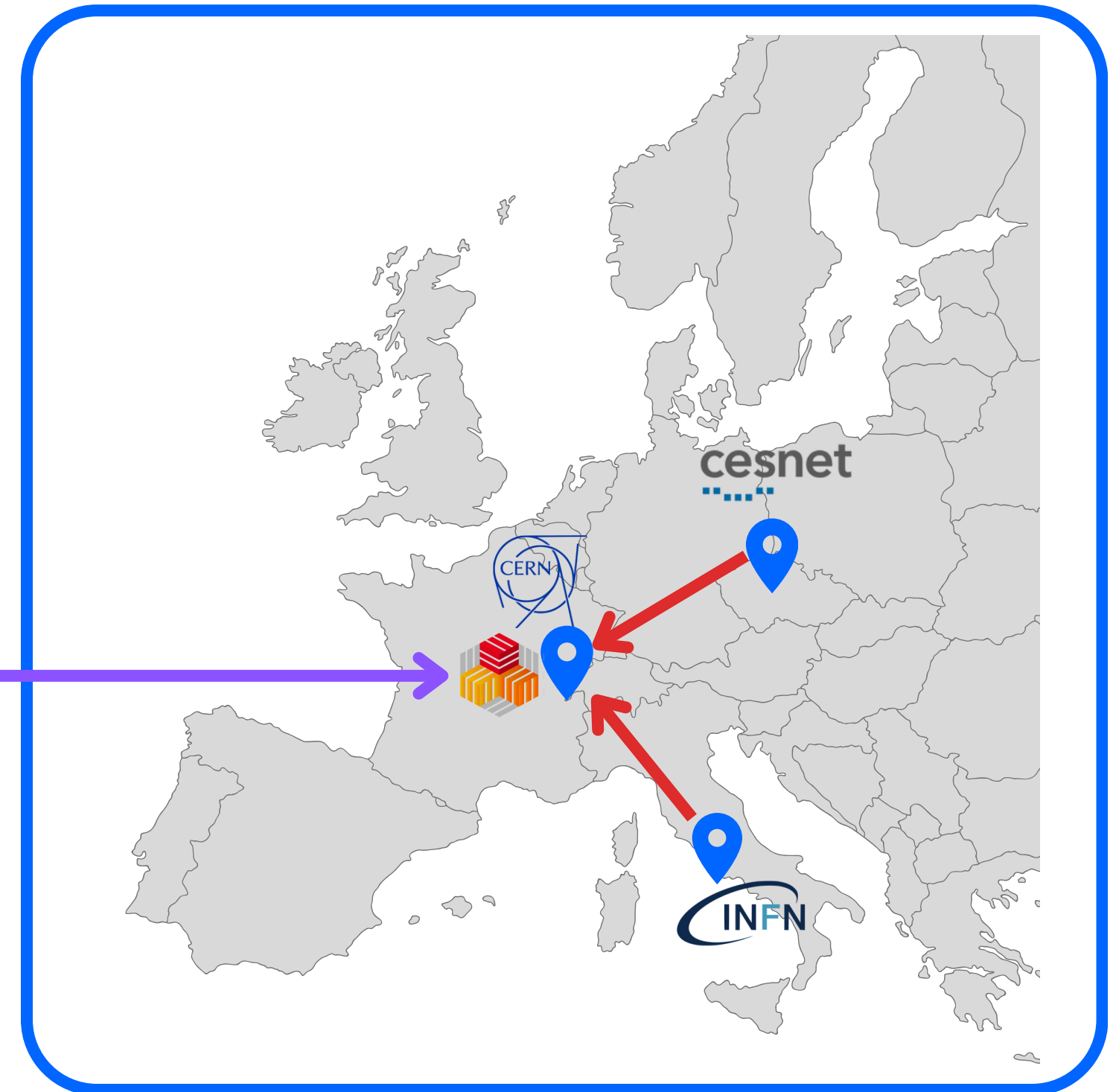
How do we SCALE OUT?



FUSE mount

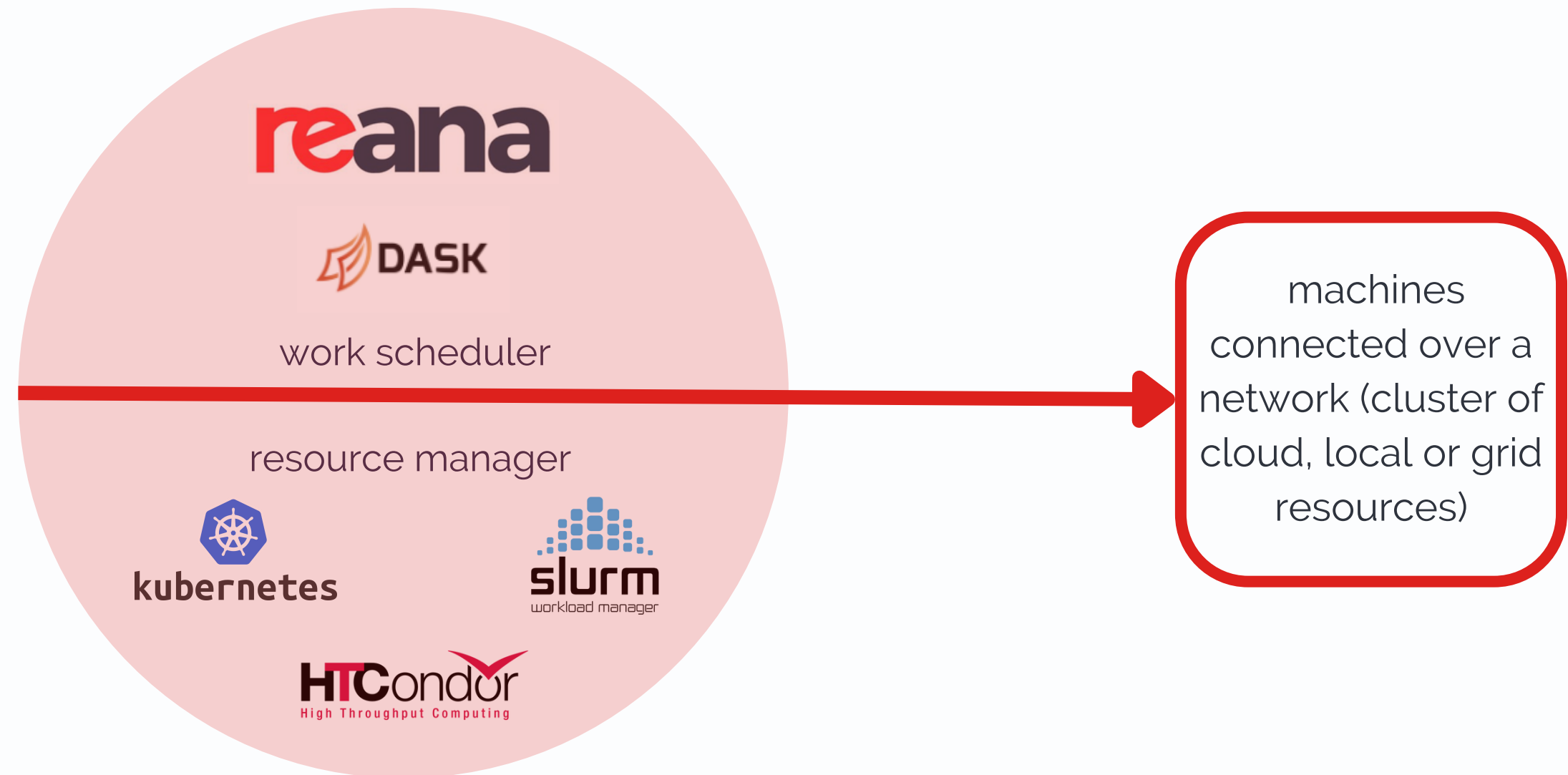
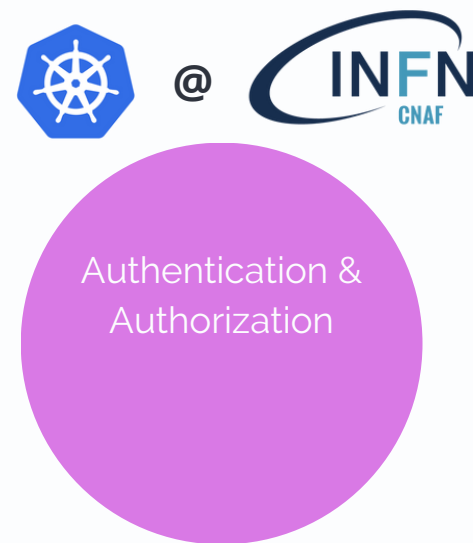


Data Lake

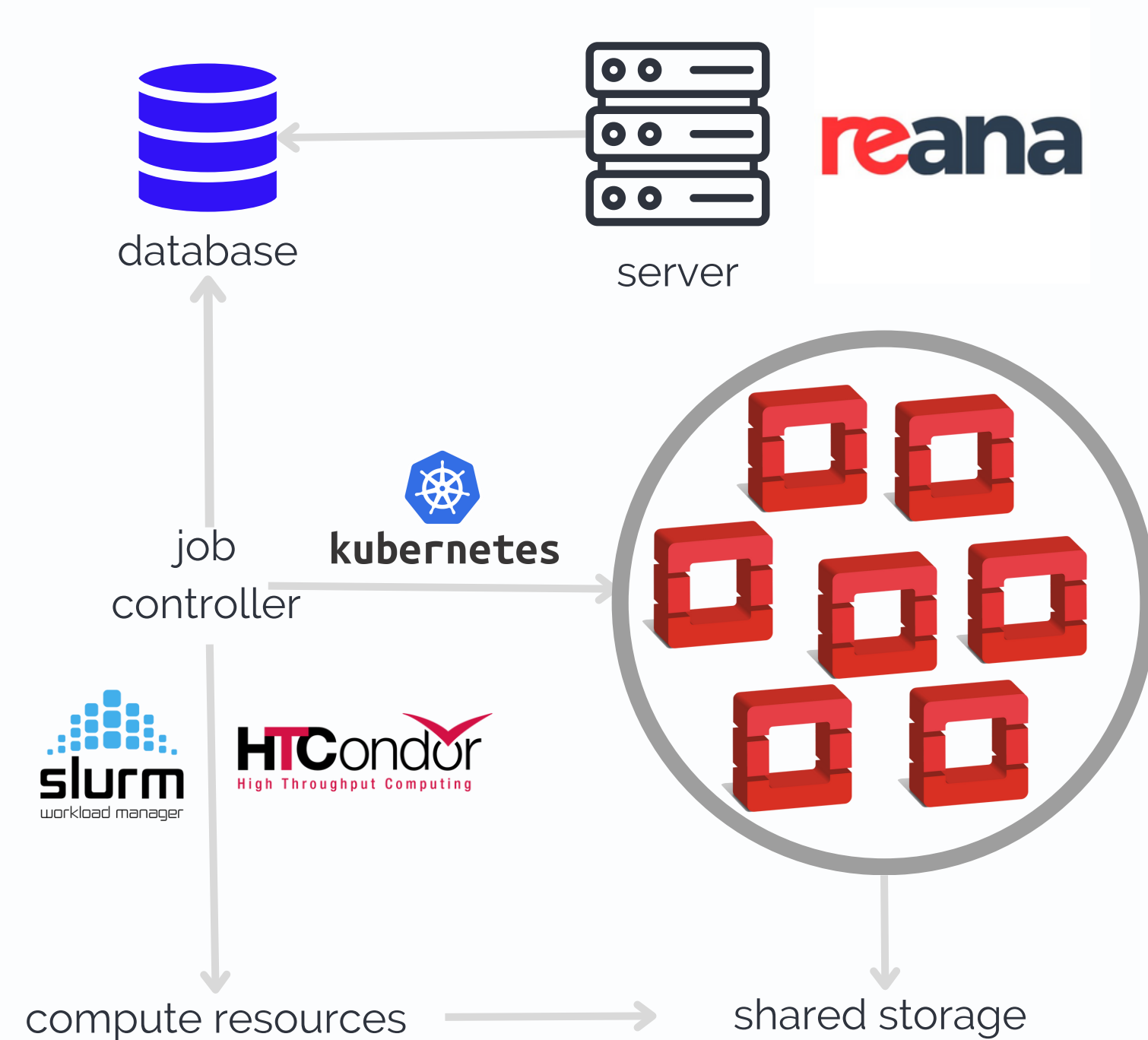


Computing

- **Distribute** the analysis
 - **resource managers** (Kubernetes, HTCondor (High Throughput Computing (HTC)) and Slurm (High Performance Computing (HPC))
 - **work schedulers** (Dask, Reana, Spark)
- **Preserve** the analysis for reuse
 - work schedulers (Reana)



Analysis preservation and distribution



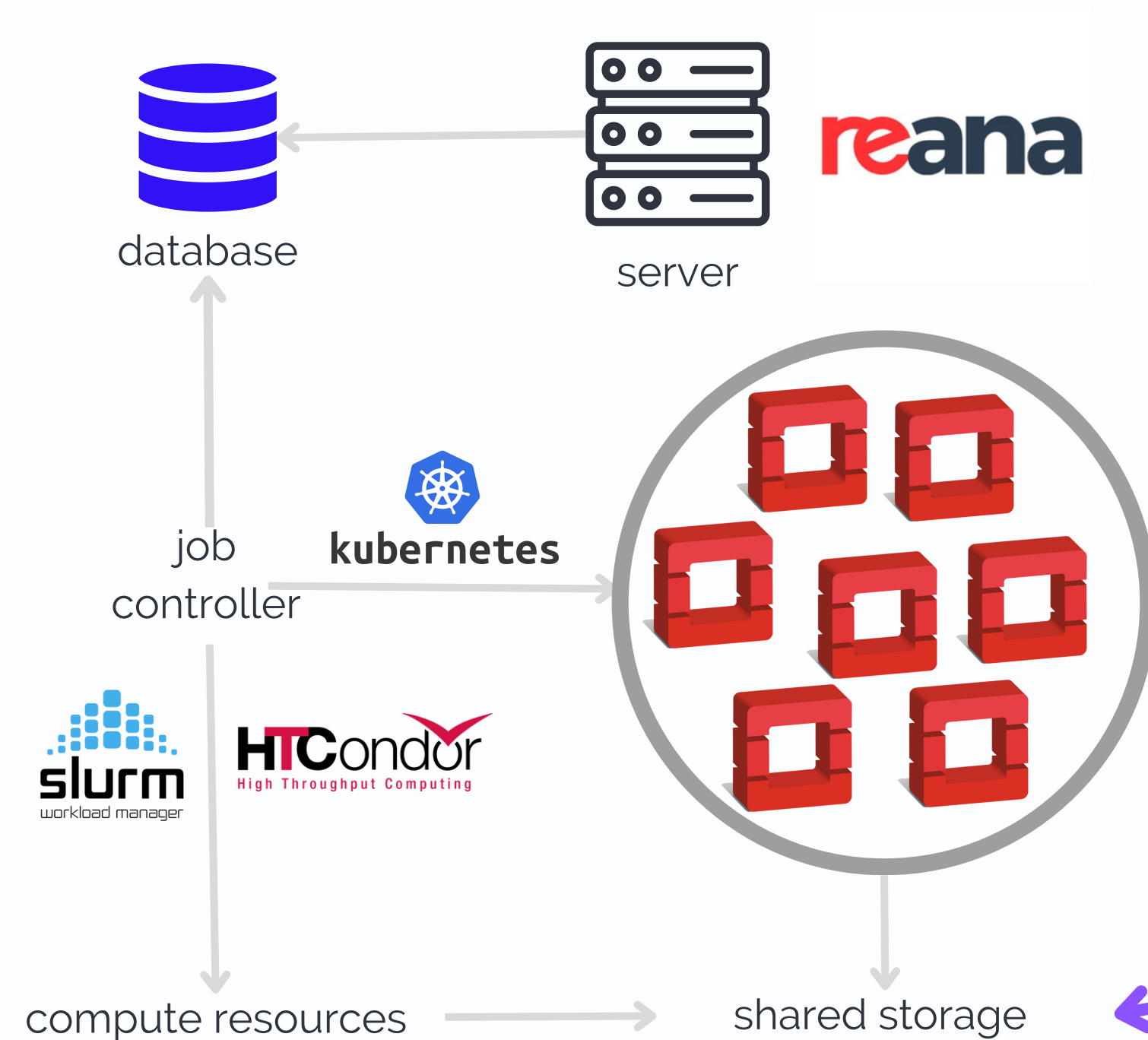
Reana is a reproducible analysis project developed at CERN, to make the preservation of heavier analyses seamless.

- Easily installed via Helm
- Intuitive declarative programming approach (reana.yaml file) with:
 - input data
 - environment
 - code
 - computational steps
- Isolates each step with different containers
- Supports workflow engines
 - CWL
 - Snakemake
 - Yadage --> workflow concatenation (output becomes input)

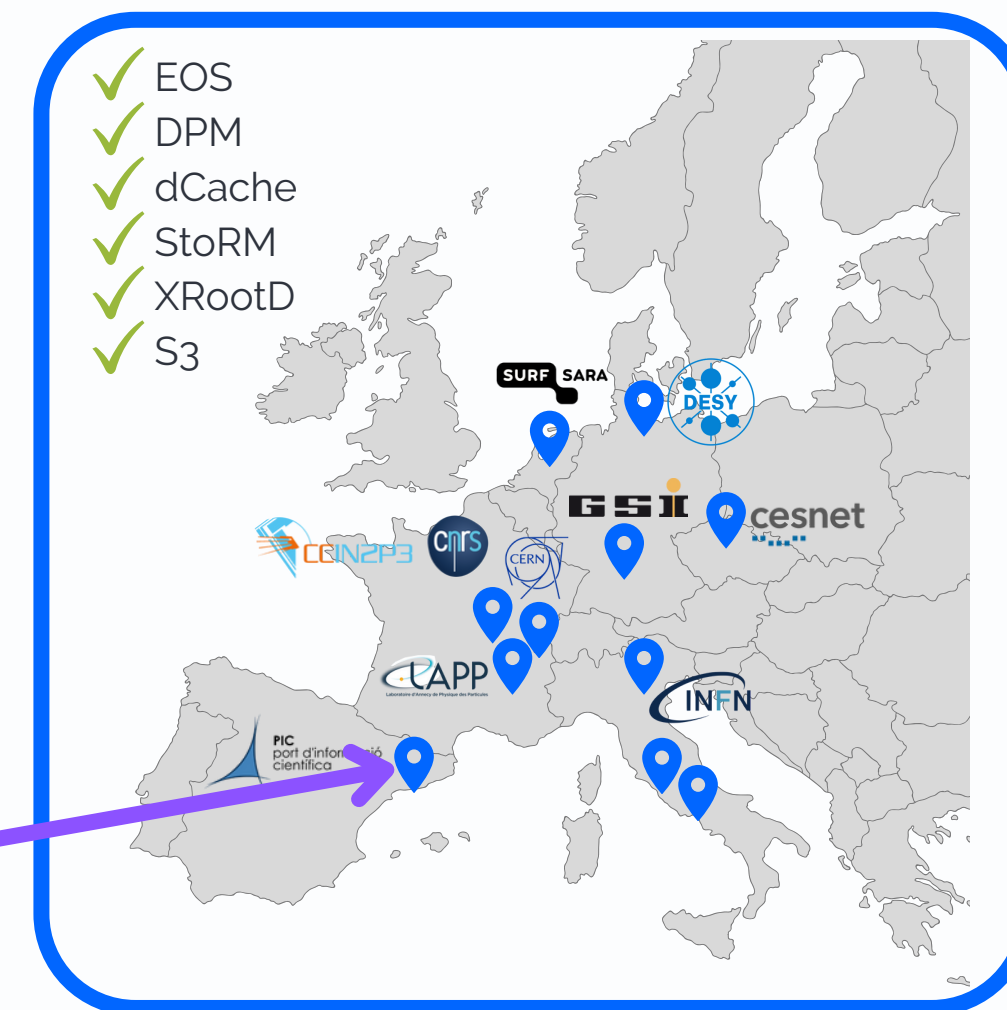
Non-local analysis preservation

From the Reana client:

- authenticate via IAM to Rucio with a side-car container
 - get data from distributed storage
- the analysis can be reproduced fully and **independently from local storage**

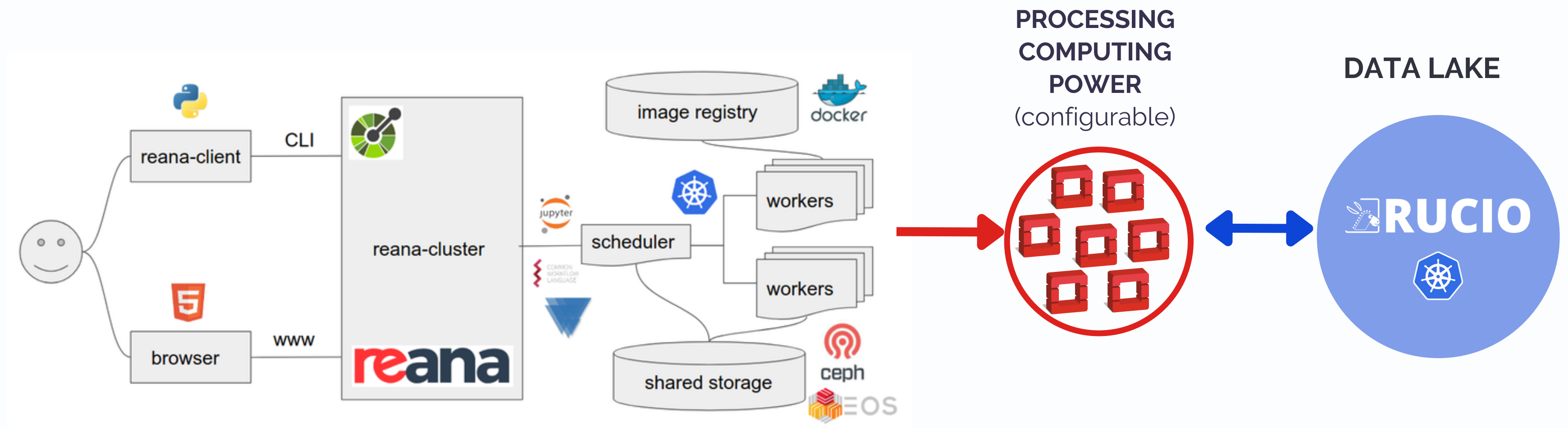


Data Lake



Analysis preservation and distribution

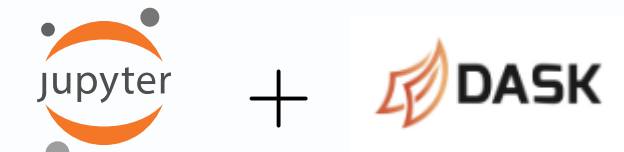
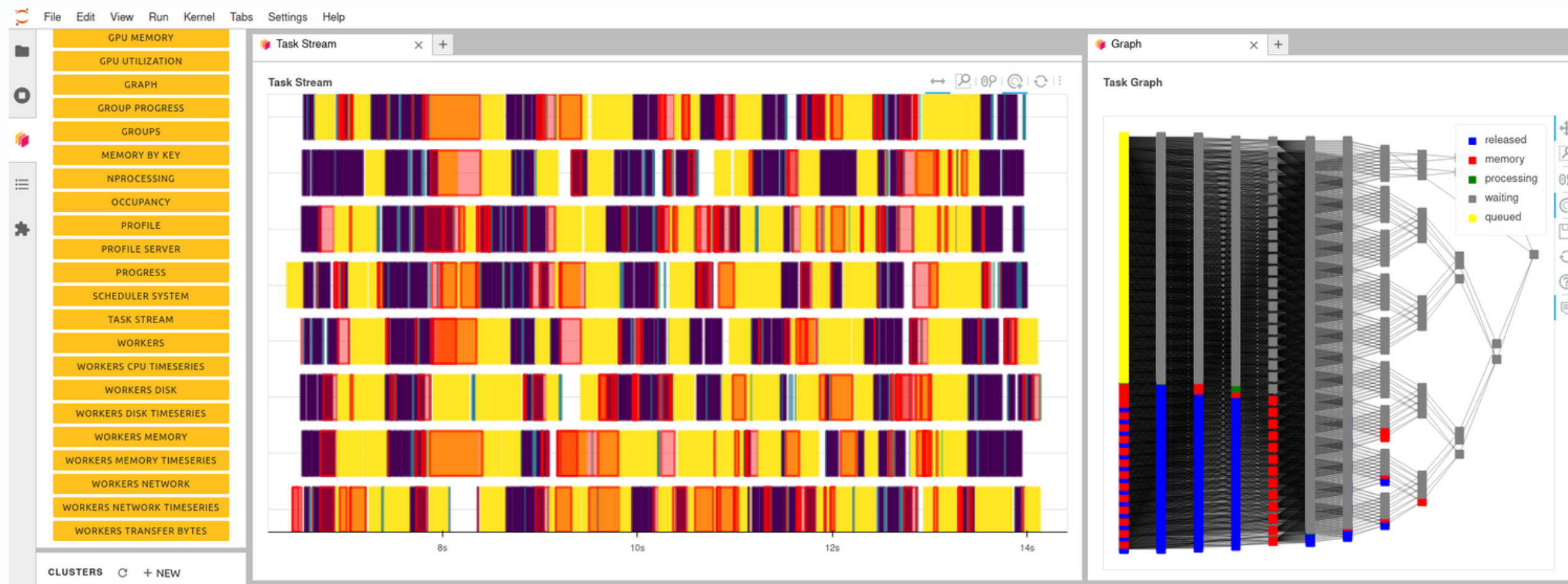
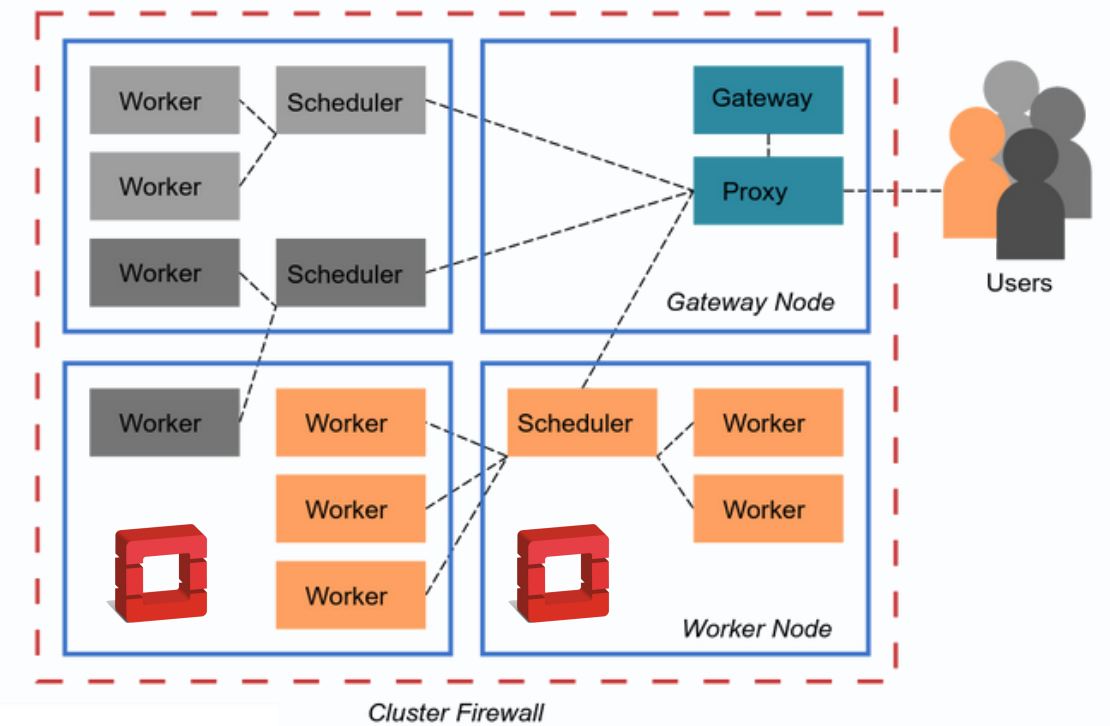
Reana makes preservation of heavier analyses seamless



Workflow distribution with Dask

Daskhub helm chart: Dask Gateway + Jupyterhub

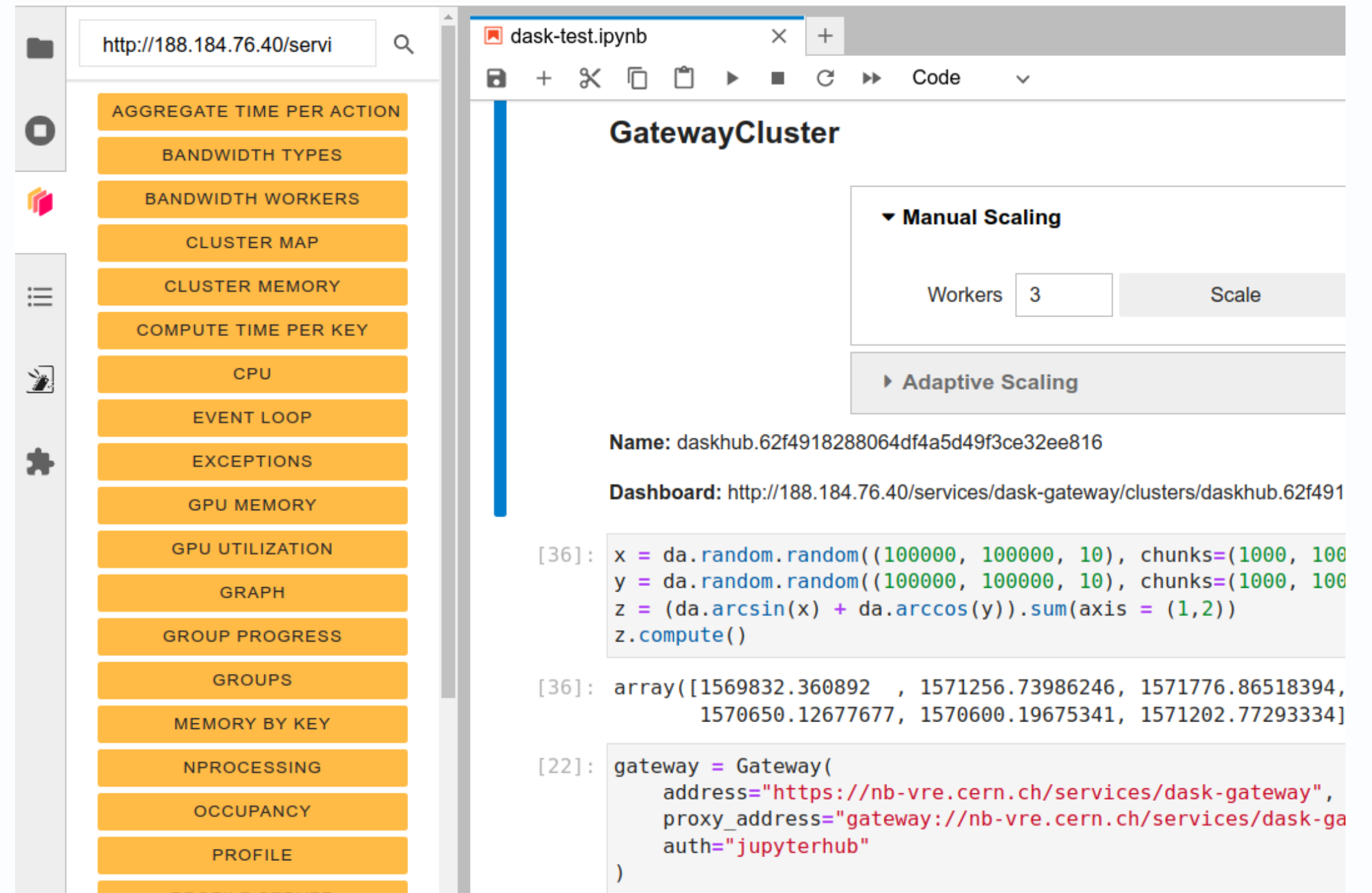
- multi-user, configurable usage profiles
- gateway to distribute access to all cloud nodes of the VRE
- code needs to be adapted
- dashboards of work progress



Workflow distribution with Dask

Work in progress:

Docker image with Rucio Jupyterlab extension and Dask, giving the possibility to spawn a cluster to each user



The screenshot displays a JupyterLab interface. On the left, a sidebar contains a search bar with the URL `http://188.184.76.40/servi` and a list of menu items: AGGREGATE TIME PER ACTION, BANDWIDTH TYPES, BANDWIDTH WORKERS, CLUSTER MAP, CLUSTER MEMORY, COMPUTE TIME PER KEY, CPU, EVENT LOOP, EXCEPTIONS, GPU MEMORY, GPU UTILIZATION, GRAPH, GROUP PROGRESS, GROUPS, MEMORY BY KEY, NPROCESSING, OCCUPANCY, PROFILE, and PROFILE SERVER. The main area shows a **GatewayCluster** dashboard for a cluster named `daskhub.62f4918288064df4a5d49f3ce32ee816`. The dashboard includes a **Manual Scaling** section with a `Workers` input field set to `3` and a `Scale` button, and an **Adaptive Scaling** section. Below the dashboard, a code cell [36] contains the following Python code:

```
[36]: x = da.random.random((100000, 100000, 10), chunks=(1000, 1000, 10))
      y = da.random.random((100000, 100000, 10), chunks=(1000, 1000, 10))
      z = (da.arcsin(x) + da.arccos(y)).sum(axis = (1,2))
      z.compute()
```

The output of the code cell is:

```
[36]: array([1569832.360892 , 1571256.73986246, 1571776.86518394,
          1570650.12677677, 1570600.19675341, 1571202.77293334])
```

Below the code cell, another code cell [22] shows the `Gateway` class initialization:

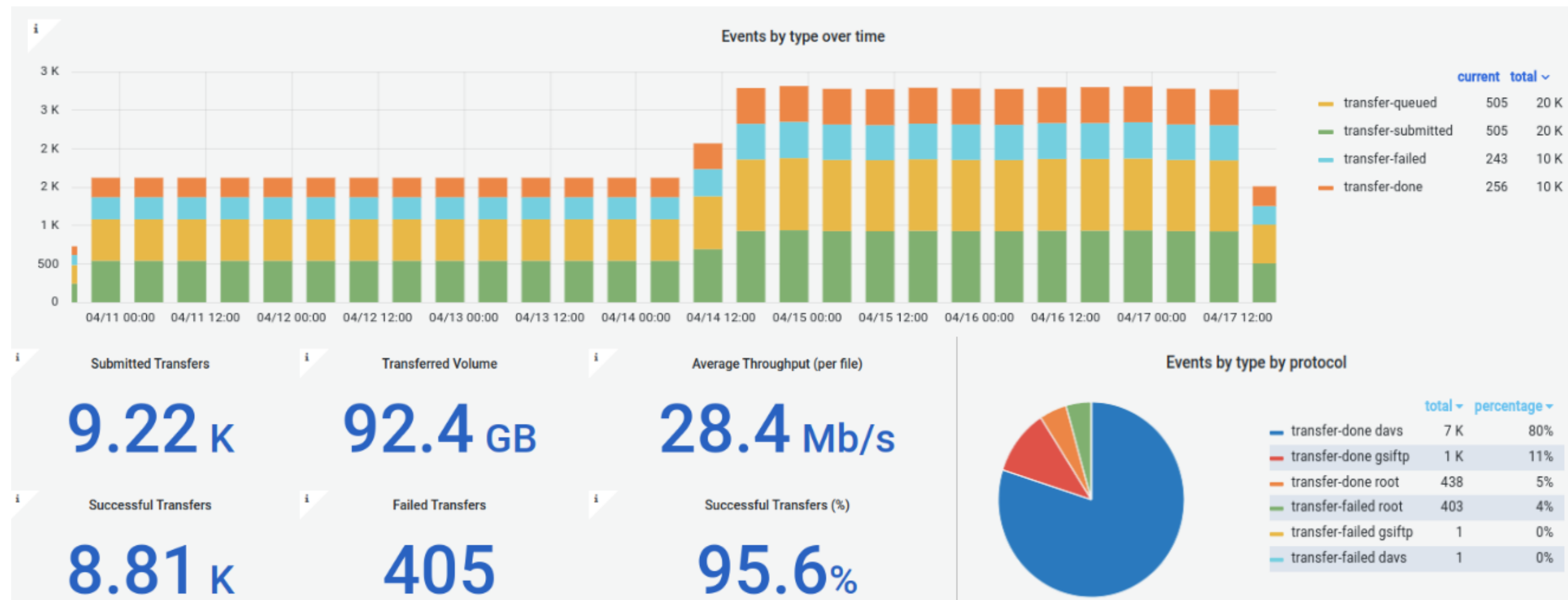
```
[22]: gateway = Gateway(
      address="https://nb-vre.cern.ch/services/dask-gateway",
      proxy_address="gateway://nb-vre.cern.ch/services/dask-ga",
      auth="jupyterhub"
    )
```



Monitoring, testing, dashboards, on-boarding

- Continuous **monitoring and testing** of transfers between Rucio Storage Elements (RSEs) is in place on Grafana dashboards hosted at CERN.

<https://monit-grafana-open.cern.ch/d/PJ65OqBVz/vre-rucio-events?orgId=16&from=now-7d&to=now>



Monitoring, testing, dashboards, on-boarding

- **Rucio and Reana UI** interfaces deployed with K8s allow to explore and debug failed transfers and workflows.

<https://reana-vre.cern.ch/>

<https://vre-rucio-ui.cern.ch>

AnalysisElenaNontuples #3
Finished 16 days ago

finished in 3 min 44 sec
step 4/4

Engine logs Job logs Workspace Specification

Step htupleAnalysisEl finished in 47 seconds Kubernetes ghcr.io/vre-hub/atlas-dilepton:latest \$ echo 'Current Directory' echo \$PWD I...

```
-rw-rw-r--. 1 root root 26222 Apr 21 10:32 prunSelector.py
drwxrwxr-x. 1 root root 25 Apr 21 10:34 recast
-rw-rw-r--. 1 root root 11825 Apr 21 10:32 runSelector.py
-rw-rw-r--. 1 root root 172 Apr 21 10:32 runprunSelector.py
-----
Error in <TChain::LoadTree>: Cannot find tree with name nominal in file
ntuples/mc16a/user.dummy.recastSignal.mc16_13TeV.500353.MGPy8EG_MET_50_lv_lds_mZp_500_ee_minitrees.root/user.dummy.dummy._000001.
minitrees.root
Error in <TChain::LoadTree>: Cannot find tree with name nominal in file
ntuples/mc16a/user.dummy.recastSignal.mc16_13TeV.500353.MGPy8EG_MET_50_lv_lds_mZp_500_ee_minitrees.root/user.dummy.dummy._000001.
minitrees.root
Error in <TChain::AddBranchToCache>: Could not load a tree
Error in <TChain::LoadTree>: Cannot find tree with name nominal in file
ntuples/mc16a/user.dummy.recastSignal.mc16_13TeV.500353.MGPy8EG_MET_50_lv_lds_mZp_500_ee_minitrees.root/user.dummy.dummy._000001.
minitrees.root
user.dummy.recastSignal.mc16_13TeV.500353.MGPy8EG_MET_50_lv_lds_mZp_500_ee_minitrees.root
Number of events to process: 0
```

Name	Account	RSE Expression	Creation Date	Remaining Lifetime	State
elena_test:2023.03.16-11.19.03.txt	egazzarr	EULAKE-1	2023-05-07T13:22:23.000Z	7d	STUCK
user.ron:test_from_CERN-030523_1643.txt	garcia	SURF-IOP-EXP	2023-05-04T10:35:14.000Z	-	STUCK
user.ron:test_from_CERN-030523_1643.txt	garcia	EULAKE-1	2023-05-03T14:43:27.000Z	-	OK
user.ron:mytestfile_2	garcia	DESY-DCACHE	2023-05-03T14:35:27.000Z	-	OK
elena_test:test-file-rucio-2023-04-24-01.txt	egazzarr	PIC-DCACHE	2023-04-24T14:13:33.000Z	-	OK
elena_test:test-file-rucio-2023-04-24-02.txt	egazzarr	PIC-DCACHE	2023-04-24T14:12:45.000Z	-	REPLICATING
elena_test:test-file-rucio-2023-04-24-01.txt	egazzarr	EULAKE-1	2023-04-24T14:12:12.000Z	-	OK
elena_test:test-file-rucio-2023-04-20-04.txt	egazzarr	IN2P3-CC-DCACHE	2023-04-20T15:08:51.000Z	-	REPLICATING
elena_test:test-file-rucio-2023-04-20-03.txt	egazzarr	DESY-DCACHE	2023-04-20T15:06:00.000Z	-	REPLICATING
elena_test:test-file-rucio-2023-04-19-01.txt	egazzarr	SURF-IOP-EXP	2023-04-19T15:53:19.000Z	-	STUCK
elena_test:test-file-rucio-2023-04-19-01.txt	egazzarr	IN2P3-CC-DCACHE	2023-04-19T15:42:32.000Z	-	OK
elena_test:test-file-rucio-2023-04-19-01.txt	egazzarr	EULAKE-1	2023-04-19T15:35:53.000Z	-	OK
elena_test:test-file-rucio-2023-04-19-01.txt	egazzarr	DESY-DCACHE	2023-04-19T15:33:53.000Z	-	OK
elena_test:test-file-rucio-2023-04-19-01.txt	egazzarr	CESNET-S3	2023-04-19T15:33:34.000Z	-	OK

Monitoring, testing, dashboards, on-boarding

- **Documentation** is hosted on Github pages and is made easy for both users and system administrators who would like to get inspired by the VRE model.

<https://vre-hub.github.io/>

The VRE

A comprehensive analysis platform to serve the particle physics and astrophysics community.

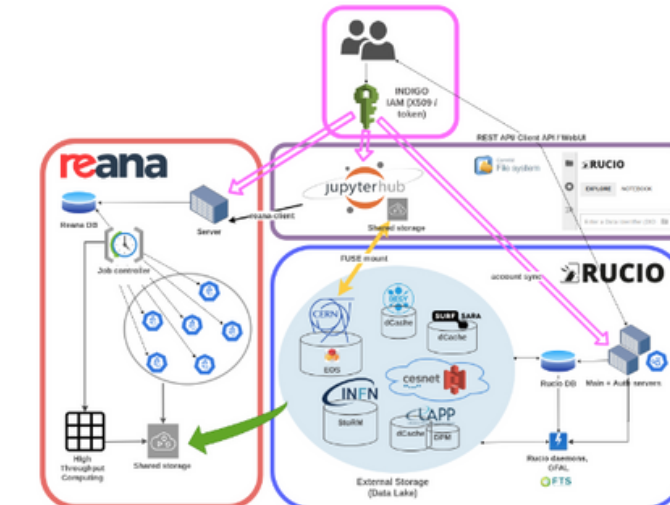
[View My GitHub Profile](#)

The Virtual Research Environment

The Virtual Research Environment is an analysis platform developed at CERN serving the needs of scientific communities involved in European Projects. Its scope is to facilitate the development of **end-to-end physics workflows**, providing researchers with access to an **infrastructure** and to the digital content necessary to produce and preserve a scientific result in compliance with **FAIR** principles. The platform's development is aimed at demonstrating how sciences spanning from High Energy Physics to Astrophysics could benefit from the usage of common technologies, initially born to satisfy CERN's **exabyte-scale data** management needs.

The Virtual Research Environment's main components are:

1. A federated and reliable **Authentication and Authorization** layer
2. A **federated distributed storage** solution (the Data Lake), providing functionalities for data injection and replication through a Data Management framework (Rucio)
3. A **computing** cluster supplying the processing power to run full analyses with Reana, a re-analysis software
4. An enhanced **notebook interface** with containerised environments to hide the infrastructure's complexity from the user.



The deployment of the Virtual Research Environment is open-source and modular, in order to make it easily reproducible by partner institutions; it is publicly accessible and kept up to date by taking advantage of state of the art IT-Infrastructure technologies.

The Science Projects which are using the VRE are described [here](#).

If you are a scientist or a new user curious to use the above resources, please refer to the following documentation:

1. [AAI](#)
2. [Rucio Data Lake](#)
3. [Reana cluster](#)
4. [Notebook service](#)

Hosted on GitHub Pages — Theme by [orderedlist](#)

Deployment

VRE public Github repository hosts

- cloud deployment of the infrastructure components with Helm, Flux, Terraform and K8s
- Science Projects software to produce the environments for the Jupyterhub instance
- scientific code to be shared
- reana.yaml files to reproduce the analysis
- forums and discussions

<https://github.com/vre-hub>



Virtual Research Environment
Technologies developed by CERN within the EOSC Future project to promote open science and collaboration between astrop...

3 followers Switzerland <https://eoscfuture.eu> @EOSCFuture vre-admin@cern.ch

Overview Repositories 10 Discussions Projects 1 Packages Teams 1 People 5

README .md

Virtual Research Environment

EOSC Future is an EU-funded H2020 project that is implementing the European Open Science Cloud (EOSC). EOSC will give European researchers access to a wide web of FAIR data and related services.

Our team at CERN is developing and contribution to the infrastructure code base of [EOSC](#).

More information can be found on our [website](#).

Pinned

- vre** Public
VRE infrastructure template running at CERN
Shell 3
- environments** Public
VRE user environment images for workflows and notebooks
C++
- science-projects** Public
VRE example science projects
Jupyter Notebook
- vre-hub.github.io** Public
VRE user documentation
HTML

Repositories

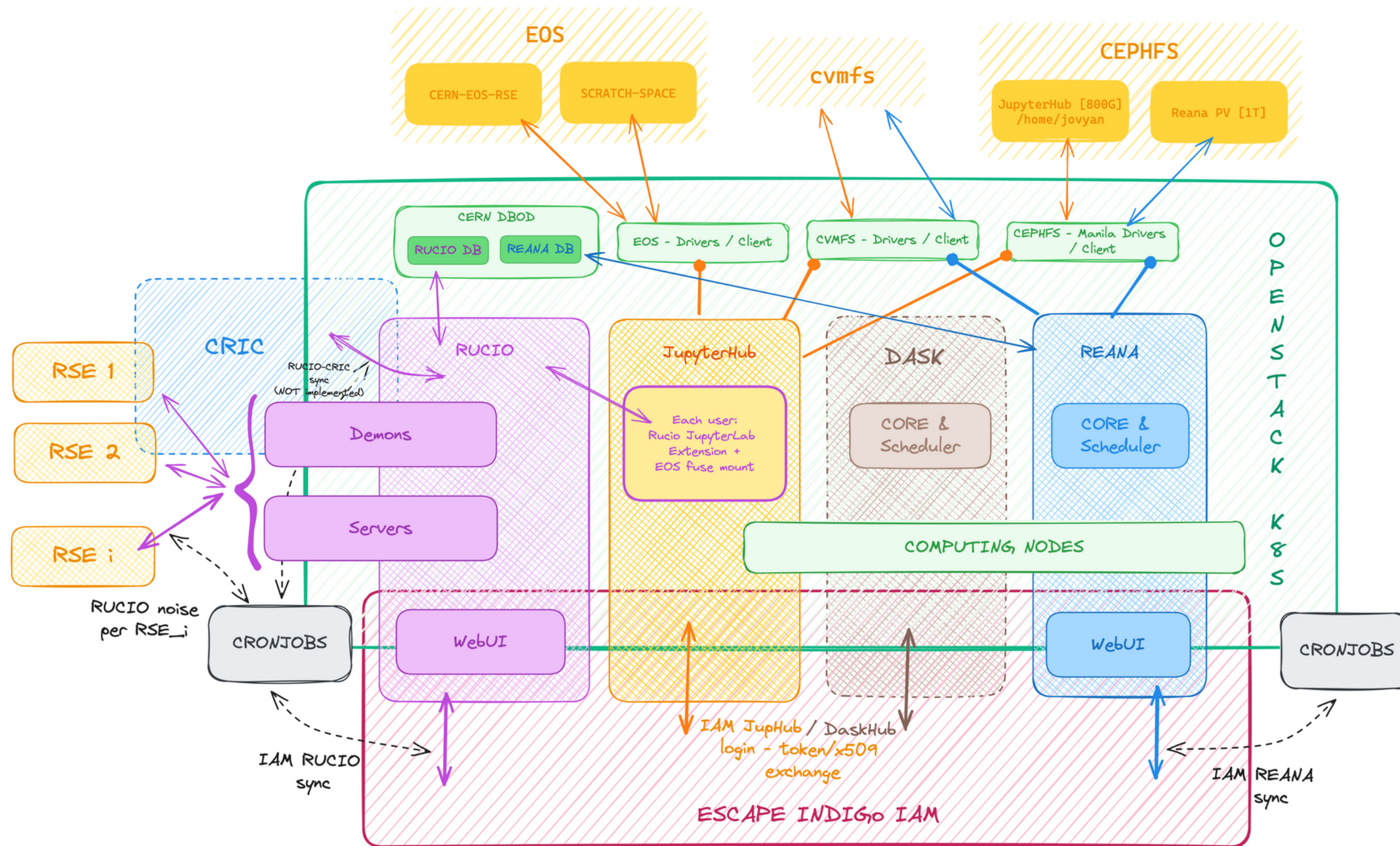
Find a repository... Type Language Sort New

- environments** Public
VRE user environment images for workflows and notebooks
C++ 0 stars 0 forks 0 issues 0 pull requests Updated last week
- vre** Public
VRE infrastructure template running at CERN
Shell 3 stars 0 forks 0 issues 0 pull requests Updated 2 weeks ago

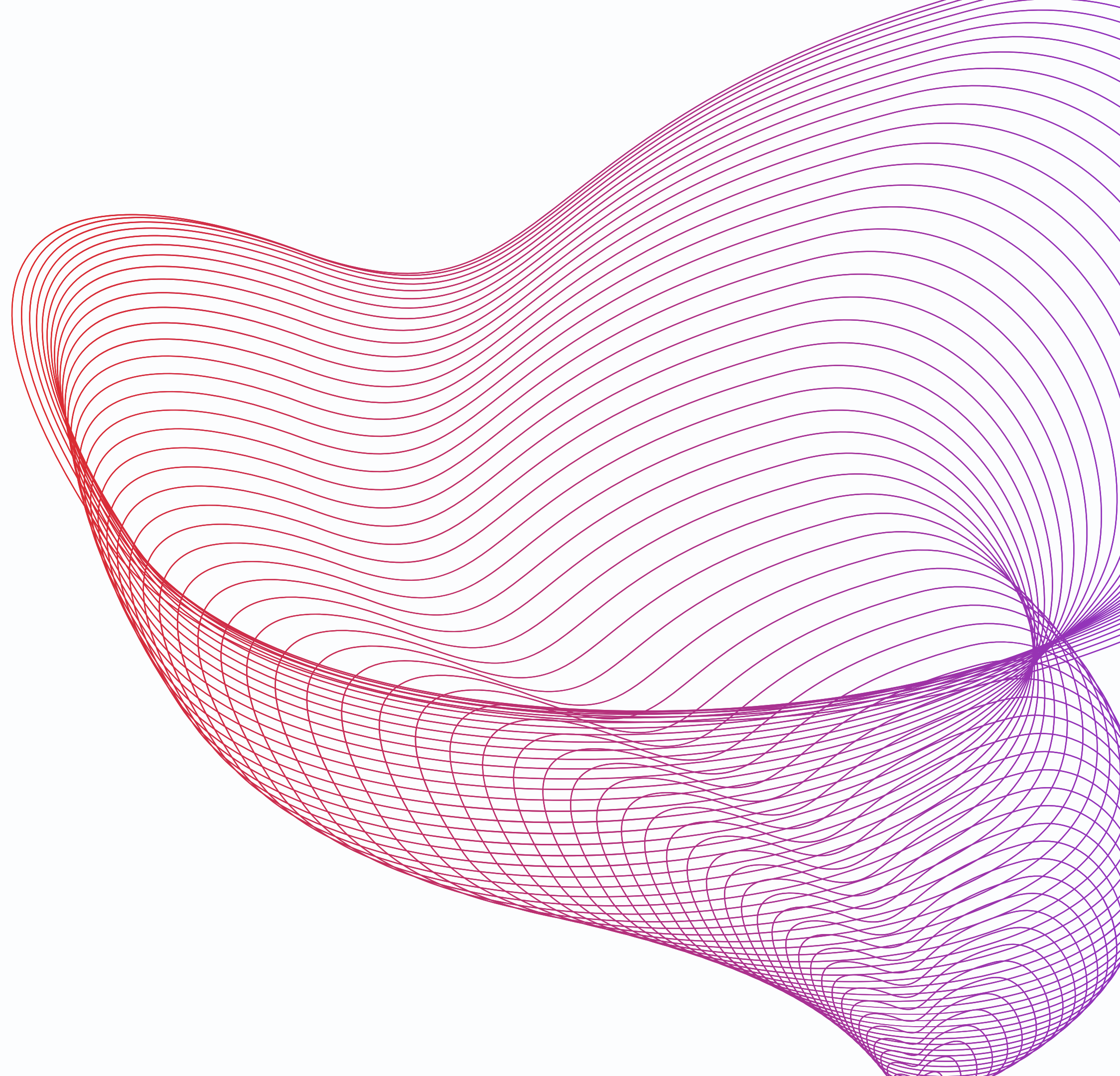
Support and meetings

- VRE users support meeting every 2 Tuesdays @14
- VRE working group meeting 1st Thursday of the month @11
 - for developers and system administrators who are building and deploying scientific infrastructures within the broad field of scientific analysis platforms

CERN VRE architecture: a closer look

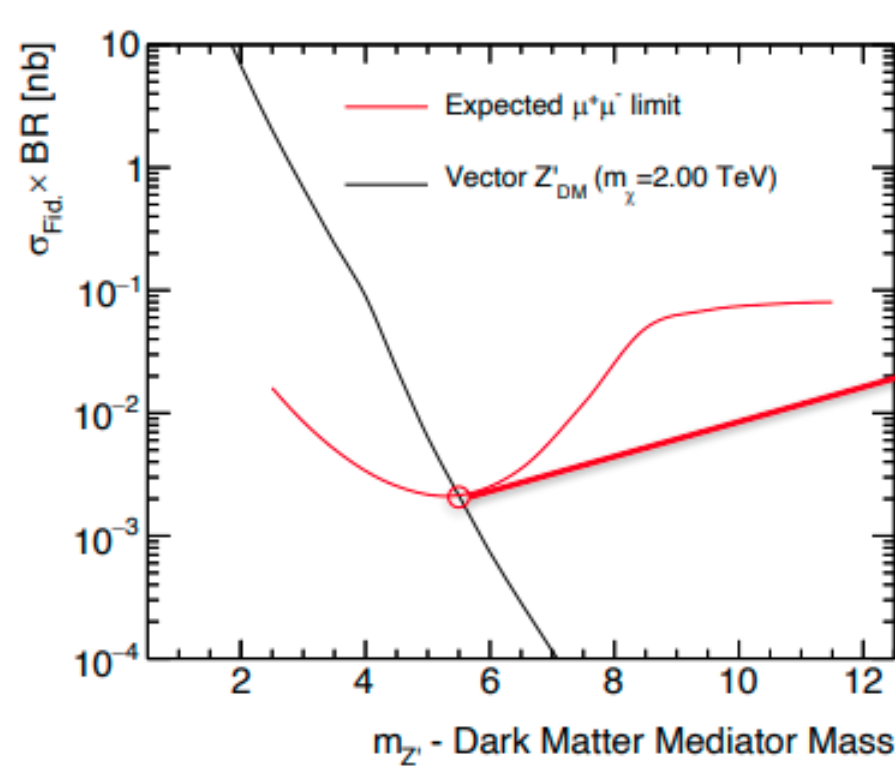


Demo

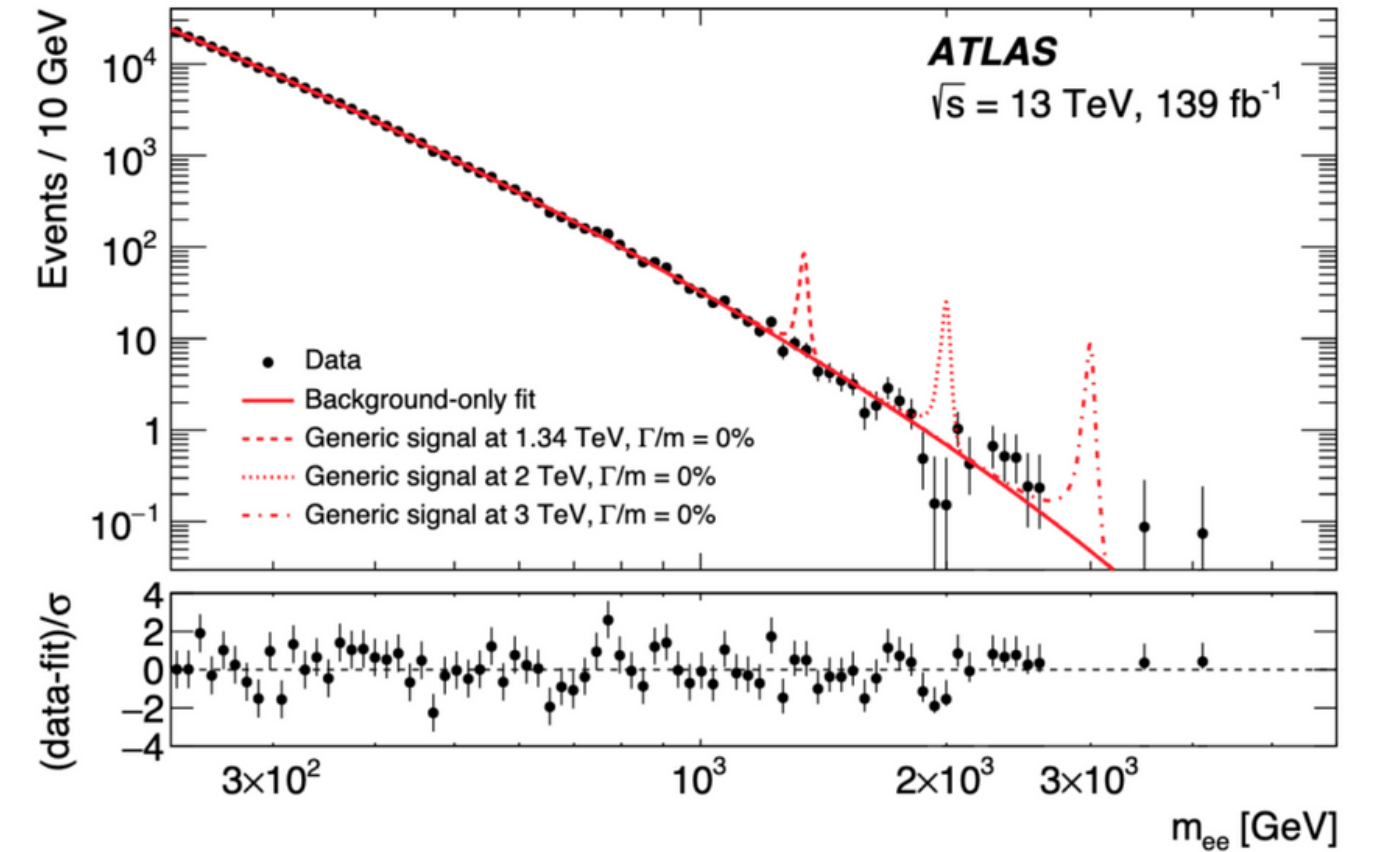
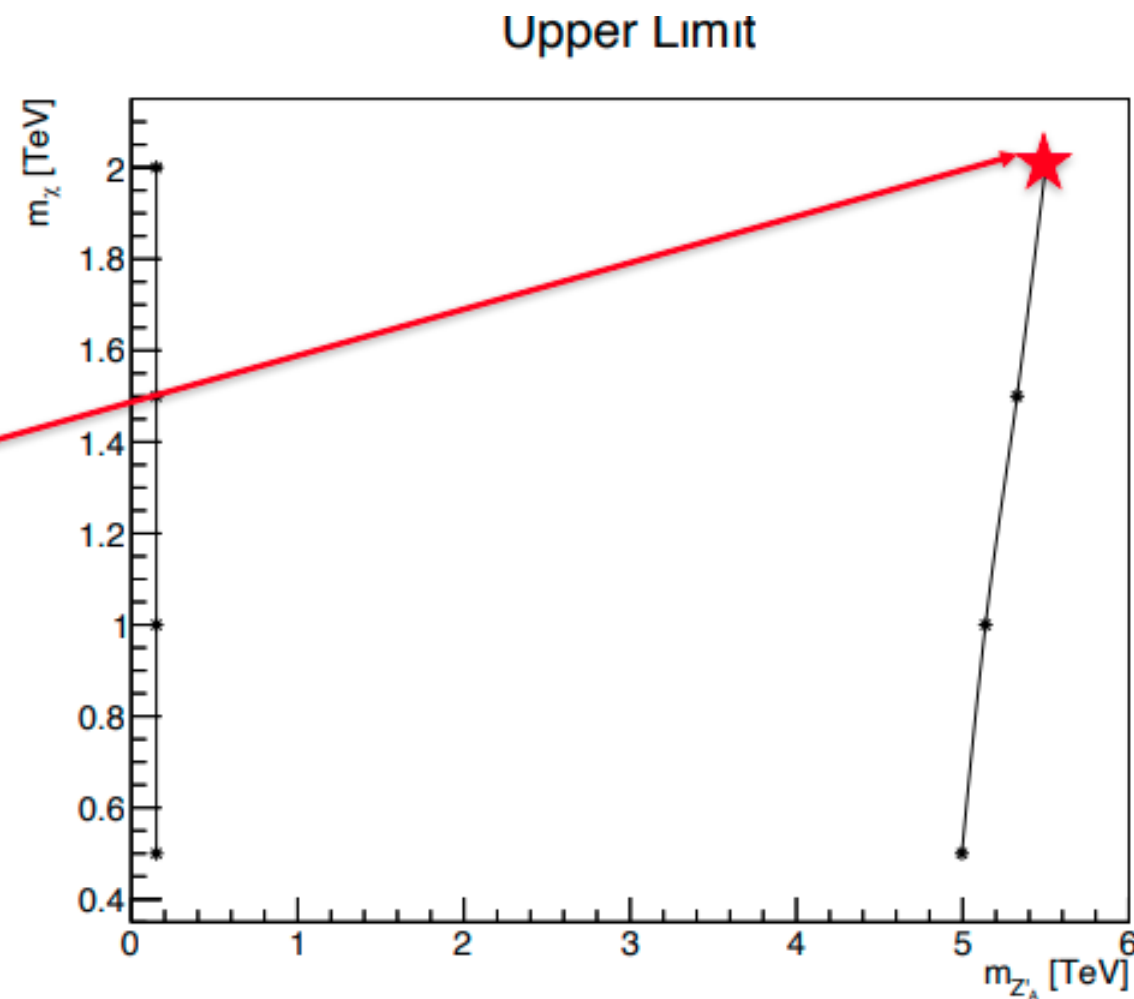


DM@LHC with ATLAS

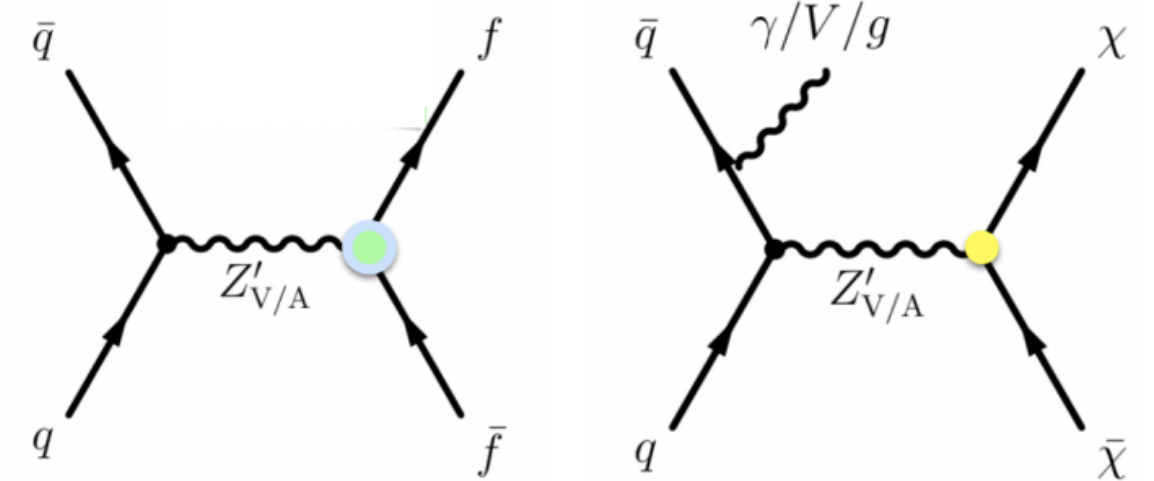
1. **Dark Matter Reinterpretation:** setting limits on High-Luminosity LHC constraints on $Z' \rightarrow \chi\chi$ (Z' mediated Dark Matter models).
2. The **dilepton** inclusive search (right) concluded in 2019
 - a. objective: projecting limits to 14 TeV and computing the fiducial cross-sections in **lower mass regions.**



Expected DM limits at 14TeV.



Dilepton Inclusive Search. Results of this analysis demonstrate good agreement with SM predictions.



See yesterday's talk by J. Little



Your workflows

Refreshed at 07:48:12 UTC

Search...

Status Latest first

rucio #28 **pending**
 Created a few seconds ago step 0/0

rucio #27 **created**
 Created a few seconds ago step 0/0

rucio #26 **finished** in 44 seconds



Watch on YouTube

https://www.youtube.com/watch?v=hvJLo_7xXc&ab_channel=ElenaGazzarrini



Success stories

- Escape Open Collaboration Agreement ensures the collaboration and joint common activities across scientific communities in the development of VREs
- VRE awoke interest from scientific domains who are in early-stage prototype phase (i.e. Einstein telescope)
- Interest from new digital models (i.e. digital twins) developed within European projects

Future outlook

VRE future steps:

- connection with HPCs, commercial clouds and other external computing resources
 - Caching data on distributed storage
 - Engage more scientific communities
-
- The pursuit of commonalities in Scientific Computing is fundamental to pursue economies of scale at all levels.
 - Agreed joint multi-year roadmaps is mandatory if we pursue common approaches in the areas of **Data Management, Data Analysis, Security, Networking and Software.**
 - Promoting alignment of efforts and ensuring positive return is challenging but is the way to go
 - --> **VRE + ESAP could align their interests and join their efforts**

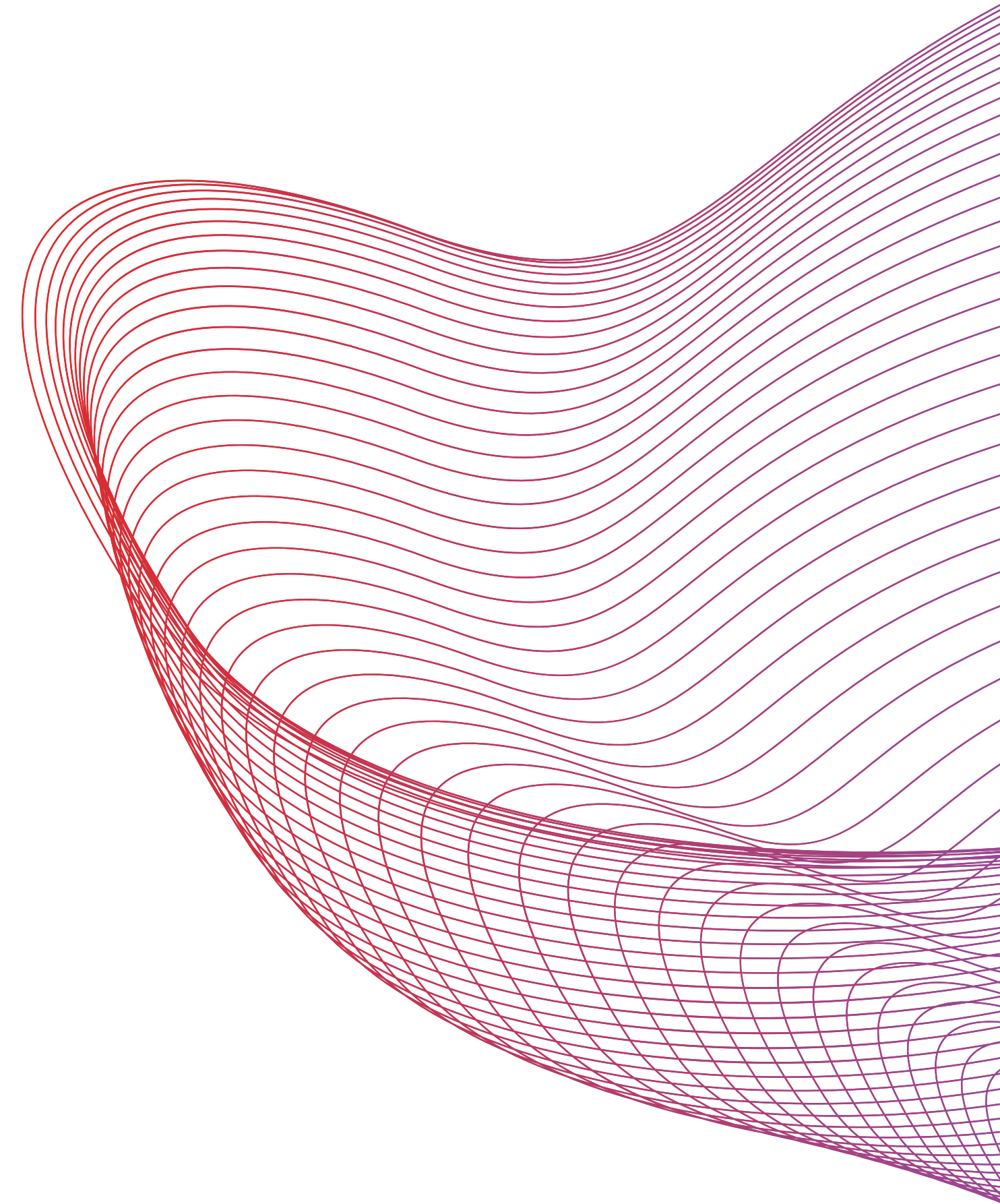
Thank you

special thanks to

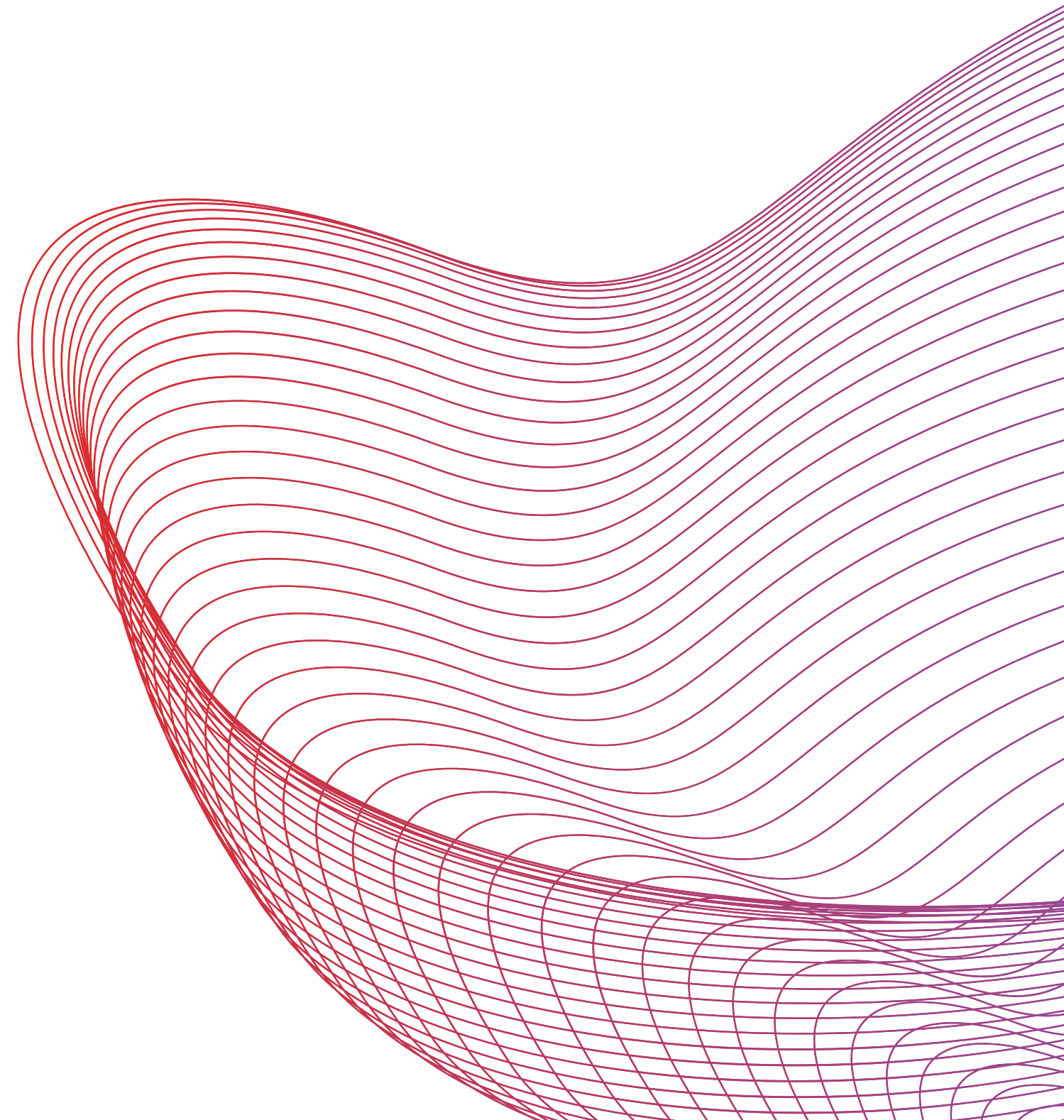
Tibor Simko & Reana team, Martin Barisits & Rucio team, Xavier Espinal, Ian Bird, CNAF IAM team and all the Science Projects researchers (Jared Little, Caterina Doglioni, Christopher Eckner, Alexander Ekman, Axel Gallen, Mikhail Smirnov, Francesca Calore, Pooja Bhattacharjee, Valerio Ippolito, Estelle Pons, Elena Cuoco, Alberto Iess, Alessandro Parisi, Dany Vohl)

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Back up



Status

The VRE is an R&D project and it is not a production system. As such, the platform is maintained by a team of 3 people.

For the moment, ~ 230 users subscribed on the IAM platform and have therefore access to the resources.

VRE documentation and links to resources at: <https://vre-hub.github.io/>.

Links to useful related works are provided by clicking on the underlined text in the slides.

vCPUs	RAM (GB)	Masters	Nodes	Remote Storage (TB)	CephFS (TB)
184	335.8	3	23	646	1.8

25 Openstack machines

- 14.6GB RAM
- 8 VCPU
- 80GB Disk
- Fedora CoreOS 35
- LINUX