Current CERN platforms for reproducible and interactive scientific analysis

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What is an analysis facility?

Analysis Facilities White Paper

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[b] Editor, [1] INFN, [2] University of Manchester, [3] Technische Universität München, [4] University of Warwick [5] University of Washington [6] Brookhaven National Laboratory [7] Morgridge Institute for Research [8] University of Chicago [9] University of Oslo [10] Ludwigs-Maximilians Universität München [11] Princeton University [12] Syracuse University [13] University of Wisconsin-Madison [14] University of Oxford [15] Technische Universität Dortmund [16] FNAL [17] CIEMAT [18] IFIC [19] TIFR [20] Purdue University [21] University of Bristol [22] Rice University [23] Paul Scherrer Institute [24] Helsinki Institute of Physics [25] University of Michigan [26] University of Illinois at Urbana-Champaign [27] University of Massachusetts Amherst [28] IFAE [29] University of Liverpool [30] University of Birmingham [31] CERN [32] University of Nebraska-Lincoln [33] SCIPP UC Santa Cruz [34] University of Hamburg [35] Massachussets Institute of Technology [36] Karlsruhe Institute of Technology

What is an analysis facility?

Analysis facility (AF): infrastructure and services that provide integrated data, software and computational resources to execute one or more elements of an analysis workflow.

- Perform fast research iterations on large datasets interactively.

- Convert interactive to batch-schedulable workloads.

- Interact with the WLCG and scale outside of the facility on occasion.

- Reproducibly instantiate desired software stack.

- Collaborate in a multi-organisational team.

- Efficiently train machine learning models for HEP.

The CERN ecosystem
A facility of Analysis Facilities

VRE@CERN

reana

SWAN

LxBatch

HTCondor

LxPlus

Kubeflow

EOS

CVMFS

SWAN at CERN
Service for Web based ANalysis

Jupyter notebooks technology

- Interactive analysis with a web browser
  - No local installation is needed
  - Based on Jupyter Notebooks
  - Calculations, input data and results "in the Cloud"

- Good for data analysis and exploration, but also for teaching

- Easy sharing of scientific results: plots, data, code

- Added value: integration with CERN infrastructure and services!

UI/Core

Analysis platforms

Compute

Software

Storage
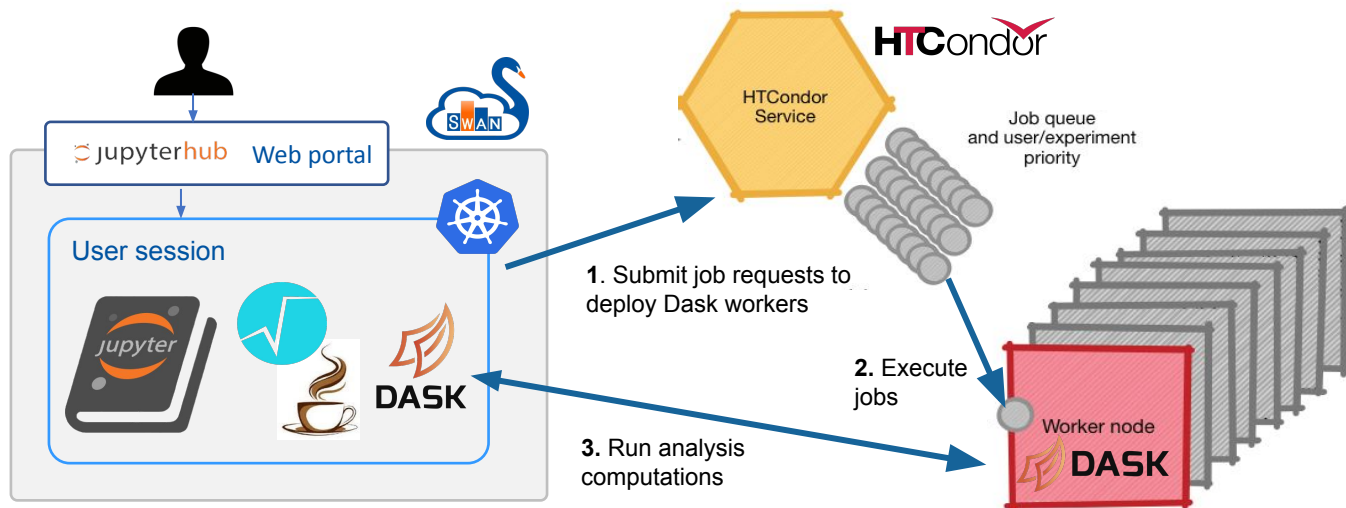
Infrastructure

SWAN at CERN
Spinning up the service

The CERN pilot Analysis Facility
Scaling columnar interactive analysis to batch

Leverages CERN resources (HTCondor)
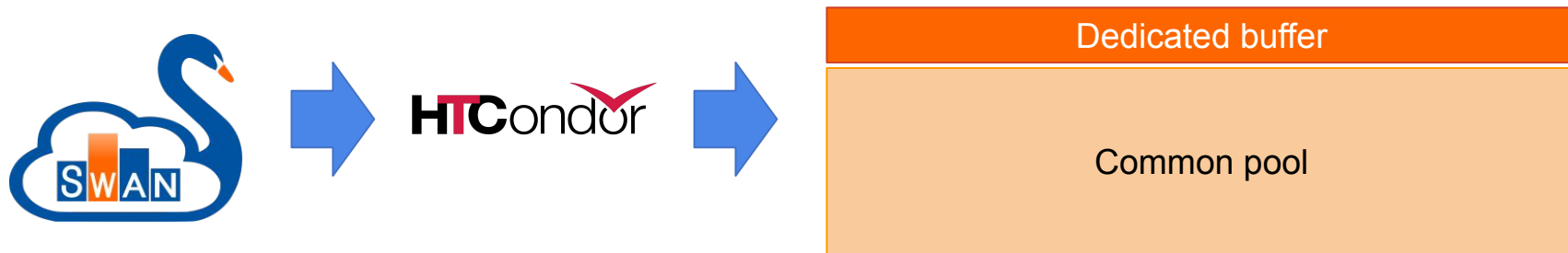- Via RDataFrame / coffea + Dask

The CERN pilot Analysis Facility
Scaling interactive analysis to batch

Pilot's interactive jobs benefit from dedicated resources in the CERN HTCondor pool
- Dedicated buffer of ~1.2k cores for quick (number) allocation of resources
- Extra resources from common pool, job start time **subject to experiment quotas**

Best test users for the pilot

User's profile

- Have a columnar-based analysis (**RDataFrame** or **Coffea)** that leverages Dask.
- Be able to submit condor batch jobs on lxplus.
- Have data stored on eos.

What feedback we would like to have

- Clarity of documentation.
- What **you like**, what you **don't like** and *what you __would__ like.*
- Signal any possible improvements so that it suits better the needs of an analyser.
- Report issues with interface, resource allocation, analysis execution, data access, software, …

More information on SWAN and the pilot at
https://swan.docs.cern.ch

Do you have a use case for the pilot?
Join the Mattermost Channel

(First join the IT-dep mattermost team)

What is an analysis facility?
A quick recap

Analysis facility: infrastructure and services that provide integrated data, software and computational resources to execute one or more elements of an analysis workflow.

- ✅ Perform fast research iterations on large datasets interactively.
- ✅ Convert interactive to batch-schedulable workloads.
- ✅ Interact with the WLCG and scale outside of the facility on occasion.
- ❓ Execute desired analysis workflows reproducibly.
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REANA

Reproducible research data analysis platform

REANA is a reproducible analysis platform allowing scientists to run **declarative computational data analysis** pipelines on containerised compute clouds.

REANA was built with the goal of **fostering computational reproducibility**.

It has installations and code distributions in Europe (e.g. AIP) and US (e.g. UChicago)

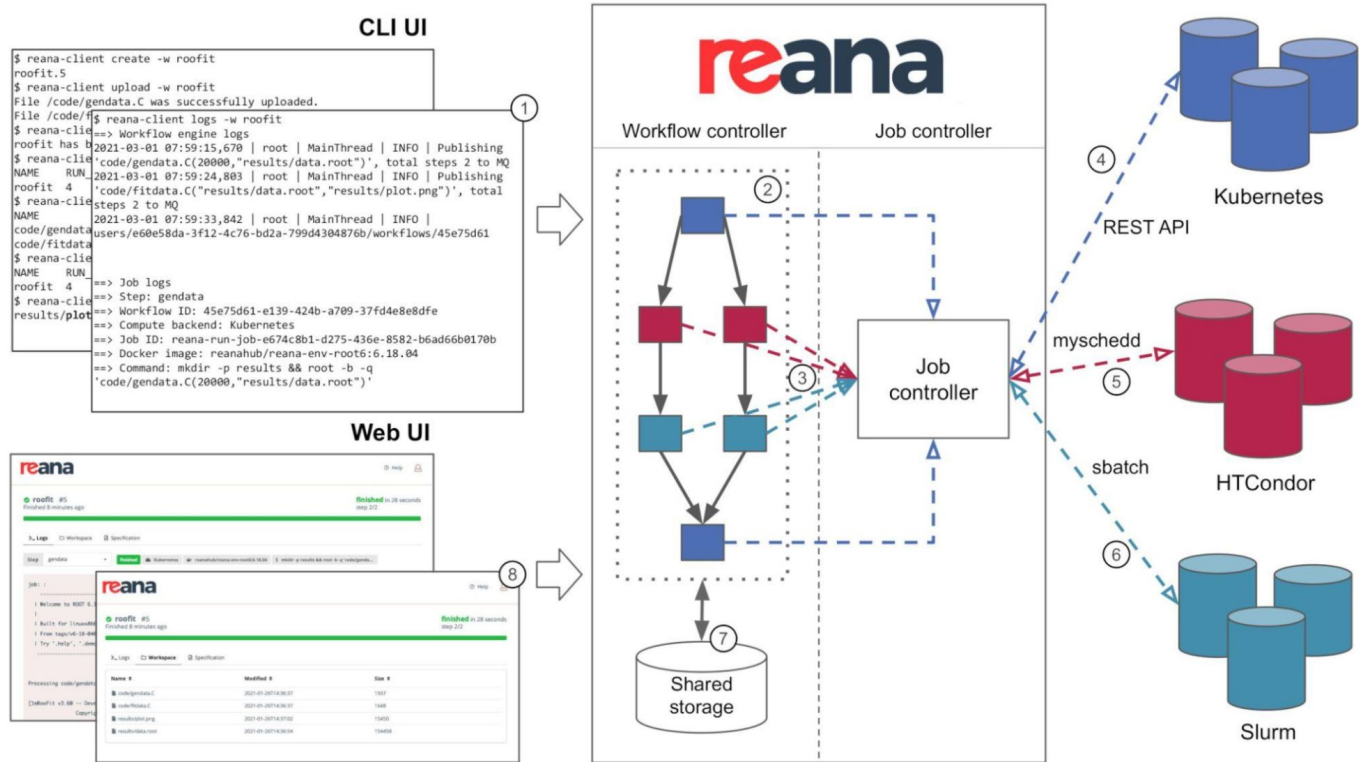| Flexible	Scalable	Reusable	Free
Run many computational workflow engines.	Support for remote compute clouds.	Containerise once, reuse elsewhere. Cloud-native.	Free Software. MIT licence. Made with ❤ at CERN.

REANA
Reproducible research data analysis platform

Multiple compute backends:
- Kubernetes
- HTCondor
- Slurm

Multiple workflow languages:
- CWL
- Serial
- Snakemake
- Yadage

Multiple means of use:
- Command-line client
- Web UI

REANA
A quickstart

```
# workflow/snakemake/Snakefile

rule all:
    input:
        "results/data.root",
        "results/plot.png"


rule gendata:
    output:
        "results/data.root"
    params:
        events=20000
    container:
        "docker://docker.io/reanahub/reana-env-root6:6.18.04"
    shell:
        """
        mkdir -p results
        root -b -q 'code/gendata.C({params.events},\"{output}\")'
        """


rule fitdata:
    input:
        data="results/data.root"
    output:
        "results/plot.png"
    container:
        "docker://docker.io/reanahub/reana-env-root6:6.18.04"
    shell:
        "root -b -q 'code/fitdata.C(\"{input.data}\",\"{output}\")'"
```

1 Structure your analysis

```
inputs:
  files:
    - code/gendata.C
    - code/fitdata.C
  directories:
    - workflow/snakemake
  parameters:
    input: workflow/snakemake/inputs.yaml
workflow:
  type: snakemake
  file: workflow/snakemake/Snakefile
outputs:
  files:
    - results/plot.png
```

more

2 Select a REANA cluster...

```
$ export REANA_SERVER_URL=https://
reana.cern.ch/
$ export REANA_ACCESS_TOKEN=XXXXXXX
```

...or install your own

```
# install kubectl 1.19+, kind 0.9+ and
helm 3.0+
$ sudo dpkg -i kubectl*.deb kind*.deb
kubernetes-helm*.deb
# create Kubernetes cluster (or use your
own!)
$ wget https://raw.githubusercontent.com/
reanahub/reana/maint-0.9/etc/kind-
localhost-30443.yaml
$ kind create cluster --config kind-
localhost-30443.yaml
$ wget https://raw.githubusercontent.com/
reanahub/reana/maint-0.9/scripts/prefetch-
images.sh
$ sh prefetch-images.sh
# deploy REANA using Helm
$ helm repo add reanahub https://
reanahub.github.io/reana
$ helm repo update
$ helm install reana reanahub/reana --wait
# create an admin user
$ wget https://raw.githubusercontent.com/
reanahub/reana/maint-0.9/scripts/create-
admin-user.sh
$ sh create-admin-user.sh default reana
john.doe@example.org mysecretpassword
```

more

3 Run your analysis

```
# create new virtual environment
$ virtualenv ~/.virtualenvs/myreana
$ source ~/.virtualenvs/myreana/bin/
activate
# install REANA client
$ pip install reana-client
# create new workflow
$ reana-client create -n my-analysis
$ export REANA_WORKON=my-analysis
# upload input code and data to workspace
$ reana-client upload ./code ./data
# start computational workflow
$ reana-client start
# check its progress
$ reana-client status
# list workspace files
$ reana-client ls
# open interactive notebook session
$ reana-client open jupyter
# download output results
$ reana-client download results/plot.png
```
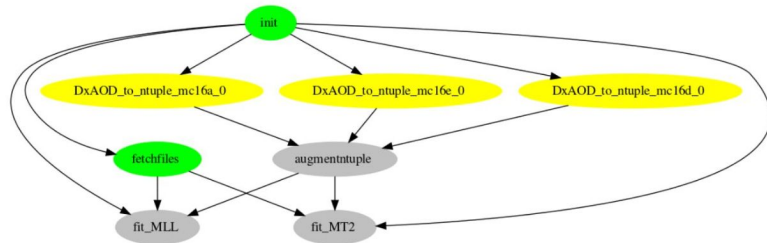
more

REANA

Usage example: pMSSM reinterpretation of ATLAS Run-2 searches
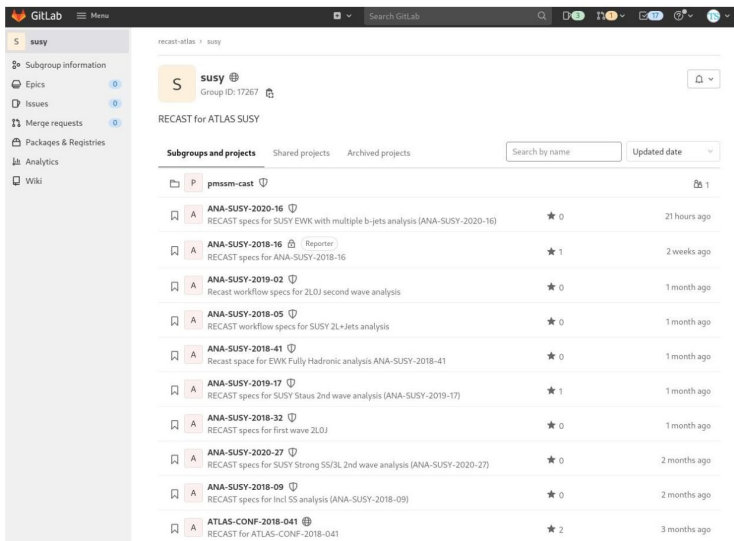

Figure 1. A screenshot of the ATLAS SUSY group analyses preserved on GitLab. Each repository is labeled with the internal ATLAS analysis identifier and contains both workflow files and additional data files needed for the computational processing.
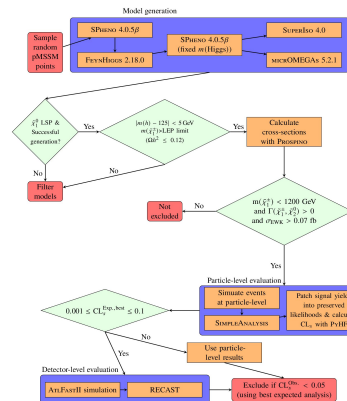
https://arxiv.org/abs/2403.03494

Figure 2. A typical pMSSM workflow. The computational runtime is about 10 minutes without systematics (test payload) and about 10 hours with all systematics (real payload).

https://arxiv.org/abs/2402.01392
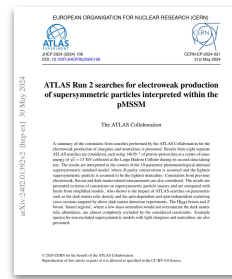
More information on REANA at
https://www.reanahub.io/

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I don't have a CERN account 😞

ESCAPE: European Science Cluster of Astronomy and Particle Physics

Consortium of 31 members, including:

- 10 ESFRI projects & landmarks: **CTA, EST, FAIR, HL-LHC, KM3NeT, SKA, LSST, VIRGO, ESO, JIVE**

- 2 pan-European International Organizations: **CERN and ESO**

- 2 European Research Infrastructures: **EGO and JIV-ERIC**

- 4 supporting European consortia: **APPEC, ASTRONET, ECFA and NuPECC**

Budget: **15.98 M€**

Duration: **48 months** (1/2/2019 -31/1/2023)

ESCAPE has received funding from the European Union's Horizon 2020 research and innovation programme under **Grant Agreement no. 824064**.
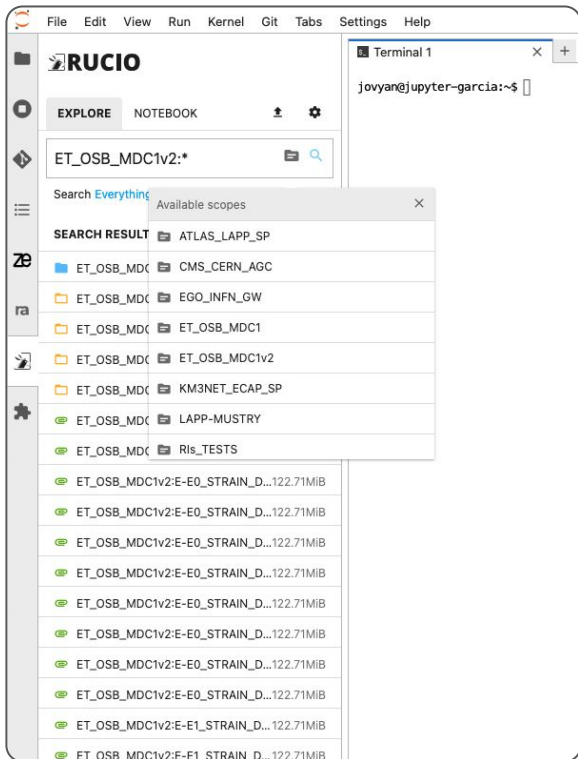
The CERN Virtual Research Environment
A CERN-agnostic version of SWAN

Authentication and authorization
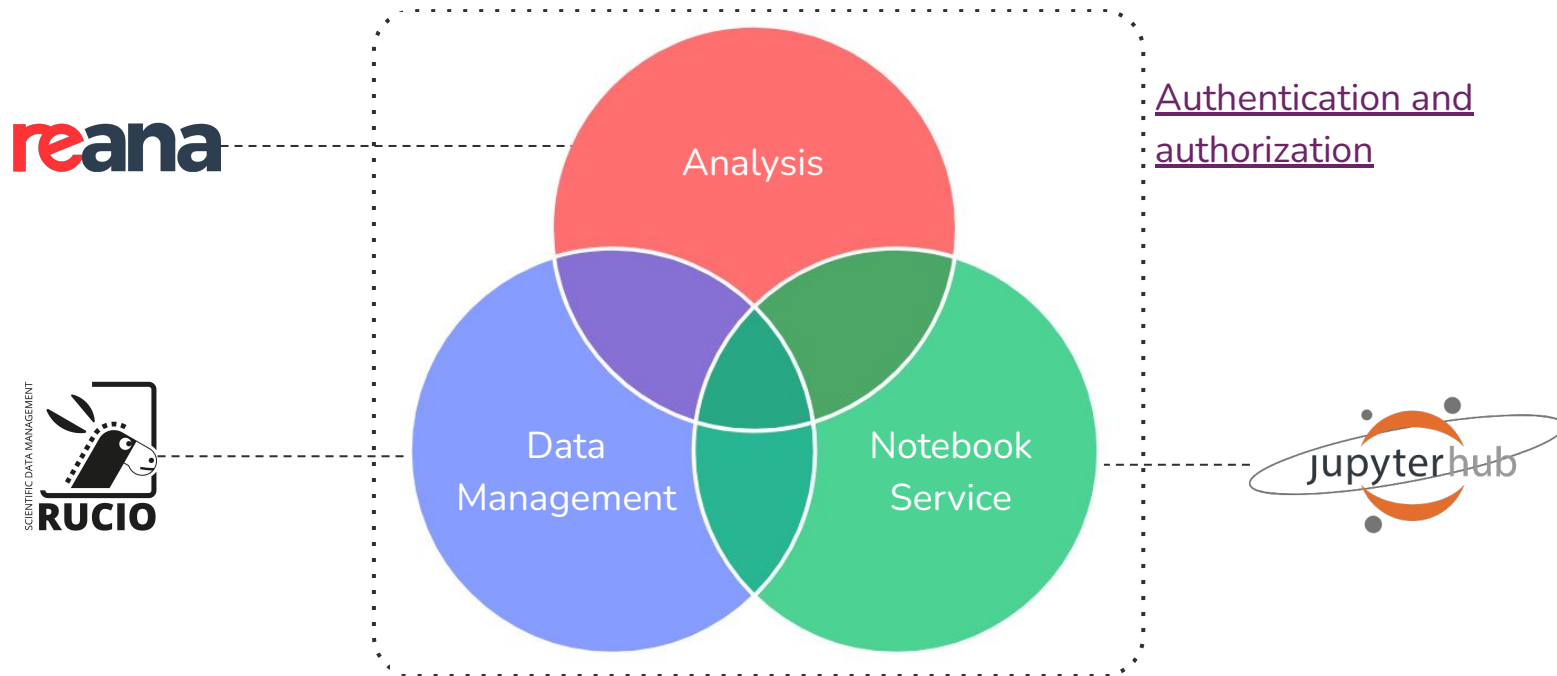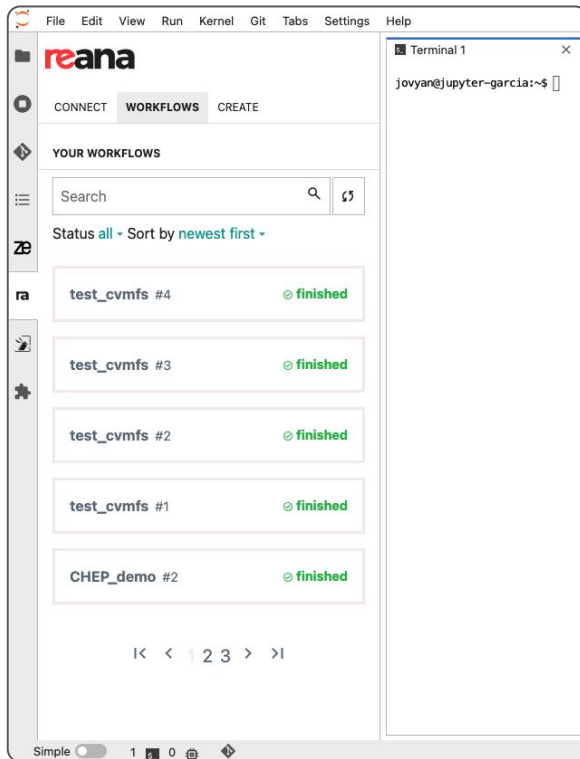
User's interactions with the VRE

Comparison
(is the thief of joy)

SWAN

Available at the click of a button ✅

Data persistence ✅

No account restrictions ❌

Change easily the software stack ✅

Access >200 cores ✅

Access to batch ✅

Access to GPUs ✅

Integration with Data Lake tech. ❌

Integration with REANA ❌

Production service
Can sustain heavy workloads

VRE@CERN

✅ Available at the click of a button

✅ Data persistence

✅ No account restrictions

✅ Change easily the software stack

❌ Access >200 cores

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✅ Integration with Data Lake tech.

✅ Integration with REANA

Proof of concept platform
Features more functionalities

More information on the VRE at
https://vre-hub.github.io/

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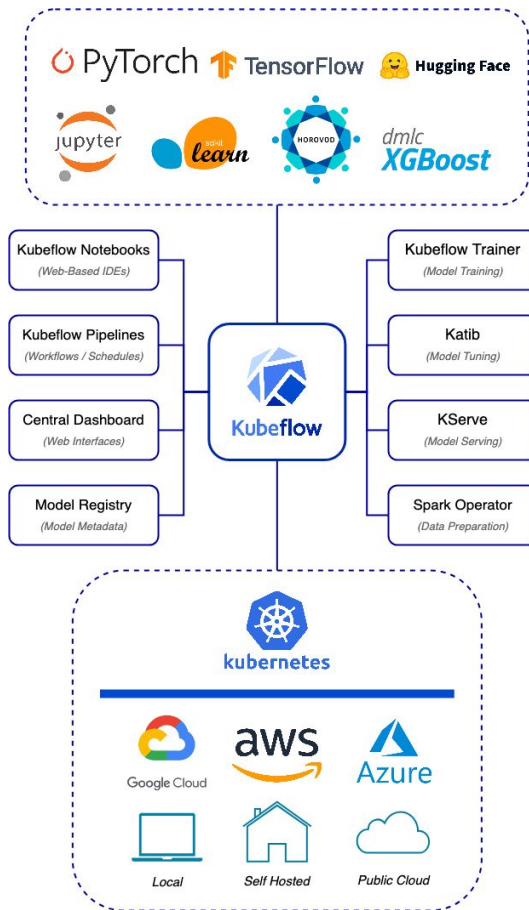
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ml.cern.ch
Run machine learning workloads

What is Kubeflow?

Kubeflow is a community and ecosystem of **open-source** projects to address each stage in the ML lifecycle

- **Community & Ecosystem:** Open-source projects addressing each stage of the ML lifecycle.

- **Purpose:** Simplifies, makes AI/ML on Kubernetes portable and scalable.

- **Audience:** Researchers, data scientists, ML engineers, developer teams.

- **Modular & Scalable Tools:** From building to deploying ML models for AI applications.

More information on ml.cern.ch at
https://ml.cern.ch/

Summary

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