Virtual Research Environment

Towards a comprehensive analysis platform

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Agenda

Motivation

Science use case

Components

Demo
Motivation
Data volumes growing not only at LHC

The LHC at CERN was the first large scientific experiment to generate and manage multi PBs of data per year.

Technologies to manage and process data initially developed at CERN are being adopted by other collaborations, as new generation of detectors, antennas and telescopes are producing and processing large data volumes as well.

See plenary talk by Rosie Bolton


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The challenge

A common infrastructure across Research Infrastructures would foster:

- economy of scale
- collaboration across domains
- scientific reuse
- sustainability
Have you failed to reproduce a result?

- 70% researchers tried and failed to reproduce others’ results
- > 50% researchers failed to reproduce own results

Baker, M. 1,500 scientists lift the lid on reproducibility. NatBure 533, 452–454 (2016).
EU collaborations

EU-funded projects promote cross-fertilisation across Research Infrastructures and scientific domains to find common, consistent and useful solutions to challenges of...

- Federated Data Management and Transfer Services
- Distributed Data Processing
- Software Sustainability
- Analysis Preservation and Reusability

... all in one common Analysis Platform!

See yesterday’s talk by G. Lamanna
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.
Timeline

- **ESCAPE project**
  - 2020: First ESCAPE Data Lake prototype
  - 2021: initial VRE design
  - 2022: Science Projects onboard the VRE
  - 2023: CHEP2023

- **EOSC-Future project**
Science Use Case
Experimental data generated at site in data centres

Analysis workflow

- **Data collection**: Experimental data generated at site.
- **Storage**: Data storage is required to hold large volumes of data.
- **Data processing**: Formats for the data are reduced to make it suitable for analysis.
- **Analysis**: Analysis is performed with preserved, versioned software on computing resources.
- **Results interpretation & preservation**: Results are interpreted and preserved for future use.

Combine results, compare across workflows and share.
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

**Virtual Research Environment**

- **DARK MATTER**
- **EXTREME UNIVERSE**
- **Authentication & Authorization**
- **Data Management**
- **Analysis**
- **Notebook service**

**Context:** EOSC-Future
- Data Management
- Authentication & Authorization
- Notebook service

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Dark Matter searches

Both HEP and astrophysics and researching limits of Dark matter, and preserving analysis workflows would enable to output combined plots

See yesterday’s talk by J. Little
Extreme Universe searches

Multi-messenger astronomy: EM radiation, GW, neutrinos, cosmic rays are created by different astrophysical processes, and thus reveal different information about their sources.

<table>
<thead>
<tr>
<th>INPUT DATA</th>
<th>Binary Neutron Star Merger</th>
<th>Active Galactic Nuclei</th>
<th>Core-Collapse Supernovae</th>
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</thead>
<tbody>
<tr>
<td>STUDY</td>
<td>• GW</td>
<td>• Fast Radio Bursts</td>
<td>• Broadband follow ups</td>
</tr>
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<td></td>
<td></td>
<td>• multi wavelength</td>
<td>• Neutrinos</td>
</tr>
<tr>
<td></td>
<td></td>
<td>observations</td>
<td>• GW</td>
</tr>
<tr>
<td>EXPERIMENT</td>
<td>VIRGO</td>
<td>LOFAR</td>
<td>FermiLAT</td>
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<td></td>
<td>KM3NeT</td>
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</tbody>
</table>
VRE Components
The building blocks

- Distributed storage
- Continuous Integration / Continuous Delivery
- Container Orchestration
- Infrastructure As Code
- Analysis
- Data Management
- Authentication & Authorization
- Notebook service
- cloud, HPC
Authentication & Authorisation

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

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

Authentication & Authorization

subject mapping cronjob

Data Management

Notebook service

Analysis

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Rucio is an open-source data management and orchestration project initially developed by the ATLAS experiment to manage large volumes of data. It is now used by various CERN and non-CERN communities.

The Data Lake is a policy-driven, reliable, distributed data infrastructure able to deliver data on-demand at low latency to all types of processing facilities. It ensures data security, quality and access. The storage elements are managed by partner institutions.
Daemons for data access & replications through gridFTP, HTTP(S)/webDAV, XRoot protocols

- EOS
- DPM
- dCache
- StoRM
- XRootD
- S3

Data Lake

Central Relational Database

FTS3 and GFAL2

Main & authorisation servers

(see Mario Lassnig talk)
To facilitate interactive analysis.

**Notebook Service**

- **jupyter**: Interface to run preliminary analysis
- **docker**: Containerised environments on public repositories
- **zenodo**: Client libraries and software installed to interact with underlying services
- **ceph**: CephFS volumes provided as shared, temporary storage solution

### Server Options

- **Minimal environment**
  - Based on jupyter/scipy-notebook (active mana-client)
- **ROOT environment**
  - ROOT 6.28.10, a C++ kernel is implemented too - DAQ testing
- **Minimal environment - python 3.9.13**
  - Contains a TEAMA client
- **Virtual Observatory environment**
  - Contains Jupyter notebook examples with the basic usage of the NOA tools
- **Indirect Dark Matter Detection Environment**
  - Contains a ODC compiler and the MuForm, ARIP, ISW arms and fermatools libraries
  - No fermipy (supported)
- **Common gamma analysis tools**
  - Contains a ODC compiler and astropy, gpyol, gammapy, gammapy libraries
- **Wardon Detection Filter (WDF) project environment**
  - Contains the full WDF env
- **Compact stars Science Project environment**
  - Contains the maanamaker library
- **Kasca/S Science Project environment**
  - Contains the common gamma analysis tools and the km3io, km3ppf, and km3hdf libraries
- **Kasca/S & CTA combined analysis**
  - Compatible environment with gammapy and the km3io, km3ppf, and km3hdf libraries (en testing)
- **SKA SDC**
  - SKA environment profile for SDC
- **LOFAR environment**
  - Based on the pre-fitter container. Can be used to image LOFAR data
- **ESAP shopping basket environment**
  - Using the ESAP shopping basket library.
- **ESAP shopping basket environment (with astrophy)**
  - ESAP shopping basket and astrophy, e.g. to download and plot images from the virtual observatory
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
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?
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)

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**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
- EOS
- DPM
- dCache
- StoRM
- XRootD
- S3

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

<table>
<thead>
<tr>
<th>Name</th>
<th>Account</th>
<th>RSE Expression</th>
<th>Creation Date</th>
<th>Remaining Lifetime</th>
<th>State</th>
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<td>egazarr</td>
<td>EU-LC1-1</td>
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<td>7d</td>
<td>STUCK</td>
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<td>userran_test_from_CERN-030025-1543.txt</td>
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<td>SURF-IOC-EXP</td>
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<td></td>
<td>STUCK</td>
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<tr>
<td>userran_test_from_CERN-030025-1643.txt</td>
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<td>EU-LC1-1</td>
<td>2023-05-07T14:43:00Z</td>
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<td>OK</td>
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<td>userran_test_from_CERN-030025-1643.txt</td>
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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.
- Rucio and Reana UI interfaces deployed with K8s allow to explore and debug failed transfers and workflows.
- 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.
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
Demo
DM@LHC with ATLAS

1. Dark Matter Reinterpretation: setting limits on High-Luminosity LHC contraints 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.

See yesterday’s talk by J. Little
Behind the scenes...

K8s spawns a pod per user

Server Options

- Minimal environment
  - Based on jupyterhub notebook (active reana-client)
- ROOT environment
  - Start your ROOT analysis. A C++ kernel is implemented too
- ROOT environment (Kcache testing)
  - Run the extension in D完成后 mode
- SKA RDC1
  - SKA environment profile for SDC
- Indirect Dark Matter Detection Environment
  - Contains a GCC compiler and the ML, Fermi LAT, MSTAR, Fermi, gamma, libraries (TESTING)
- Common gamma analysis tools
  - Contains a GCC compiler and aten, sherpa, gamma, gamma, libraries

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Behind the scenes...

data gets replicated to EOS mounted storage
Behind the scenes...

```
version: 0.8.1
inputs:
directories:
  - python/
workflow:
type: serial
specification:
  steps:
    - name: fetchdata-rucio
      voms proxy: true
      rucio: true
      environment: 'projectescape/rucio-client'
      commands:
        - rucio whoami
        - rucio get ATLAS_LAPP_SP:DMsummary.dileptonReinterpretation
      name: SetLimits
      environment: 'reana/reana-env-root6.6.18.04'
      compute backend: kubernetes
      kubernetes_memory_limit: '9Gi'
      commands:
        - mkdir plots/
        - python python/MakeLimit.py
outputs:
directories:
  - plots/
```

data gets downloaded on Reana storage
Future outlook

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
  - *Einstein telescope* (next generation gravitational waves detector)
  - *NUCLEUS* experiment (elastic neutrinos scattering)
  - *VdR Würzburg* - German centre for Data-Intensive Radio Astronomy
- Interest from new digital models (i.e. **digital twins**) developed within European projects

Future plans

- connection with HPCs, commercial clouds and other external computing resources
  - FENIX and the EuroHPC Joint Undertaking work (eg: FTS delivering files to Julich-HPC with S3 protocol)
- Use VRE as a performance evaluation between workload managers
- Caching data on distributed storage
The VRE is ...

- **modular**
  - integrates software, tools and packages
  - can be configured to connect to remote storage and computing resources
- **flexible**
  - ad-hoc workflows can be created via easily editable declarative files
  - can be installed on different machines
  - independent of CERN restrictions
- **reproducible/sustainable**
  - deployment is kept simple and documented to be used as a blueprint for other research infrastructures
  - allows analysis preservation
- useful for **sharing and collaboration**
  - common entry point with same authentication for all services
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.

<table>
<thead>
<tr>
<th>vCPUs</th>
<th>RAM (GB)</th>
<th>Masters</th>
<th>Nodes</th>
<th>Remote Storage (TB)</th>
<th>CephFS (TB)</th>
</tr>
</thead>
<tbody>
<tr>
<td>184</td>
<td>335.8</td>
<td>3</td>
<td>23</td>
<td>646</td>
<td>1.8</td>
</tr>
</tbody>
</table>

25 Openstack machines
- 14.6GB RAM
- 8 VCPU
- 80GB Disk
- Fedora CoreOS 35
- LINUX
Two sides of the coin

A bipartite look at the ideal infrastructure ...

<table>
<thead>
<tr>
<th></th>
<th>SCIENTIST</th>
<th>IT ADMINISTRATOR</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>USEABILITY</strong></td>
<td>Ergonomic (onboarding, documentation)</td>
<td>Maintenance, portability, modularity</td>
</tr>
<tr>
<td><strong>DATA ACCESS</strong></td>
<td>Various FAIR data/metadata types</td>
<td>Security, varied protocols and technologies</td>
</tr>
<tr>
<td><strong>ANALYSIS</strong></td>
<td>Performance</td>
<td>Cost, energy consumption</td>
</tr>
<tr>
<td><strong>REPRODUCIBILITY / SUSTAINABILITY</strong></td>
<td>Software and analysis steps preservation</td>
<td>Easy re-deployment</td>
</tr>
</tbody>
</table>