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

Conference **ESCAPE to the Future** | 25-26 October 2022

Royal Belgian Institute of Natural Sciences | Brussels, Belgium

25 October 2022, 14:25 - 15:20

ESCAPE ESAP - Common standards to access and use data with a science platform toolkit

ESCAPE ESAP | ESFRI Science Analysis Platform

John Swinbank
ASTRON

Matthias Fueßling
CTAO

cta cherenkov telescope array | the observatory for ground-based gamma-ray astronomy

James Collinson
SKAO

SKAO

Aard Keimpema
JIVE

JIVE Joint Institute for VLBI ERIC

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European Science Cluster of Astronomy & Particle physics ESFRI research Infrastructures

ESCAPE to the Future
25-26 October 2022
Brussels, Belgium

Work Package 5

ESAP: A Science Analysis Platform Toolkit

John Swinbank — swinbank@astron.nl — WP5 Coordinator
On behalf of the WP5 team

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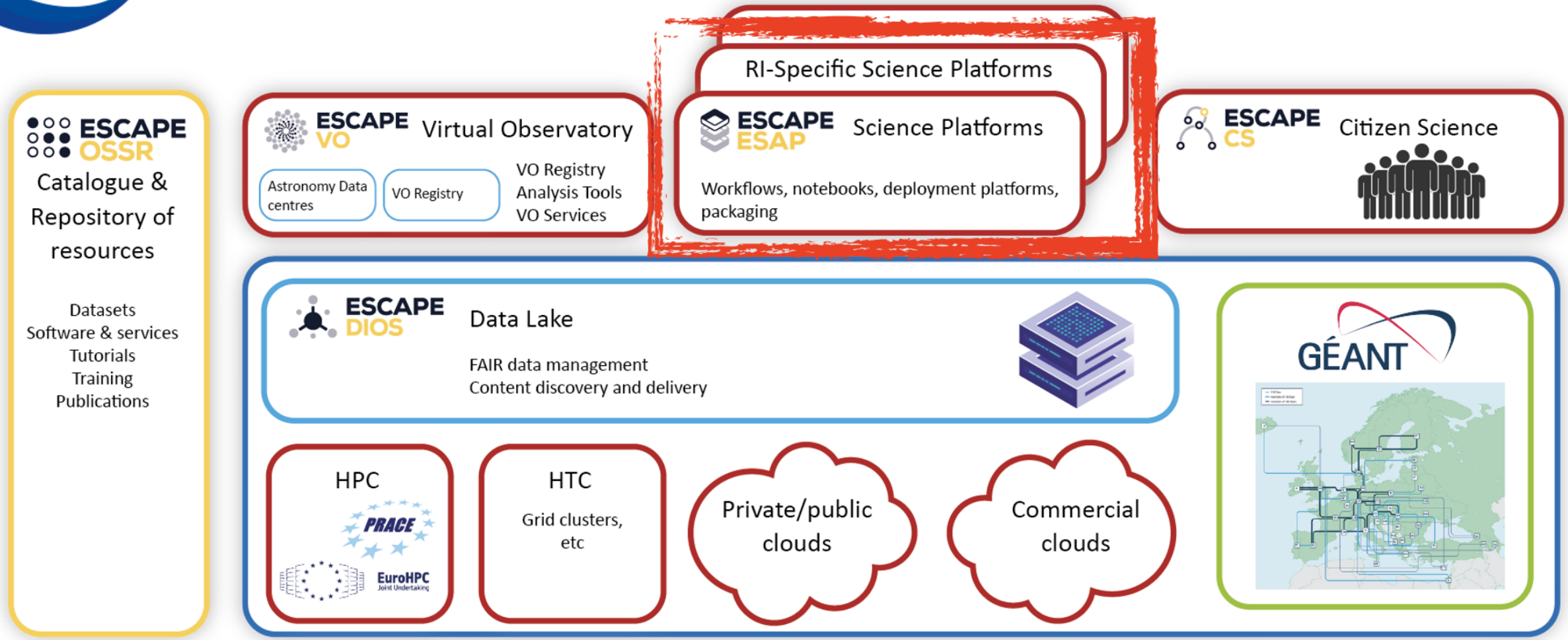
ESAP in the ESCAPE Cluster



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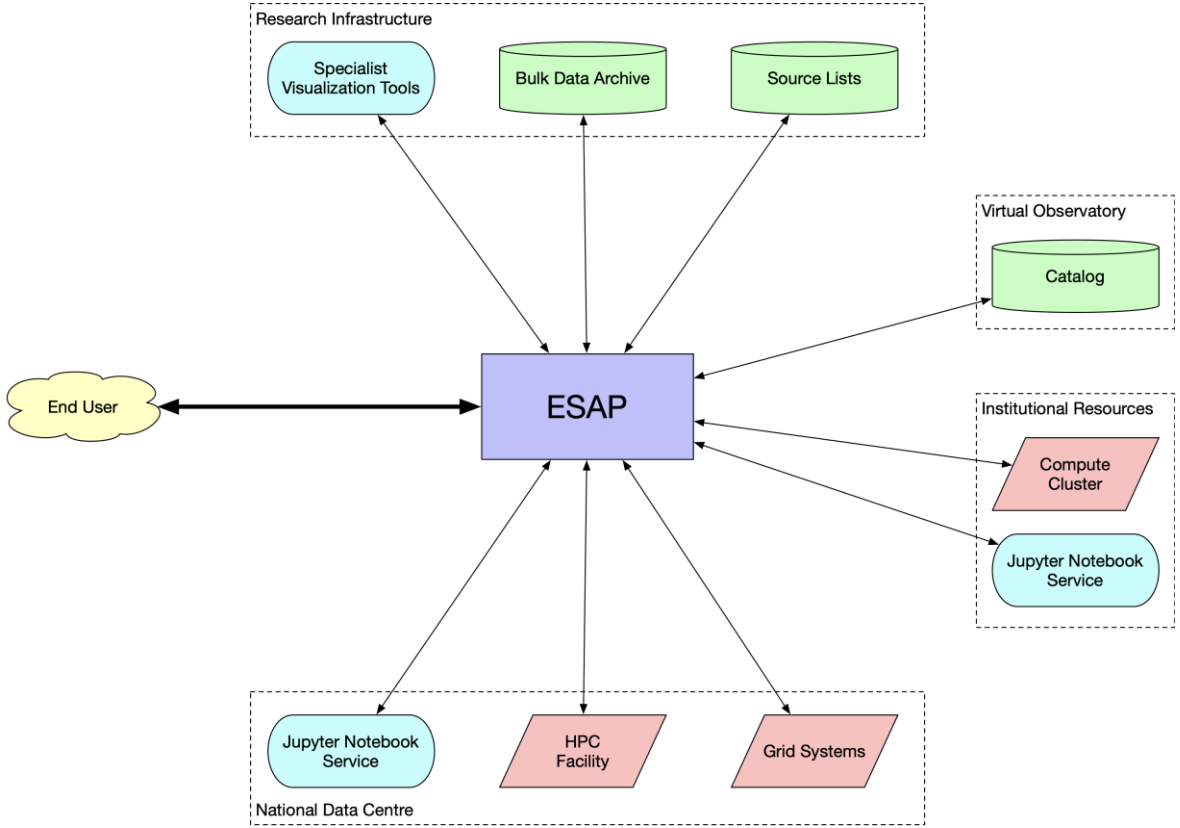
The Twin Missions of Work Package 5

- Development of **ESAP**, the ESFRI Science Analysis Platform
  - A *toolkit* for building platforms through which users can discover and interact with the data products, software tools, workflows, and services that are made available through ESCAPE and from elsewhere.
- Preparing ESFRI services, data products, and tools for integration with ESAP and their subsequent use within ESCAPE and across EOSC



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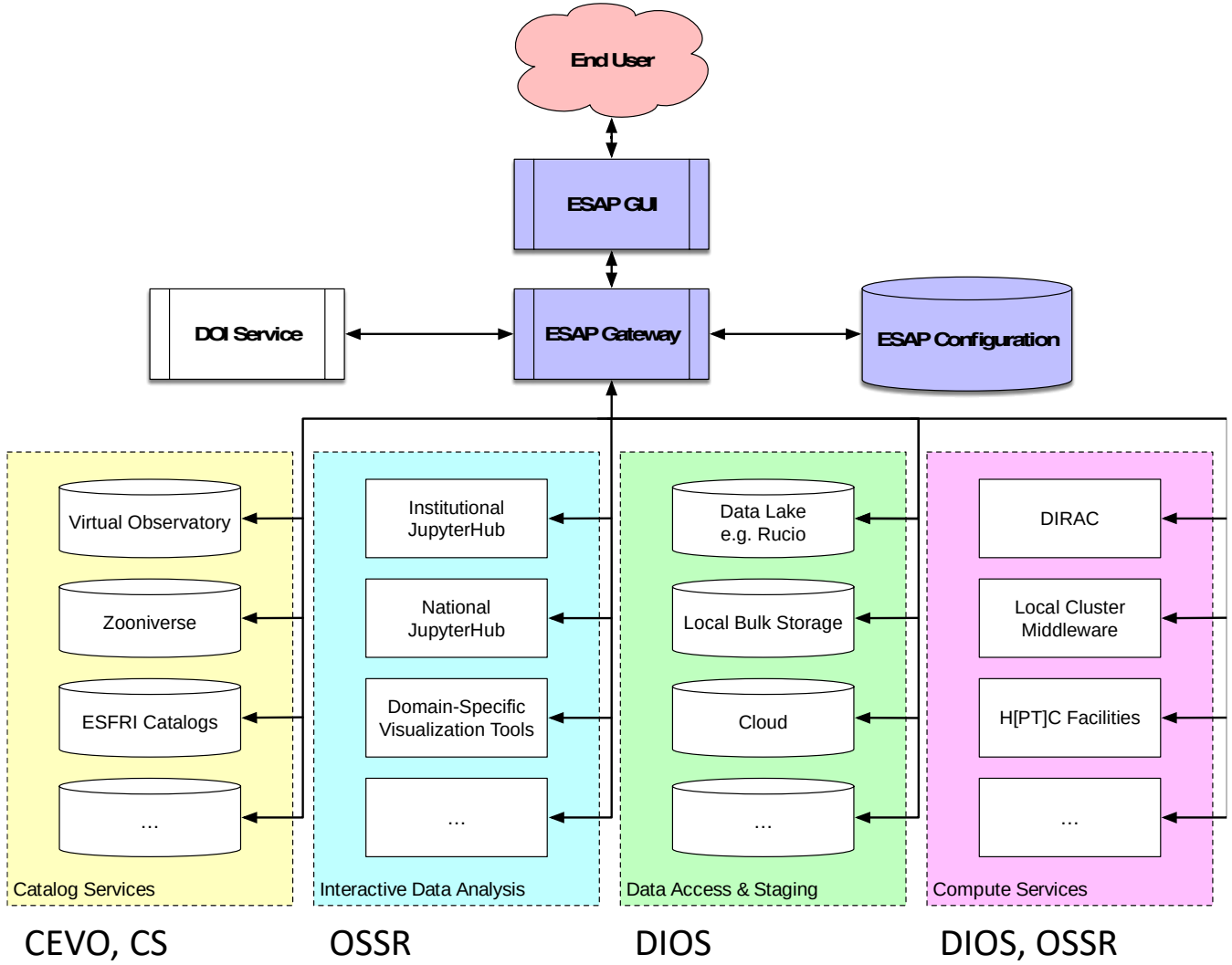
Goals and structure of ESAP

- ESAP provides the *focal point* for integrating diverse services from a range of providers.
- Two major components: GUI and Gateway.
- Focal point of a range of pluggable, independent services.
- Flexible, robust, extensible.
- A toolkit; deployable and customizable to meet the needs of different research infrastructures.



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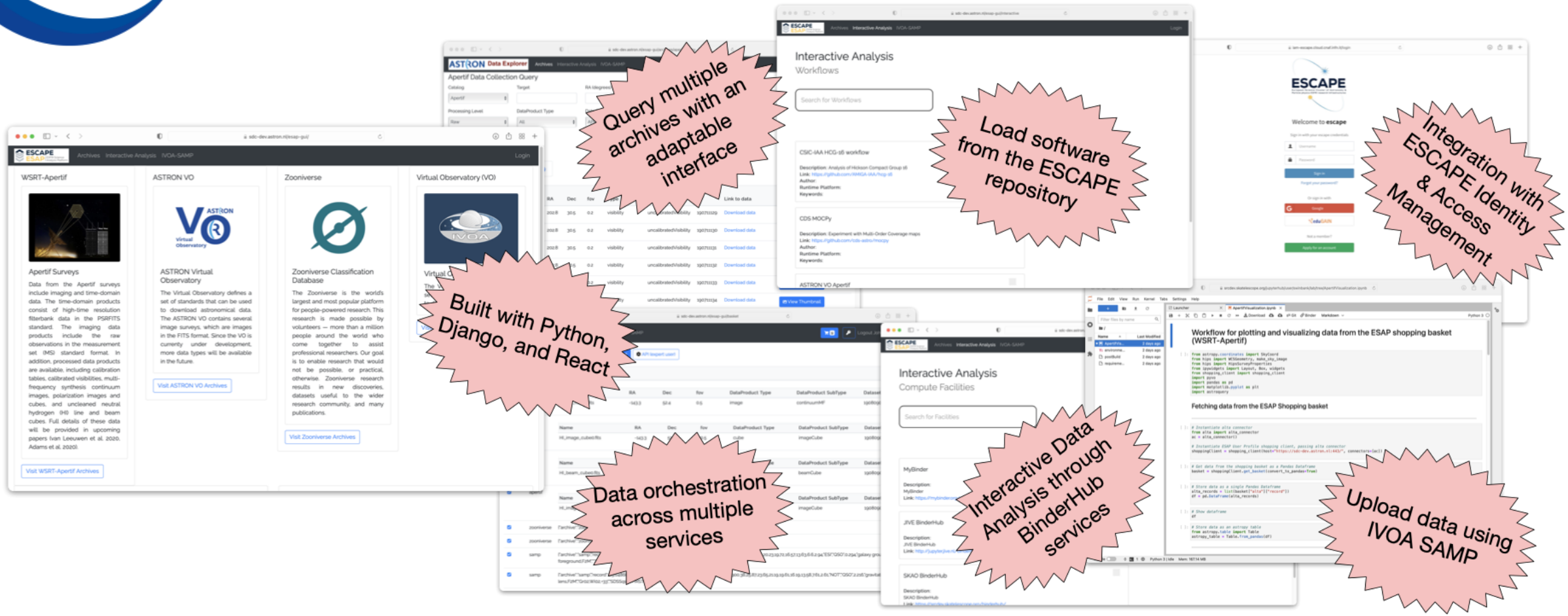
ESAP Capabilities



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Special Guest Stars

Mathias Füßling
CTAO
Cherenkov Telescope Array Observatory: Experiences with ESAP

James Collinson
SKAO
SKA Regional Centres and ESAP

Aard Keimpema
JIV-ERIC
The EVN Archive Portal: Bringing science to the data using JuypyterHub

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Cherenkov Telescope Array Observatory (CTAO): the experiences with ESAP

Matthias Füßling, Gareth Hughes (CTAO)

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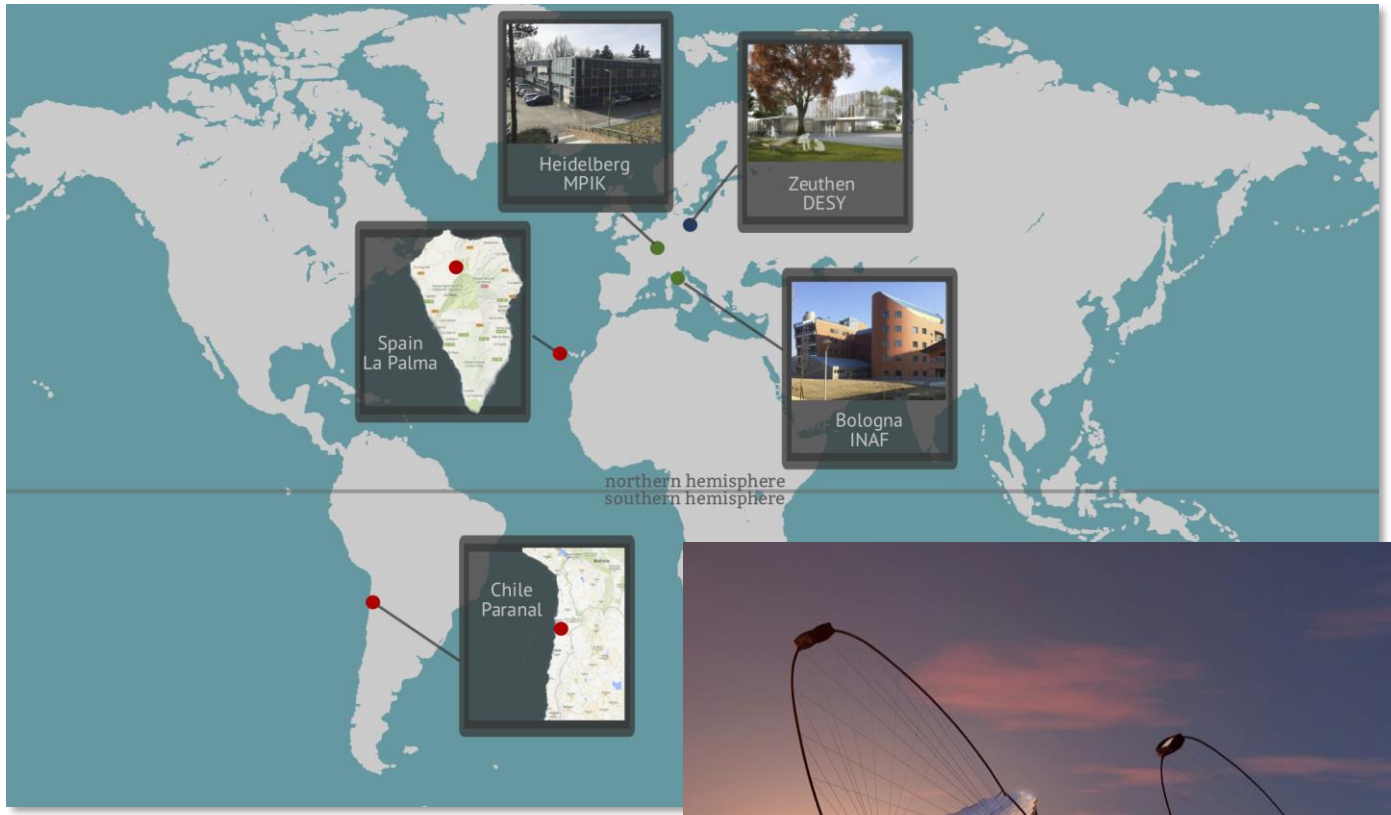
Cherenkov Telescope Array Observatory

The first ground-based gamma-ray **observatory**

- CTAO provides to the User Community:
  - a science portal for access to products and services
  - High-quality data and science tools
- ESAP offers to the ESFRIs:
  - main building blocks to build platforms tailored for specific purposes
  - ability to explore workflows:
    - CTAO users executing a science analysis (finding data, worfklow, software)
    - UIs for CTAO staff to do data management tasks (batch processing)
    - Science data challenge (interactive processing)



https://www.cta-observatory.org/

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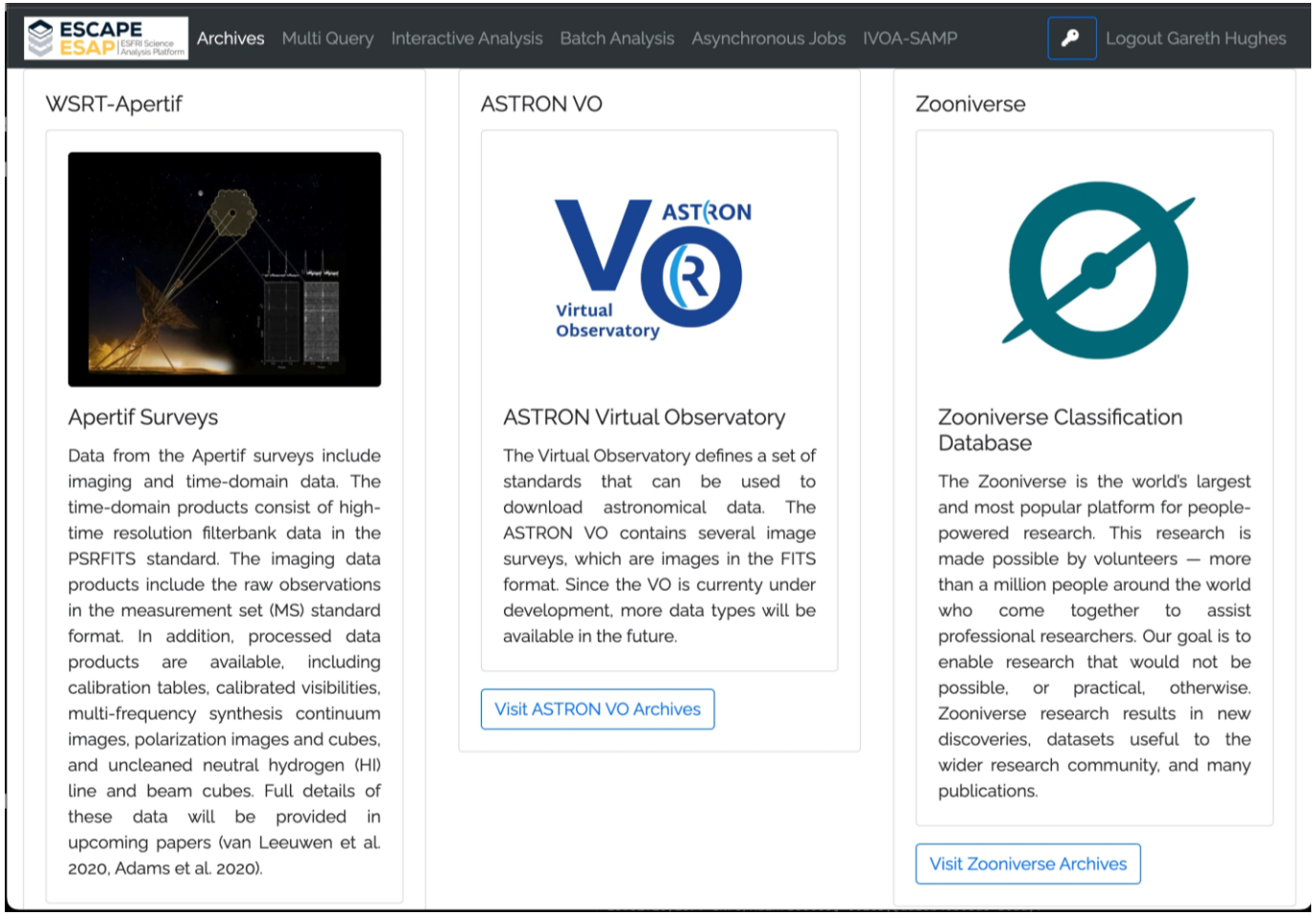
Modularity: Adding Services

- The ability to easily **add services** to a platform makes it versatile
  - The ESAP makes it simple to add an archive or service to the platform
- If a service has a REST API then it can be connected and queried through the ESAP
- Enables cross collaboration and linking of data and workflows
- A simple example of this is using the eOSSR python library developed in WP3/OSSR
  - We can now query the Zenodo archive to look for anything linked to ESCAPE and CTAO
  - For example, the CTAO Instrument response functions



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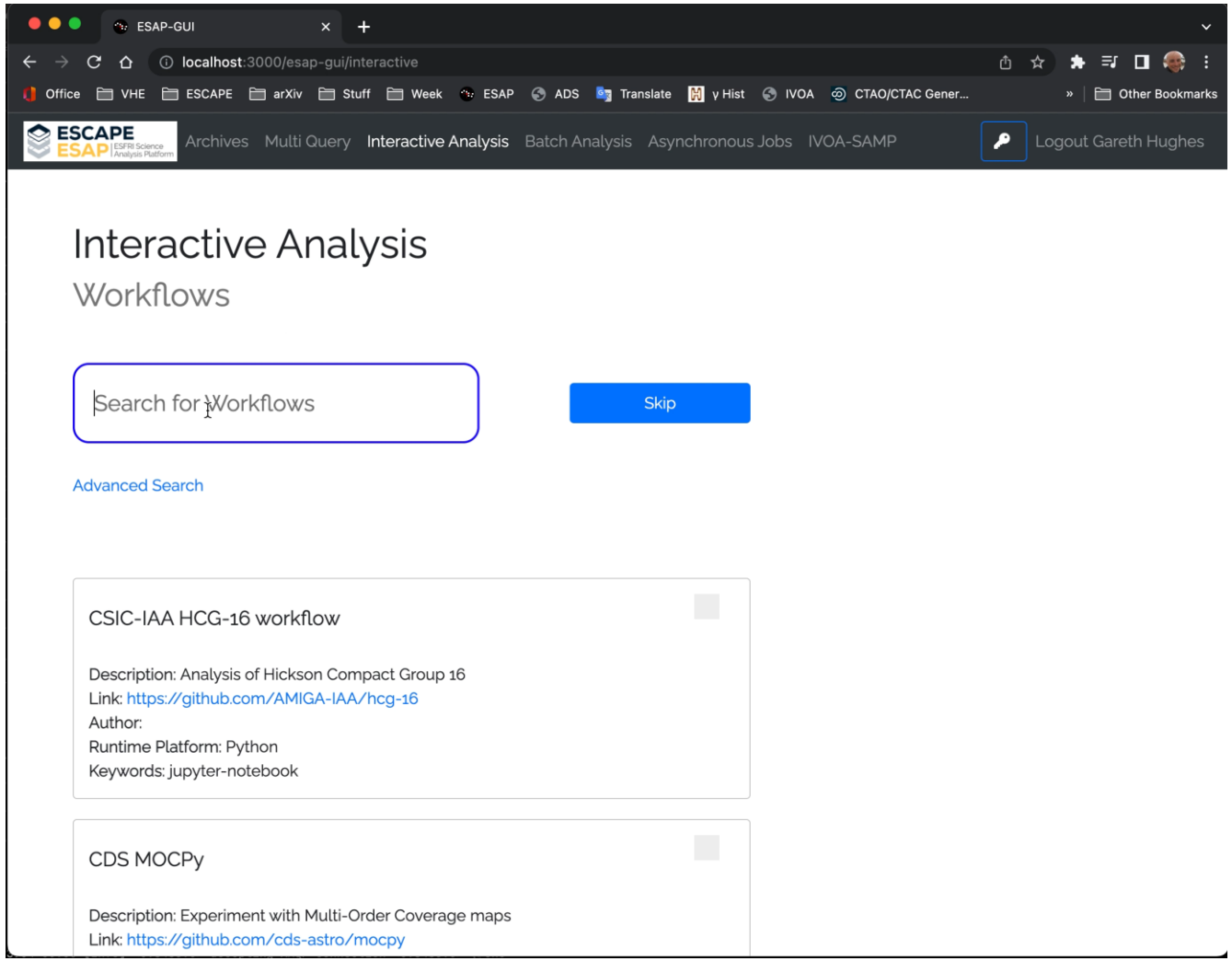
ESAP and Analysis Workflows: a tool for CTAO Users and Staff

- ESAP facilitates the connection of software, data and interactive analysis
- The CTAO Science Portal needs to offer data and services to its users and staff
  - This will allow users to interact with data
  - It can also help foster cross collaboration and joint analysis
  - Could be used to support observatory staff
- Both Gammapy and AGNpy were onboarded to the OSSR/WP3
  - Gammapy: open-source Python package for gamma-ray astromomy and will form the basis of the CTAO science analysis tools
  - AGNpy: software package developed by high-energy astrophysicists to compute of the photon spectra produced Active Galactic Nuclei
  - The workflow shown uses both Gammapy and AGNpy to fit the Spectral Energy Distribution of the BL Lacertae blasar



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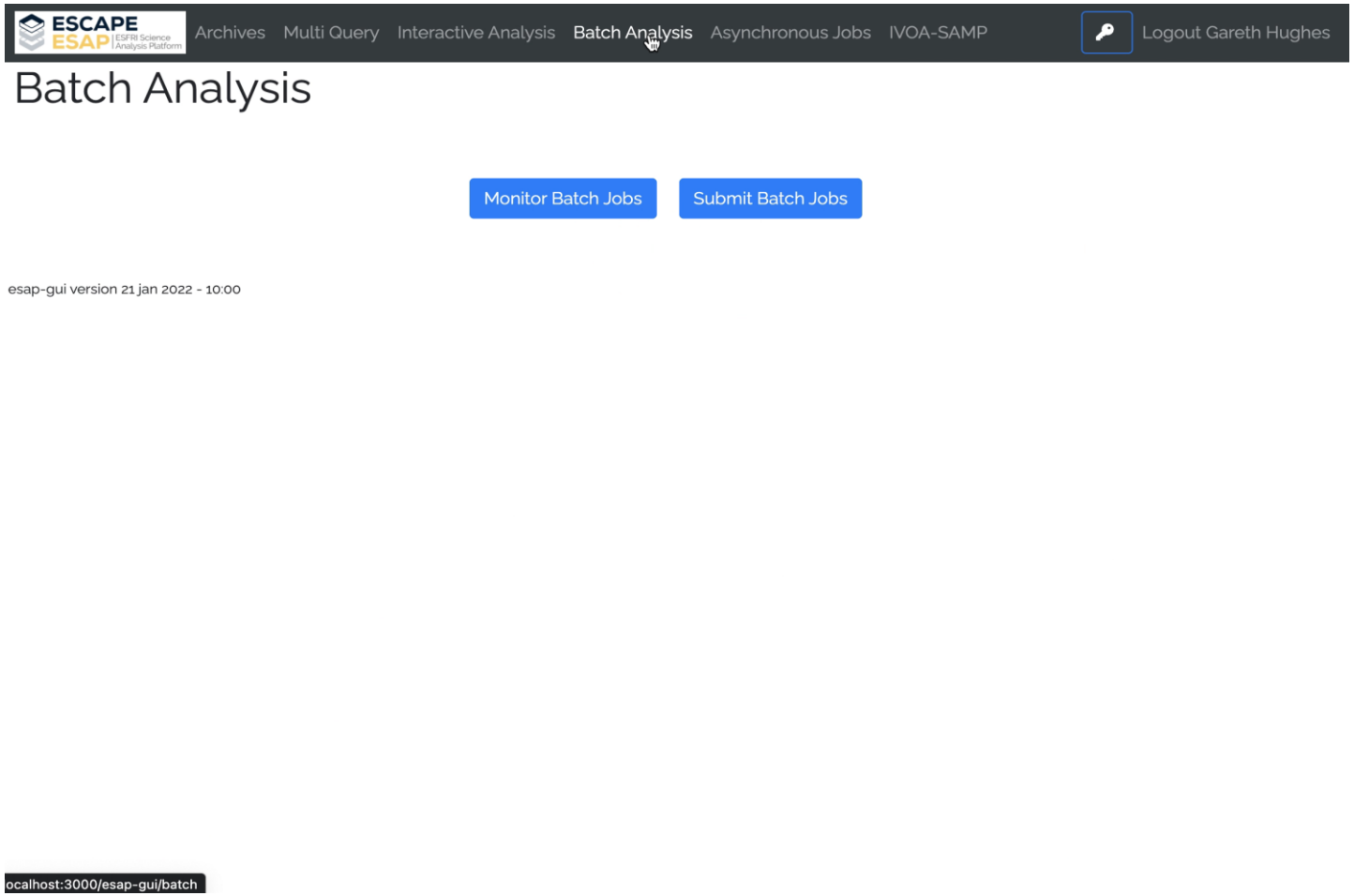
ESAP and Batch Processing

- CTAO needs to internally manage data processing at PByte-scale:
  - Service task of the Observatory
  - Automated batch processing needed
  - Data could be spread across multiple data centers
  - CTAO staff would be able to launch data management tasks
- A batch API and asynchronous worker component was developed to connect the ESAP to CTADIRAC
  - CTAO uses DIRAC as its workload management software
- Given the correct setup jobs can be launched



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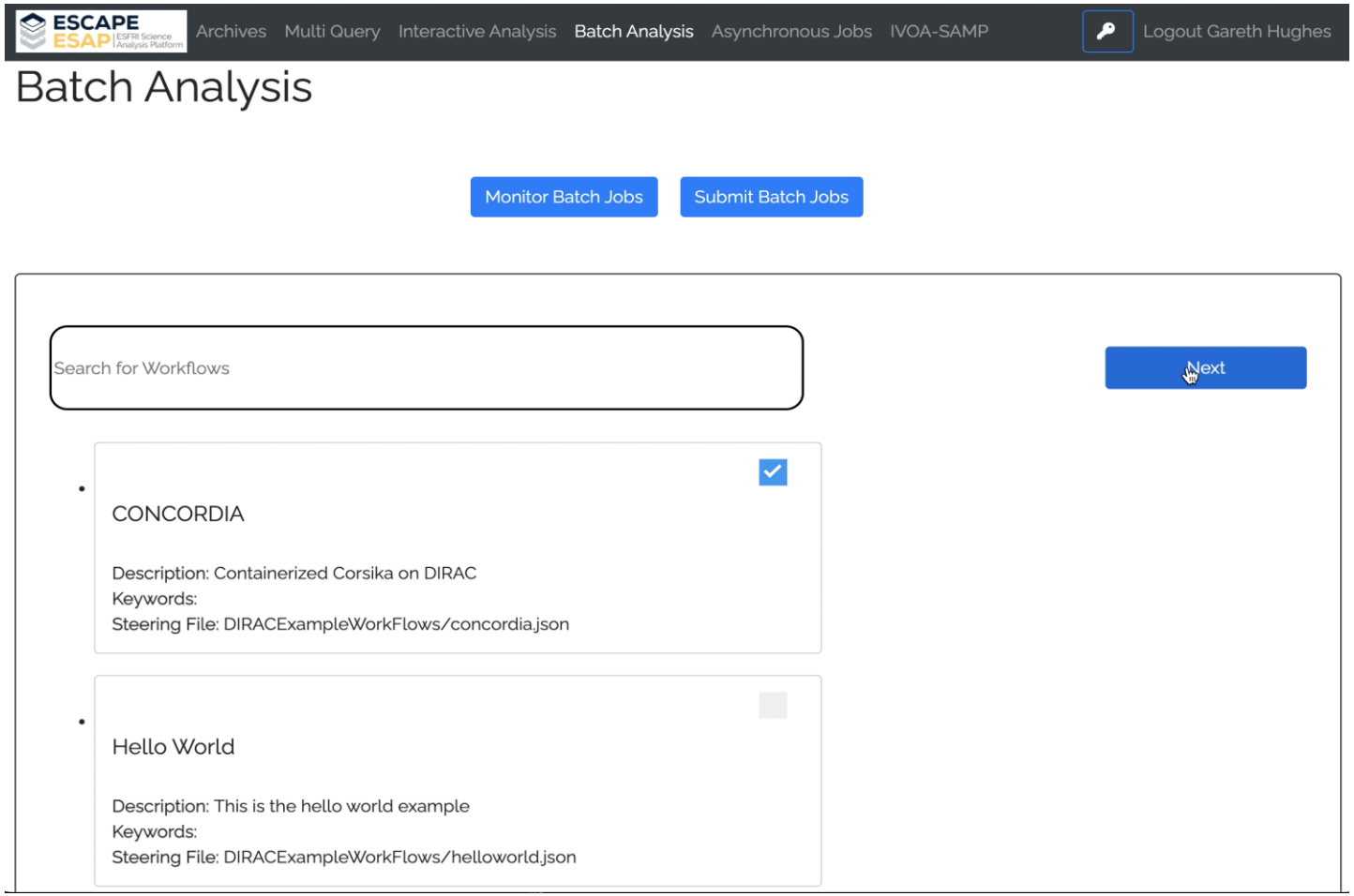
ESAP and Batch Processing

- Groups with access to a DIRAC system should be able to easily customize an ESAP to launch and monitor batch jobs
- Workflow:
  - A user can define a steering file
    - work ongoing with IVOA and CEVO to define standards
  - This tells the ESAP where to find a containerized version of your program
  - From there you can modify the parameters and submit the job
  - The jobs submitted can then be monitored via the Async worker or a custom Batch component
- Example
  - Links to WP3/OSSR CONCORDIA group
  - Potential links to ongoing and future work in WP2/DIOS
- In the future DIRAC will move to tokens making this process significantly easier



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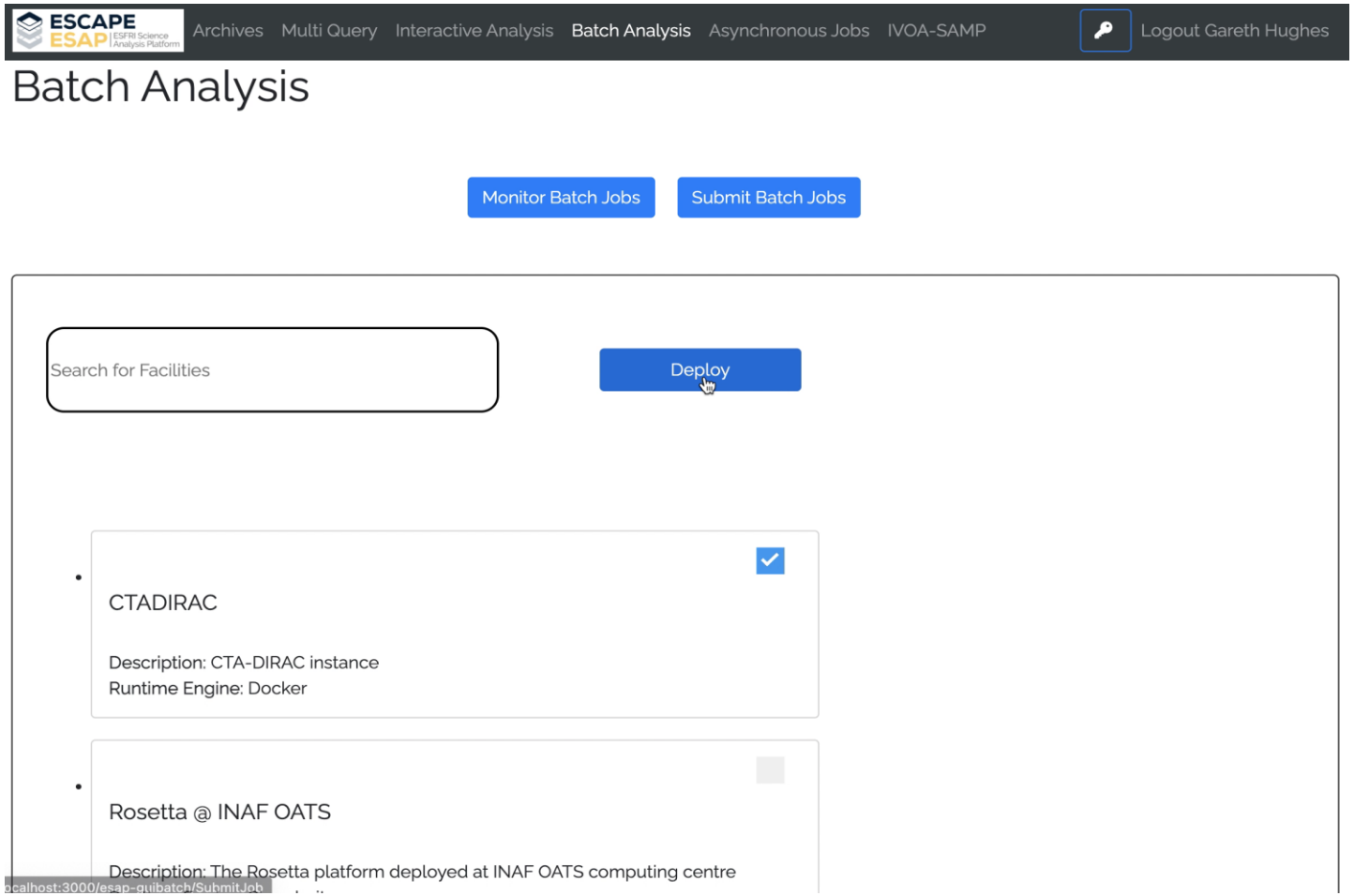

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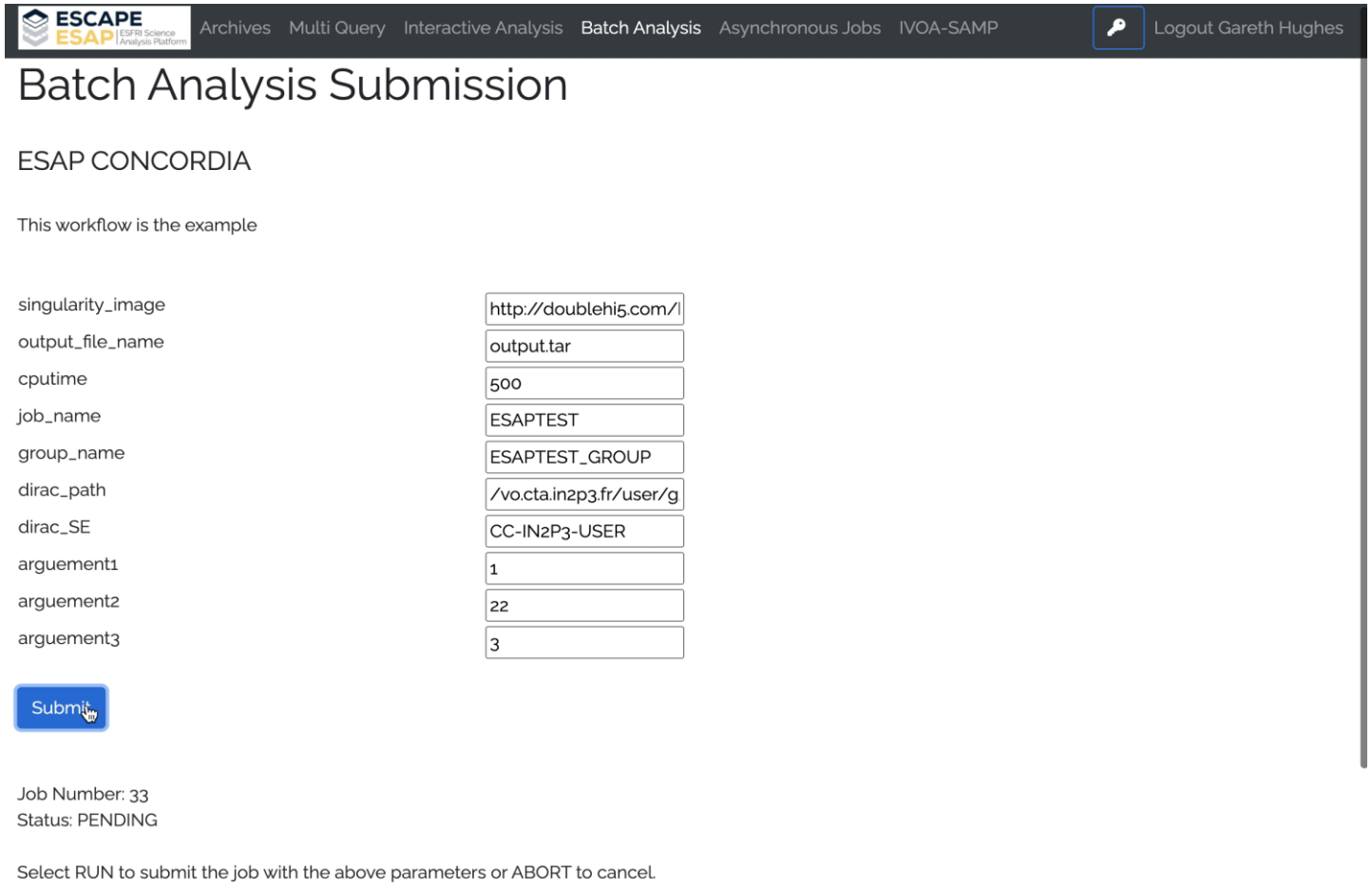

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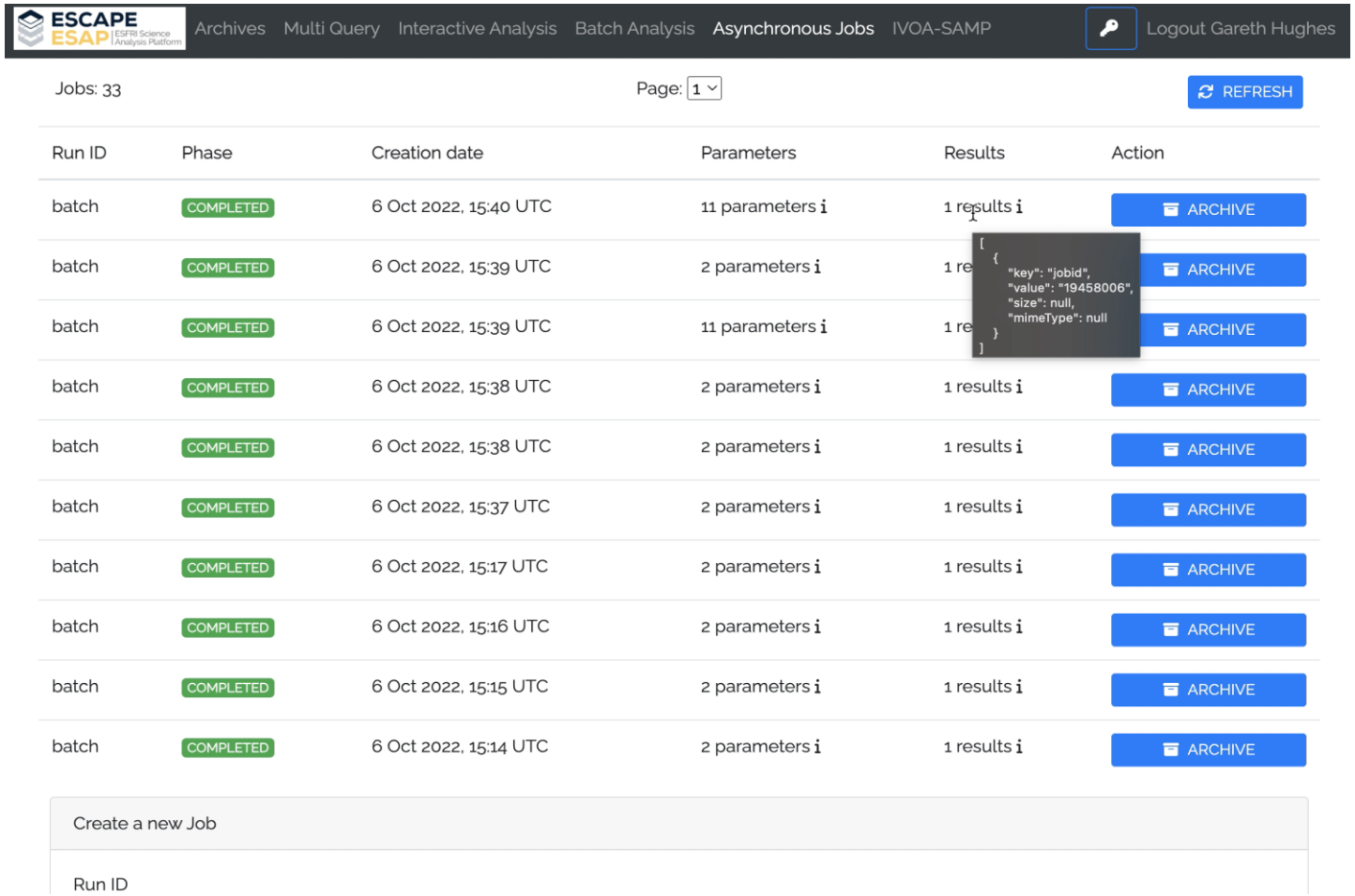

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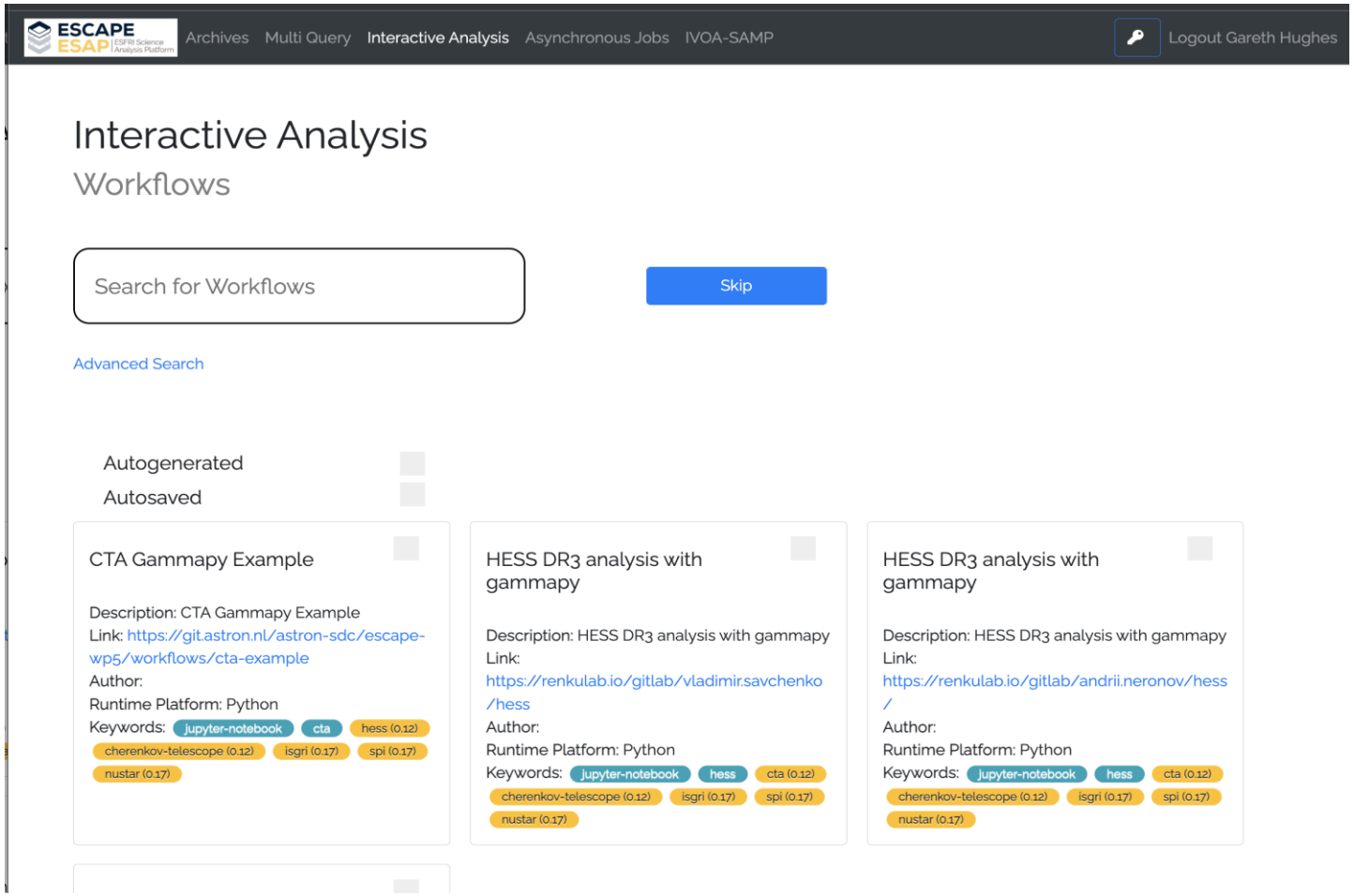
Exploring the ESAP for potential use in a Science Data Challenge

- Science Data Challenge a way to engage with CTAO users
- V. Savchenko has deployed a version of ESAP using Kubernetes on one of the future CTAO Data Centers (CSCS)
  - With the aim to investigating how it might be used for a CTAO data challenge
- They found it could be **easily customized**
  - github based login
  - addition of workflows
  - advanced search options and use of metadata
- A mybinder instance has also been added and made available to the platform
  - This work is being fed back into WP5/ESAP
- Challenge: For a Data Challenge the workflows would need to be **persistent**



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Conclusions

- CTAO has **contributed** workflows and functionality to the ESAP
- The ESAP provides an **excellent toolbox** from which one can build and tailor a Science Platform
- CTAO has been able to identify key **technologies** and ideas which it will further investigate in the future
- CSCS colleagues have been able to **deploy** their own version of the ESAP and **customize** it, to investigate possible use for a Science Data Challenge
- We look forward to further work together on these topics in future collaborations

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Thank You

- ESAP work package for their active support and engagement
  - John Swinbank
  - Klaas Kliffen
  - Nico Vermaas
  - Stelios Voutsinas
  - Hugh Dickinson
  - Zheng Mayer
  - James Collinson
  - Yan Grange

- CTAO
  - Federico Ferrini
  - Jose-Luis Contreras
  - Nuria Alvarez Crespo
  - Jordi Delgado
  - Catherine Boisson
  - Mathieu Servillat

- CSCS Team
  - Volodymyr Savchenko
  - Andrii Neronov
  - Victor Holanda

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SKA Regional Centres and ESAP

Dr James Collinson
Operations Data Scientist
SKAO

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Overview

- SKA Regional Centres (SRCs)
  - Capabilities to meet challenges of SKAO data
  - High level architectural vision
- ESCAPE prototyping activities
  - Science platform and data lake for SKAO use cases
  - Bringing compute to the data
- ESCAPE's legacy within the SKAO
  - Current SRC Network prototyping activities
  - Other benefits: collaborators, cloud techs, best practices

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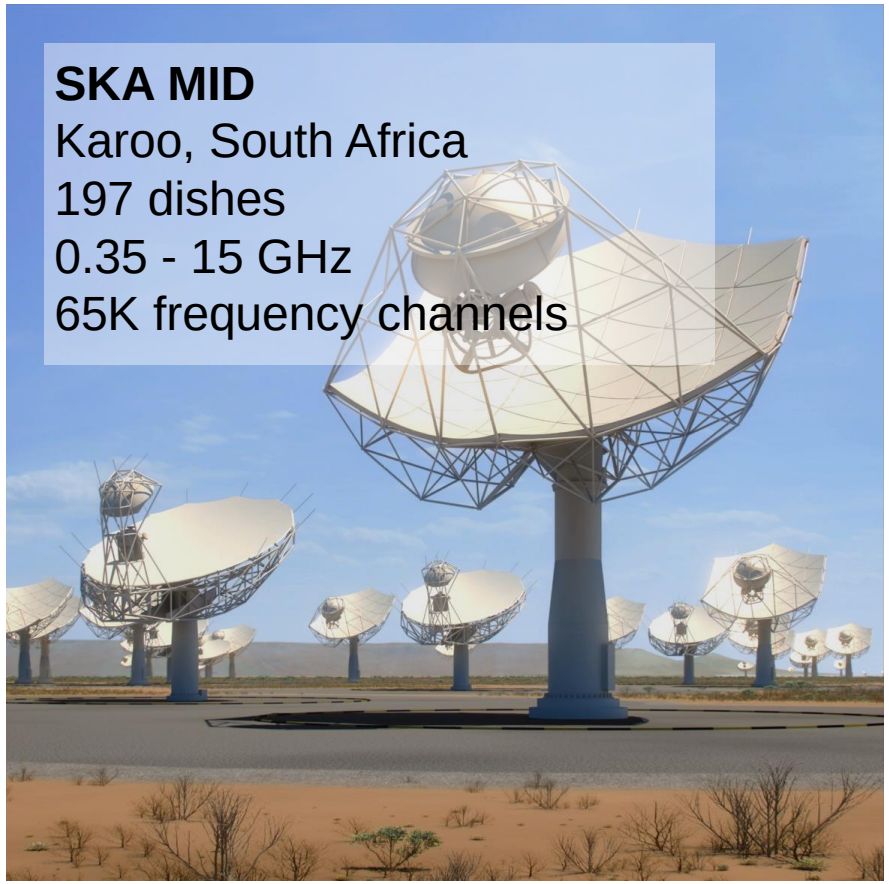
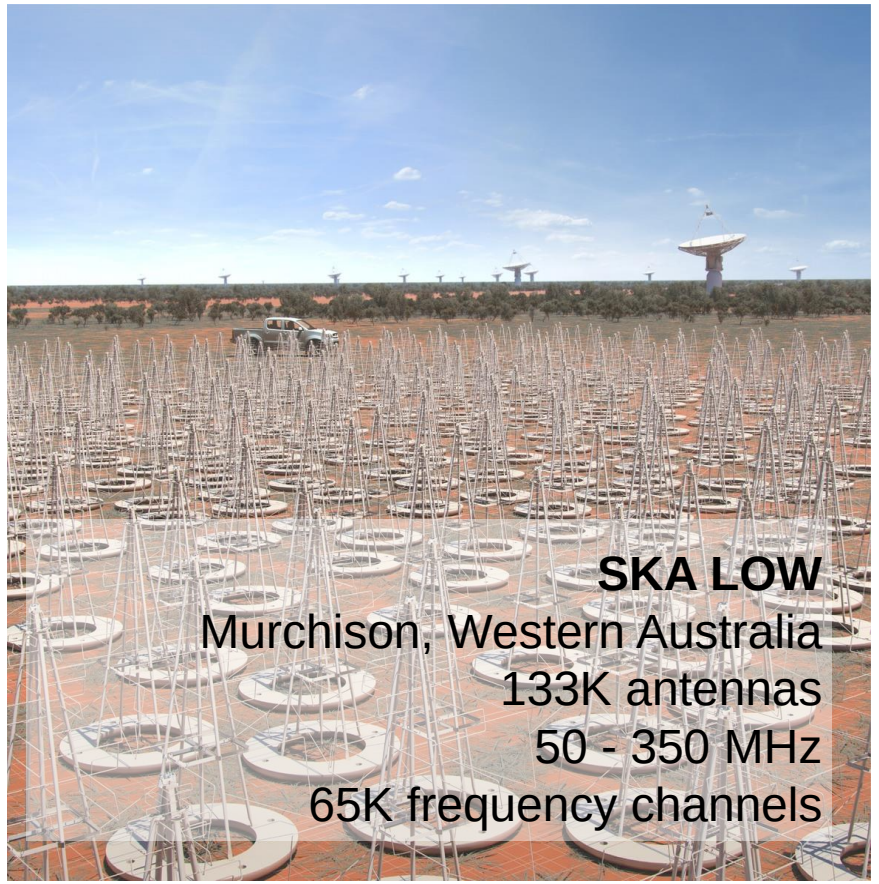
The SKAO Project





Test systems already taking data. Main science programmes from ~2028/9. 50 year lifetime.

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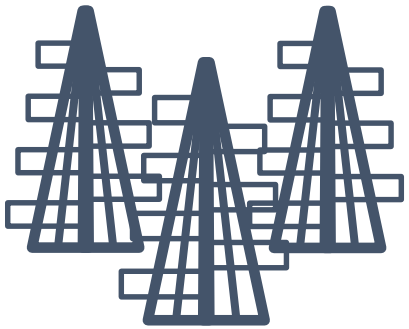
SKA Regional Centres: SKAO data processing stages



SKA LOW

2 Pb/s

SKA LOW-FREQUENCY APERTURE ARRAY

9 Tb/s

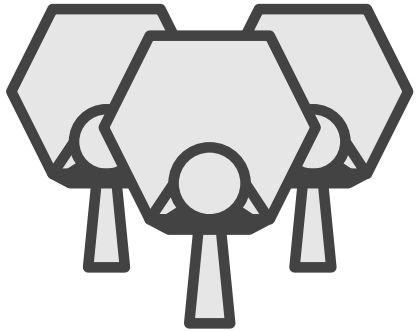
SKA CENTRAL SIGNAL PROCESSOR

8 Tb/s

SKA SCIENCE DATA PROCESSOR

100 Gb/s

SKA MID



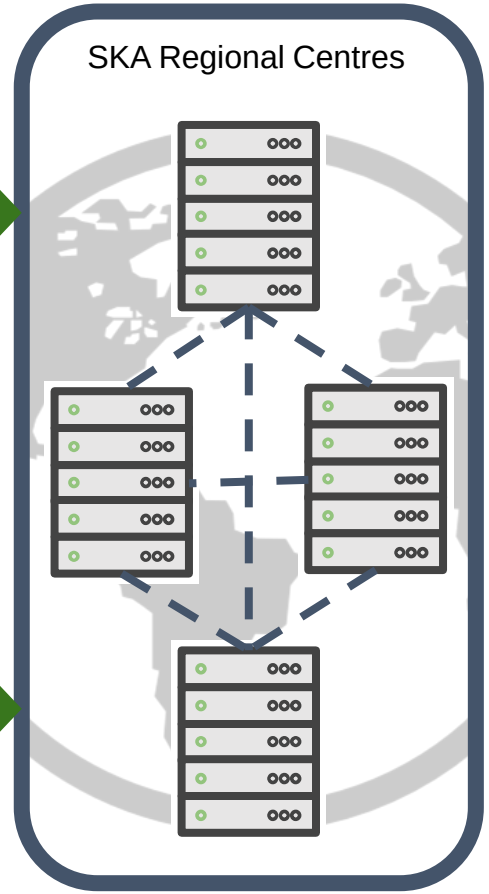
20 Tb/s

SKA CENTRAL SIGNAL PROCESSOR

9 Tb/s

SKA SCIENCE DATA PROCESSOR

100 Gb/s



* Data rates approximate

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The SRC Vision

"To ensure that scientists can access SKA data products and use them to make discoveries"

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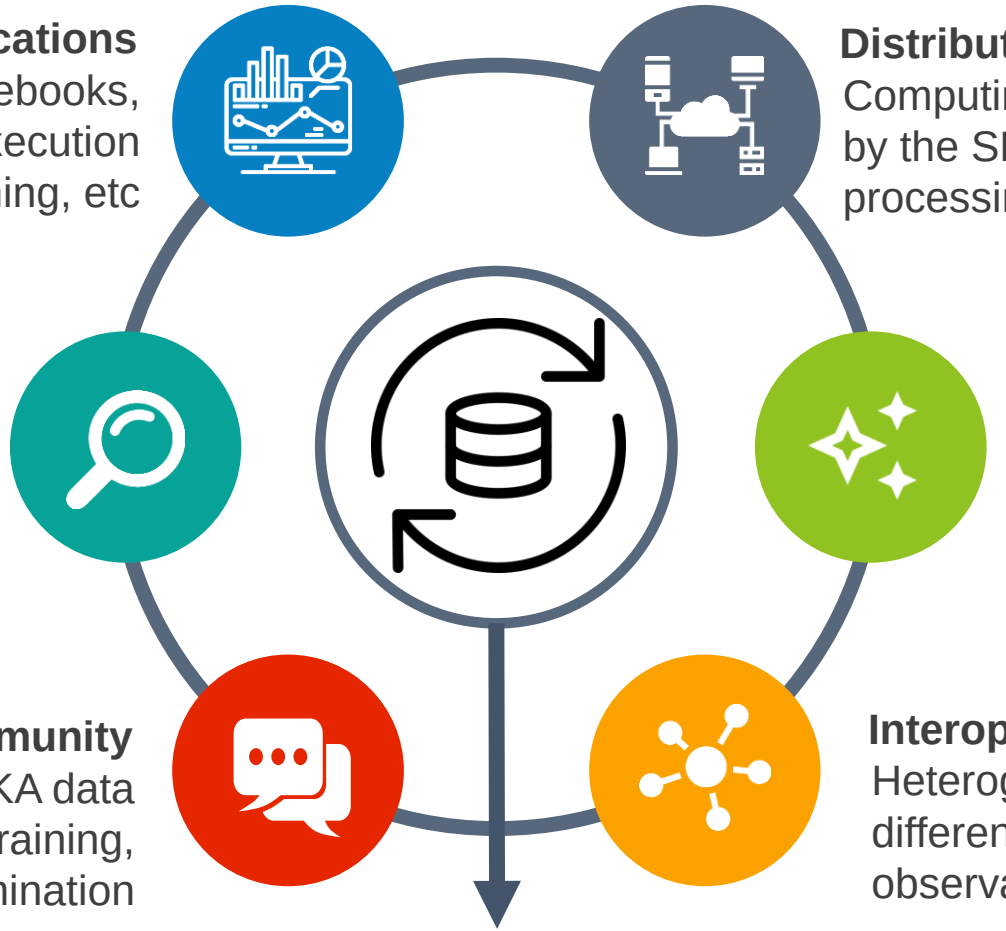
SKA Regional Centre Capabilities

Science Enabling Applications
Analysis Tools, Notebooks, Workflows execution Machine Learning, etc

Distributed Data Processing
Computing capabilities provided by the SRCNet to allow data processing



Data Discovery
Discovery of SKA data from the SRCNet, local or remote, transparently to the user

Visualization
Advanced visualizers for SKA data and data from other observatories

Support to Science Community
Support community on SKA data use, SRC services use, Training, Project Impact Dissemination

Interoperability
Heterogeneous SKA data from different SRCs and other observatories

Data Management
Dissemination of Data to SRCs and Distributed Data Storage

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Science Enabling Applications
Analysis Tools, Notebooks, Workflows execution Machine Learning, etc

Distributed Data Processing
Computing capabilities provided by the SRCNet to allow data processing

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Discovery of SKA data from the SRCNet, local or remote, transparently to the user

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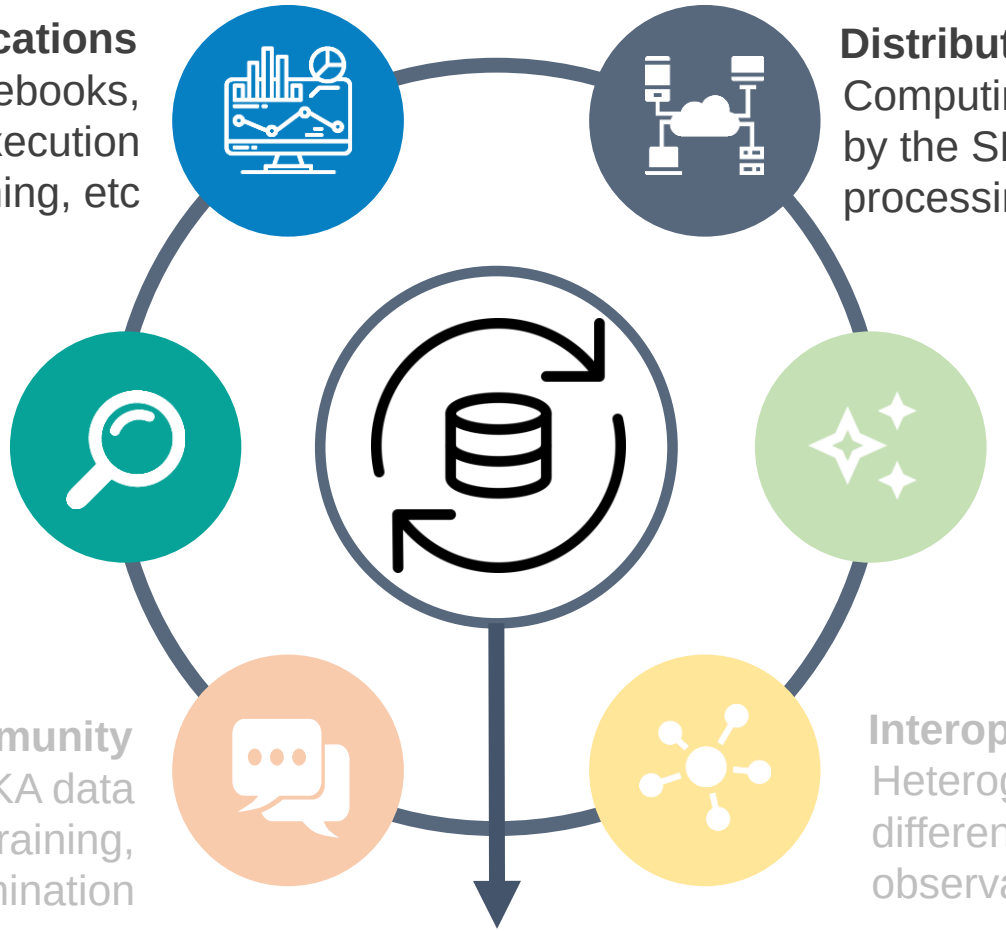

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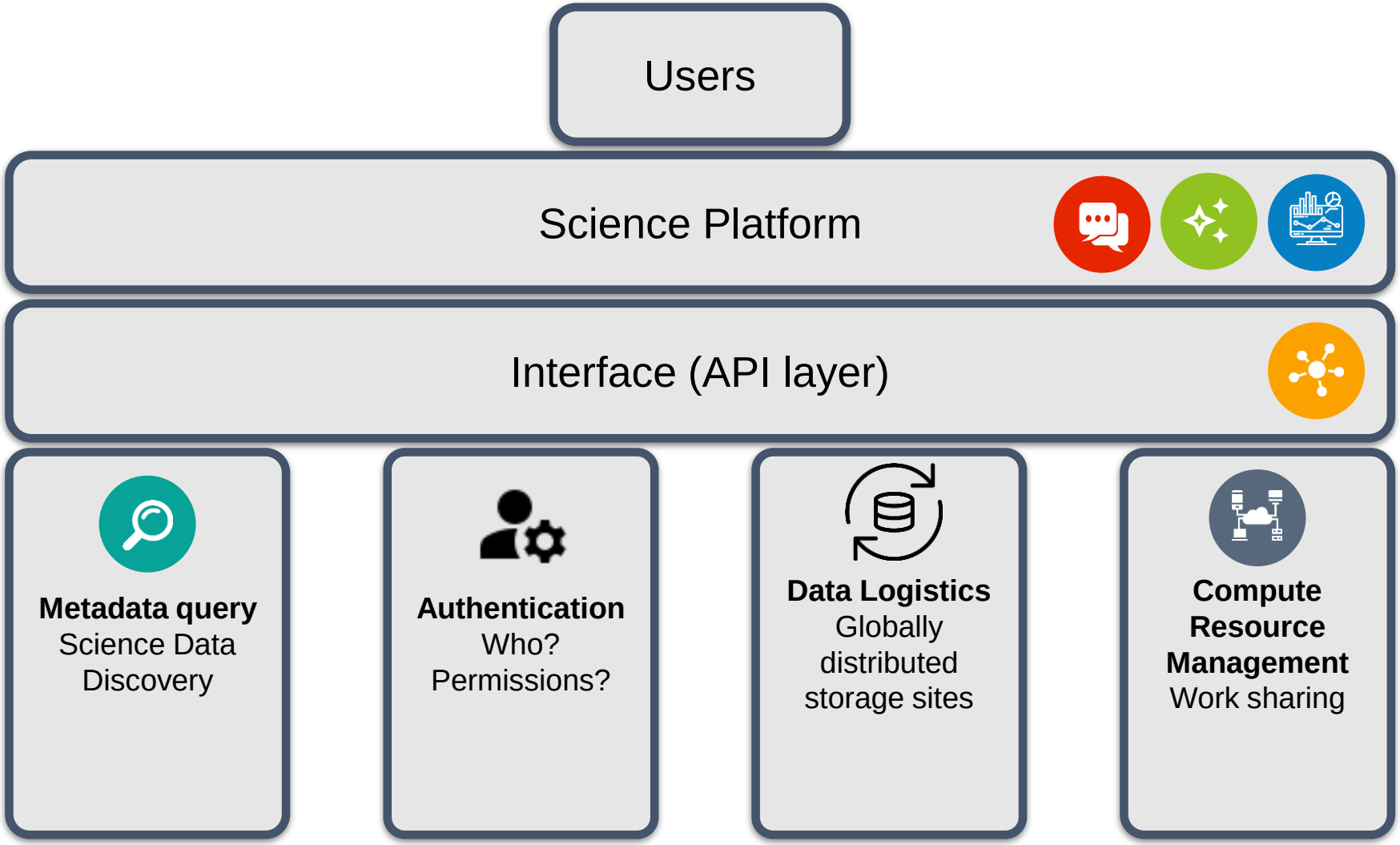
Dissemination of Data to SRCs and Distributed Data Storage

SRC Logical View



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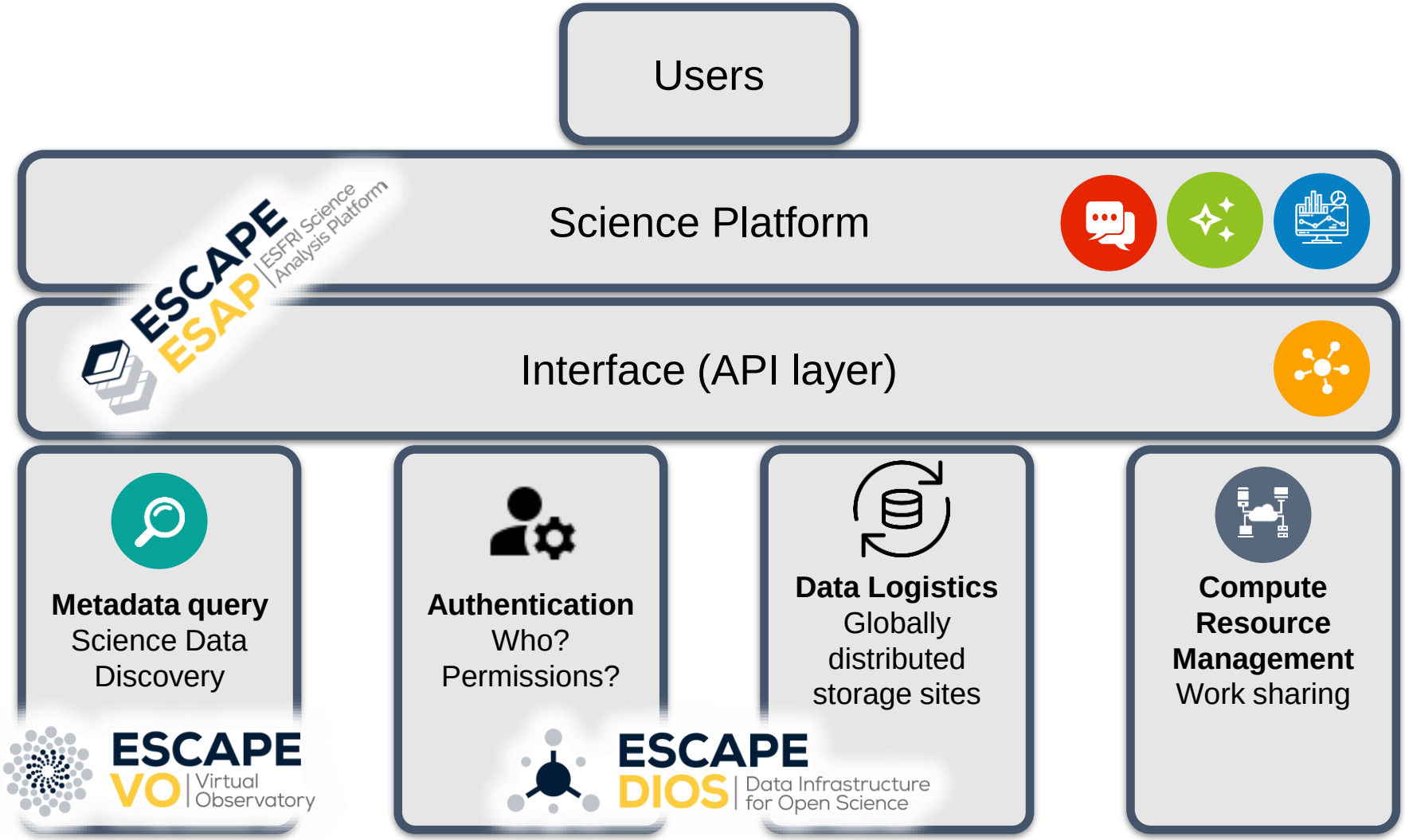

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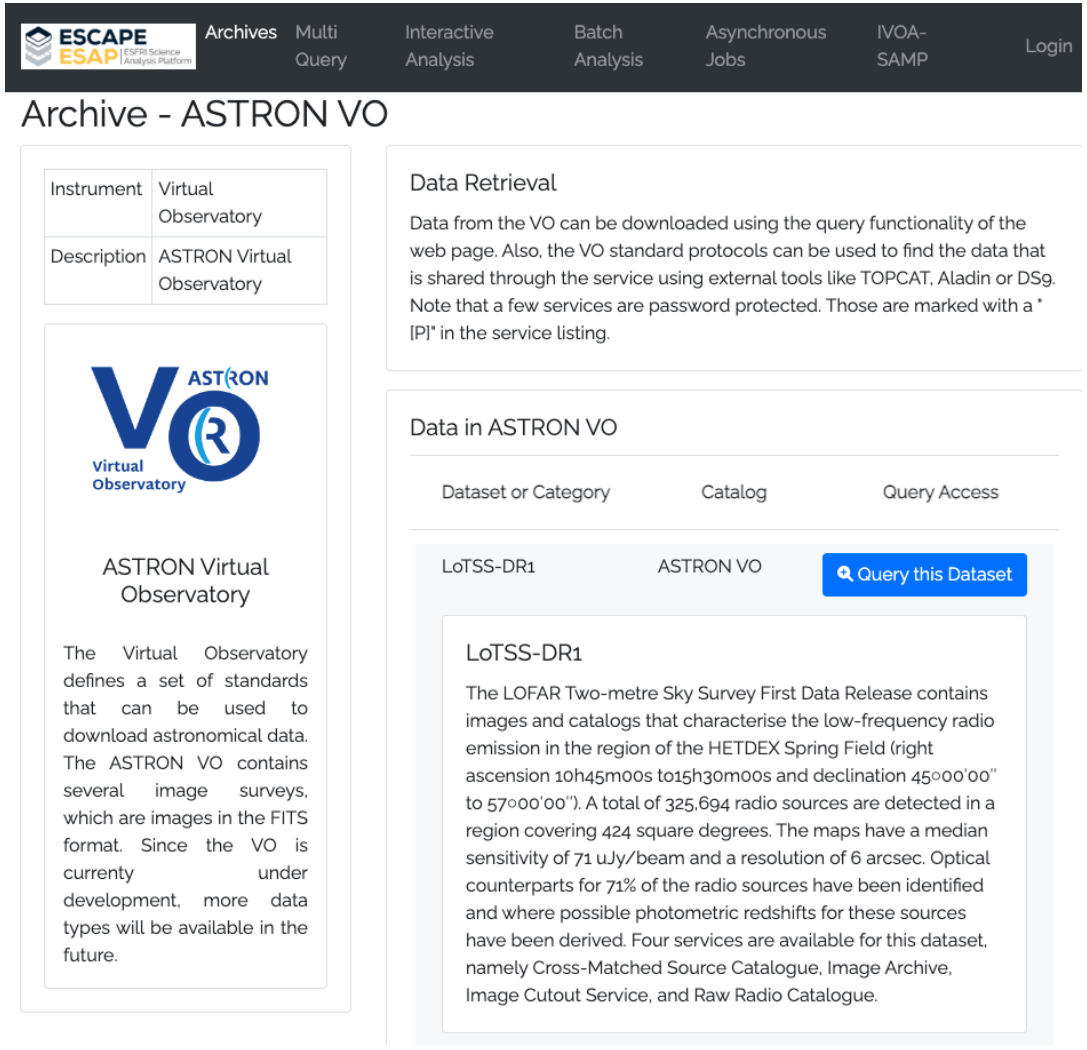
ESCAPE prototyping - SKAO

- Precursor data archives in ESAP (thanks to ASTRON folks!)
  - Helps inform decisions on archive structure



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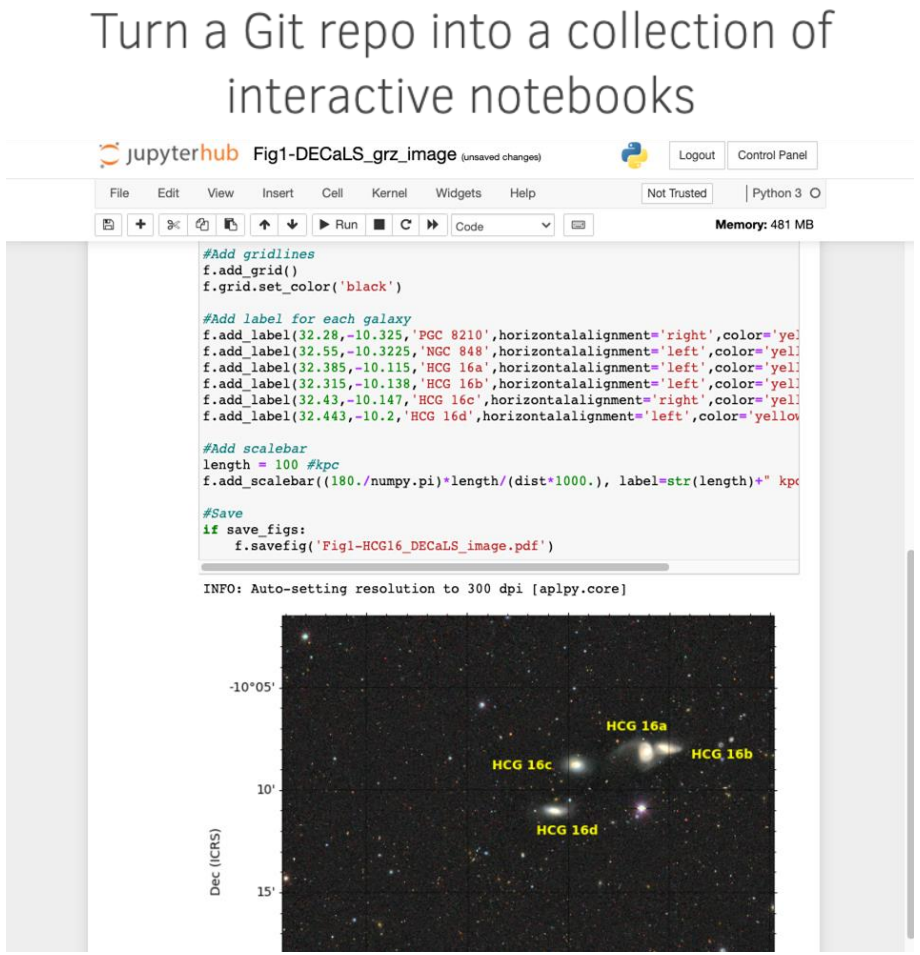
ESCAPE prototyping - SKAO

- JupyterHub on STFC Cloud
- Augmentations for SKA
  - Indigo IAM authentication
  - Persistent storage volumes
  - Binder service to dynamically build environments
  - Dask Gateway (WIP) – provision ephemeral compute clusters on demand



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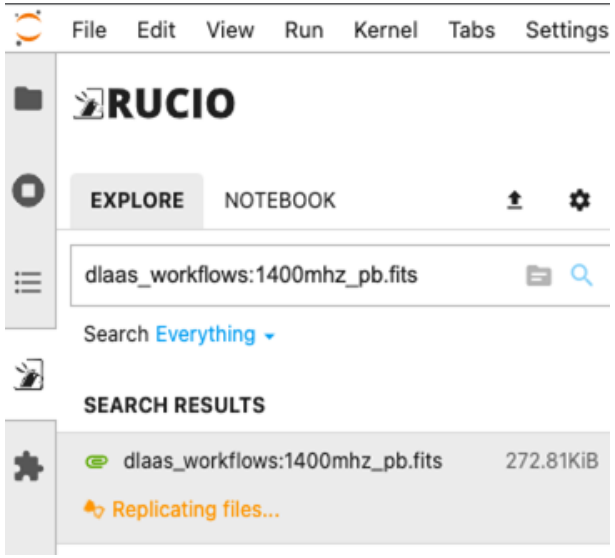
ESCAPE prototyping - SKAO

- SKAO Rucio instance
- RSEs at SKAO sites
- Full mesh automated functional tests
- Integrated with JupyterHub prototype - ‘datalake as a service’

Transfer success site matrix

Src\Dst	SPSRC_STORM	JPSRC_STORM	IMPERIAL	CNAF	AUSSRC_STORM	STFC_STORM
STFC_STORM	100%	100%	100%	100%	100%	NO DATA
SPSRC_STORM	NO DATA	100%	100%	100%	100%	100%
JPSRC_STORM	100%	NO DATA	100%	100%	100%	100%
IMPERIAL	100%	100%	NO DATA	100%	61%	100%
CNAF	100%	100%	100%	NO DATA	100%	100%
AUSSRC_STORM	100%	100%	100%	100%	NO DATA	100%



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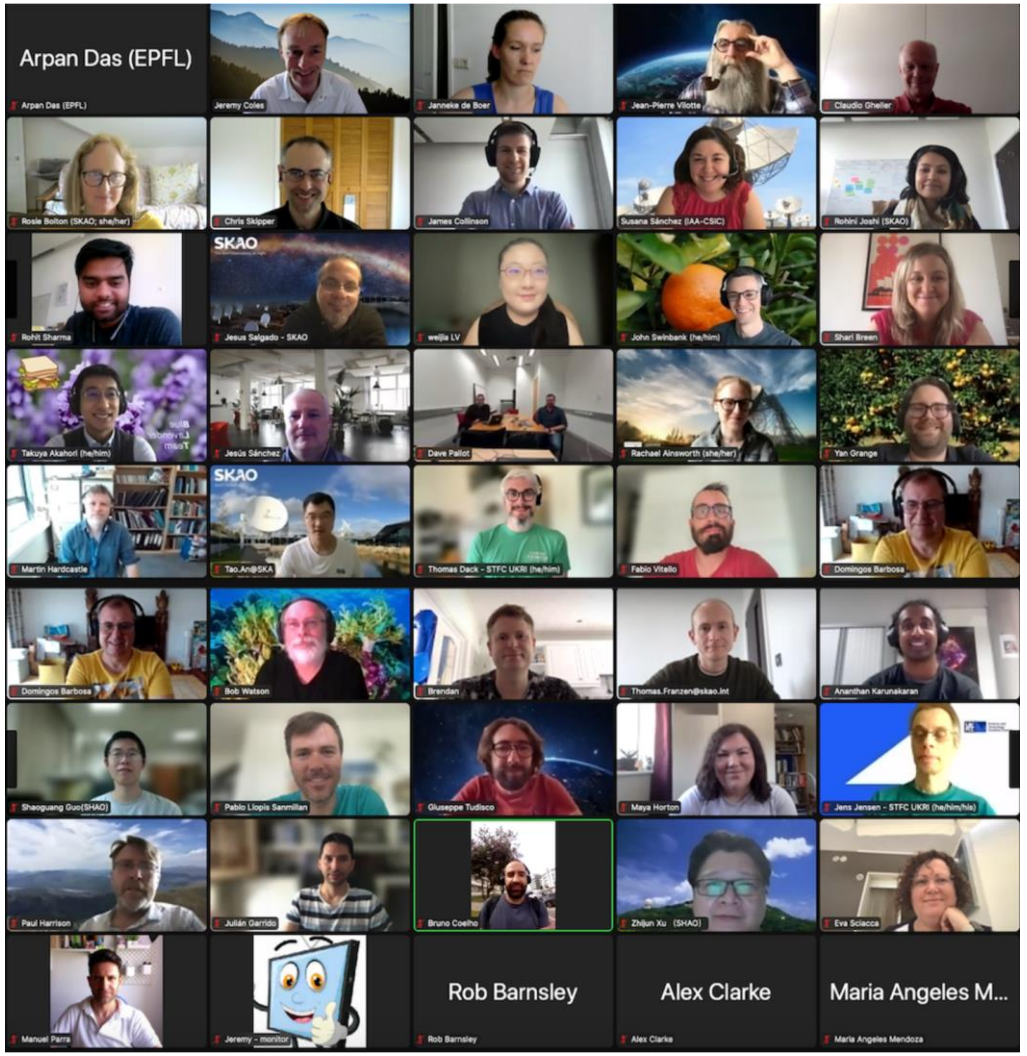
SRC Network Prototyping - 2022 onwards

- Global team of development teams
- 12 countries plus SKAO
- ~1000 dev days every 3 months, set to grow
- ESCAPE candidates further assessed include Rucio, ESAP, Indigo IAM
- ESCAPE collaborations will continue!



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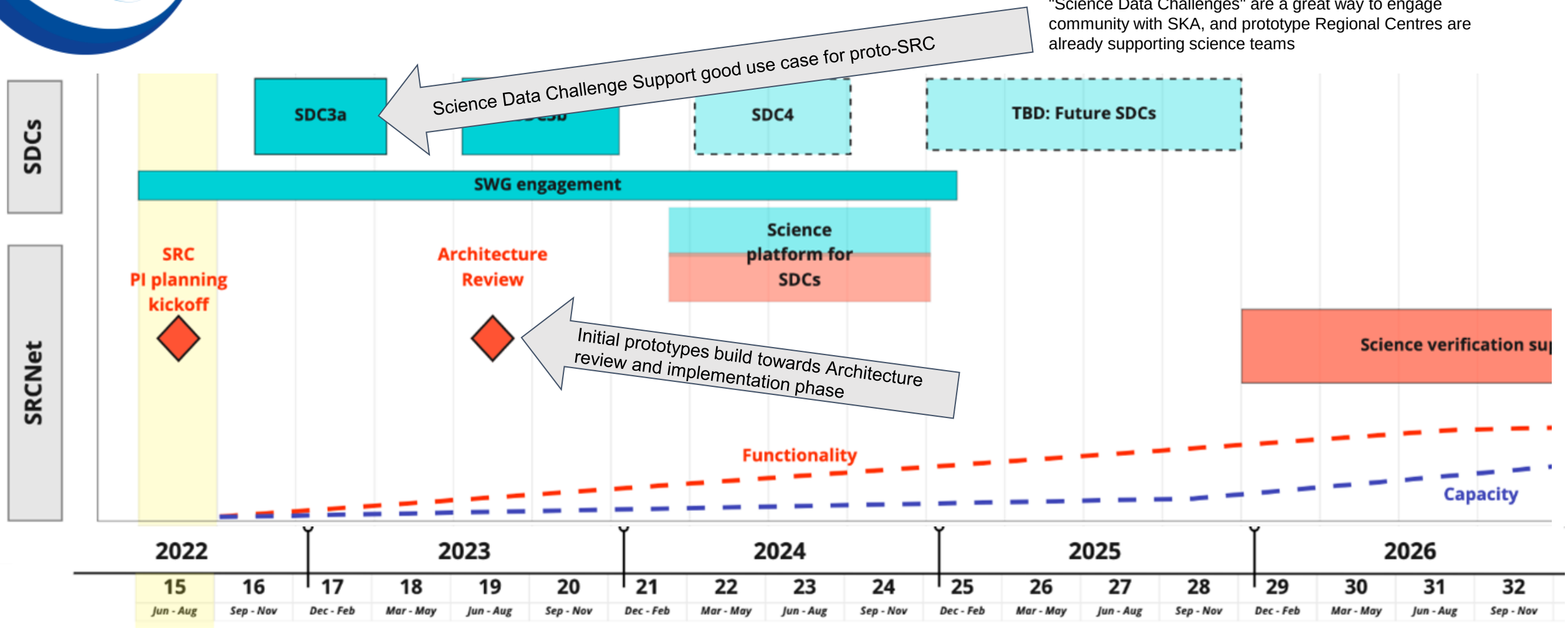
SRC Network Prototyping - 2022 onwards

"Science Data Challenges" are a great way to engage community with SKA, and prototype Regional Centres are already supporting science teams



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Other Benefits of ESCAPE

- Collaborations - experts in range of fields
  - A number of ESCAPE members are now involved in SRC prototyping (ASTRON, IAA)
  - Will continue to work with the contacts we have made (collaboration agreements with e.g. CERN/CTAO)
- Service operations experience
  - Data lake ops
  - Kubernetes deployments
  - Automated integration testing

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Thanks to all our collaborators!

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ESCAPE to the Future
25-26 October 2022
Brussels, Belgium

JIVE
Joint Institute for VLBI ERIC

The EVN Archive Portal

Bringing the science to the data using JupyterHub

Aard Keimpema

keimpema@jive.eu

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JIVE and the EVN

- JIVE is located in the Netherlands
- Technical operations and user support for the European VLBI Network
- The EVN is an *Open Skies* facility
- All EVN data is public after 1 year

The European VLBI Network

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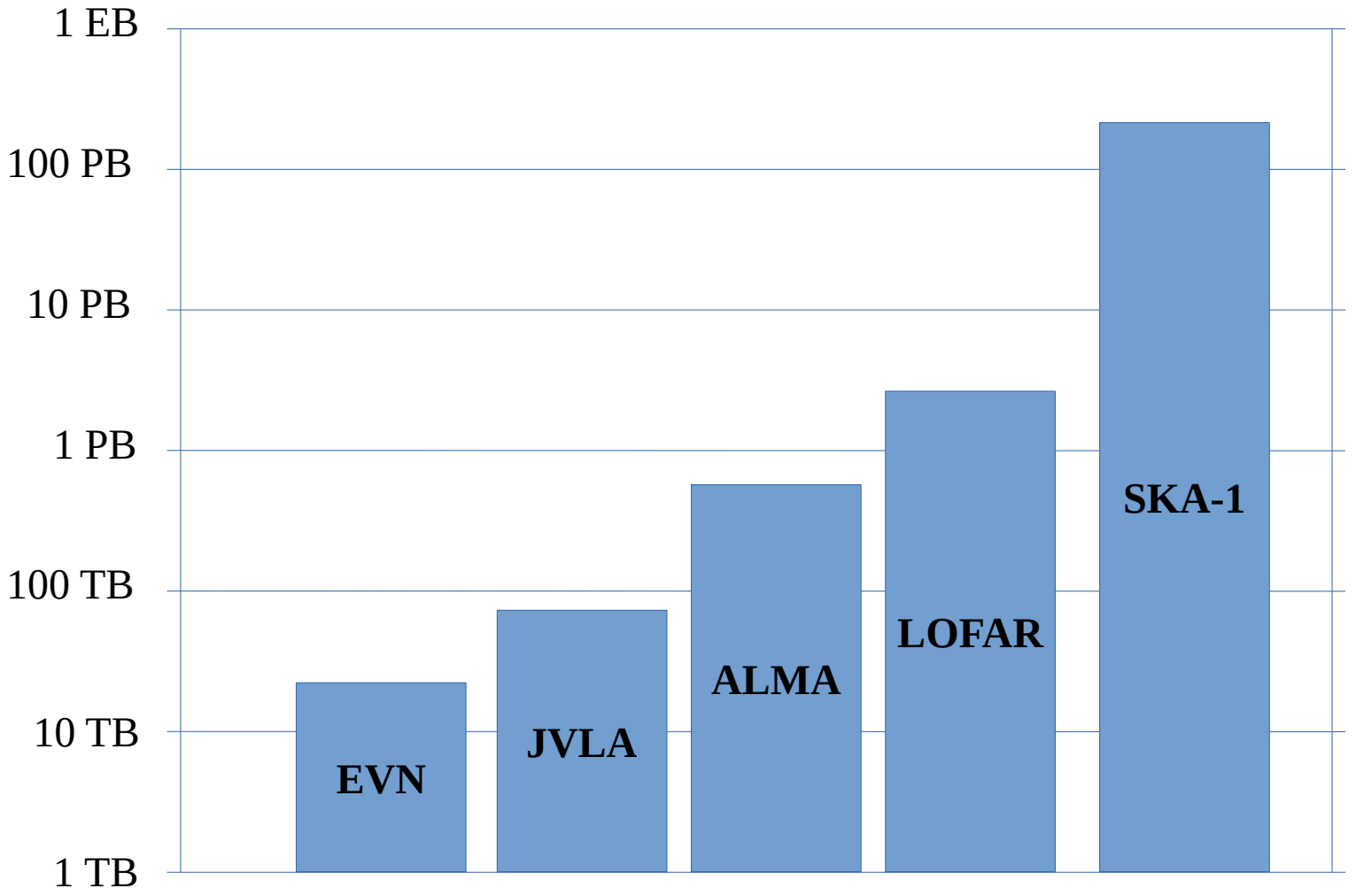
Yearly data volumes (archived data)



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Remote interactive pipelines

- Data should be processed close to where it is archived
- Solutions should accommodate both automated pipelines and interactive data processing
- Main advantages of using Jupyter for remote interactive pipelines:
  - User friendly: Notebooks are easy and intuitive to use; all results are embedded in a single document
  - Interactivity is optional: Notebooks can optionally be run as a non-interactive pipeline for batch processing
  - Accountability: Data reduction process is self-documenting and fully repeatable

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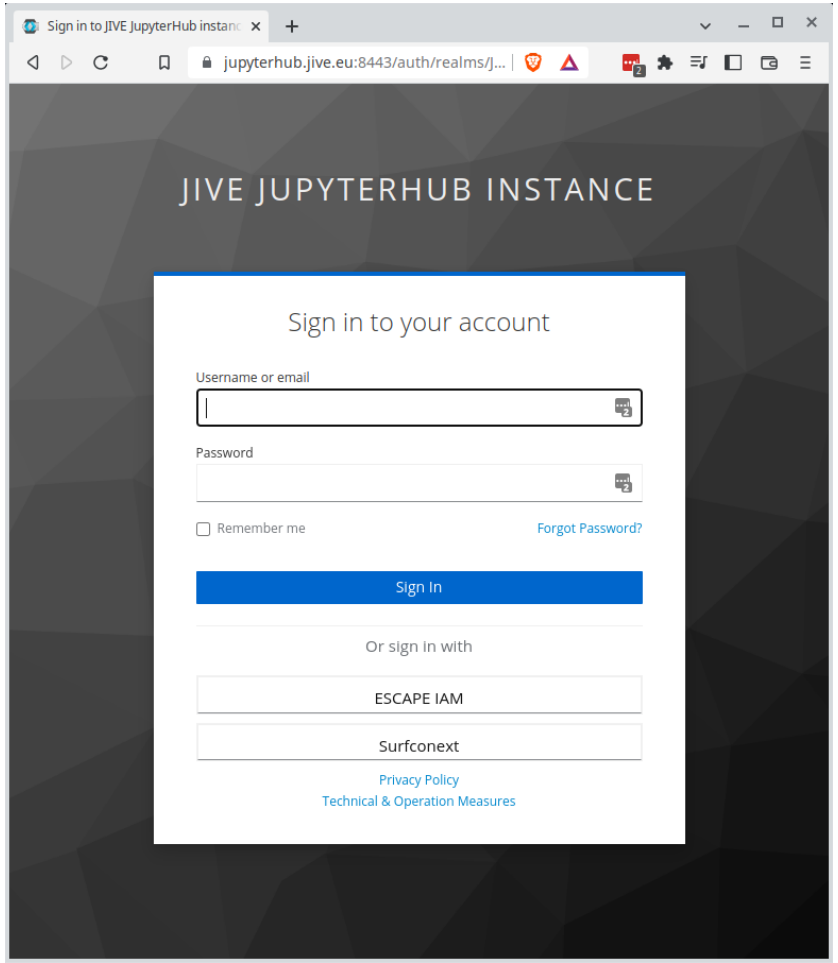
EVN Archive portal

- JupyterHub instance hosted at JIVE
- Open service: All interested users can make a free account and process any observation from the EVN archive
- Builds on the results from WP3 and WP4
- Allow federated logins: ESCAPE IAM, SurfCONEXT; Applying for eduGAIN access
- Integrated with the ESAP using BinderHub



https://jupyterhub.jive.eu

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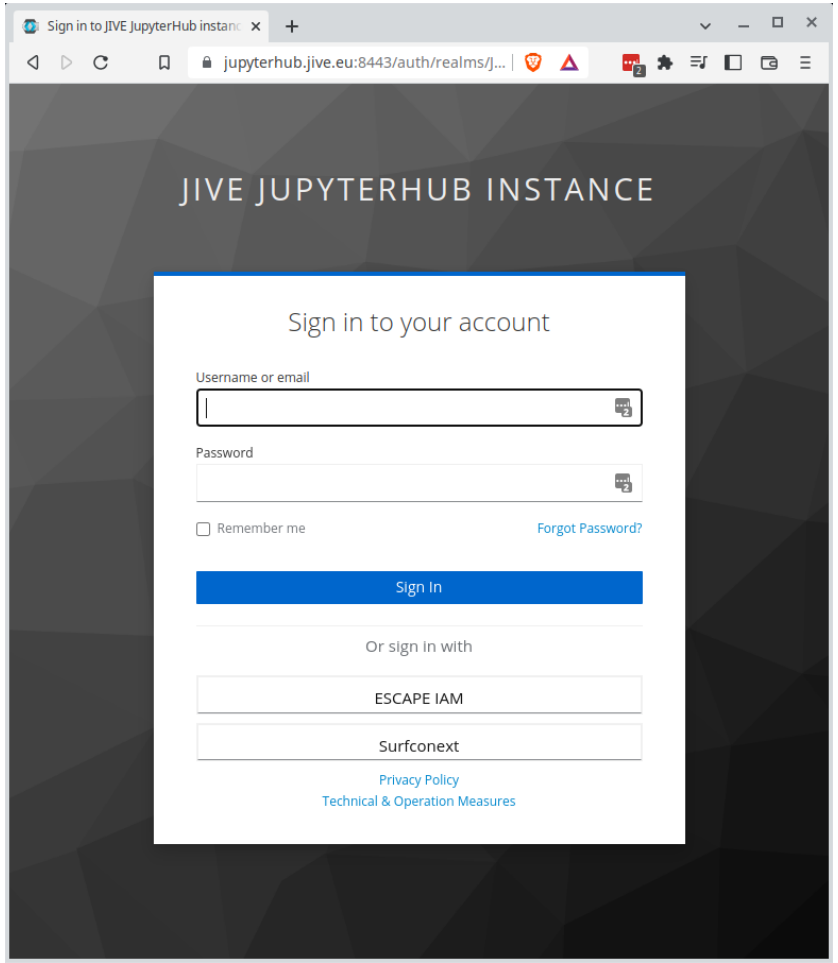
FAIR data standards

- Data on the EVN archive is
  - Findable: Through VO and web interface
  - Accessible: EVN data is public after one year and is accessible through the VO or web interface.
  - Interoperable: Only open source programs and open data formats are used (FITS, Measurement Set)
  - Reusable: Data comes with all relevant metadata and there are no restrictions on use
- Users can submit their notebooks back to the EVN archive allowing other researchers to reproduce their results



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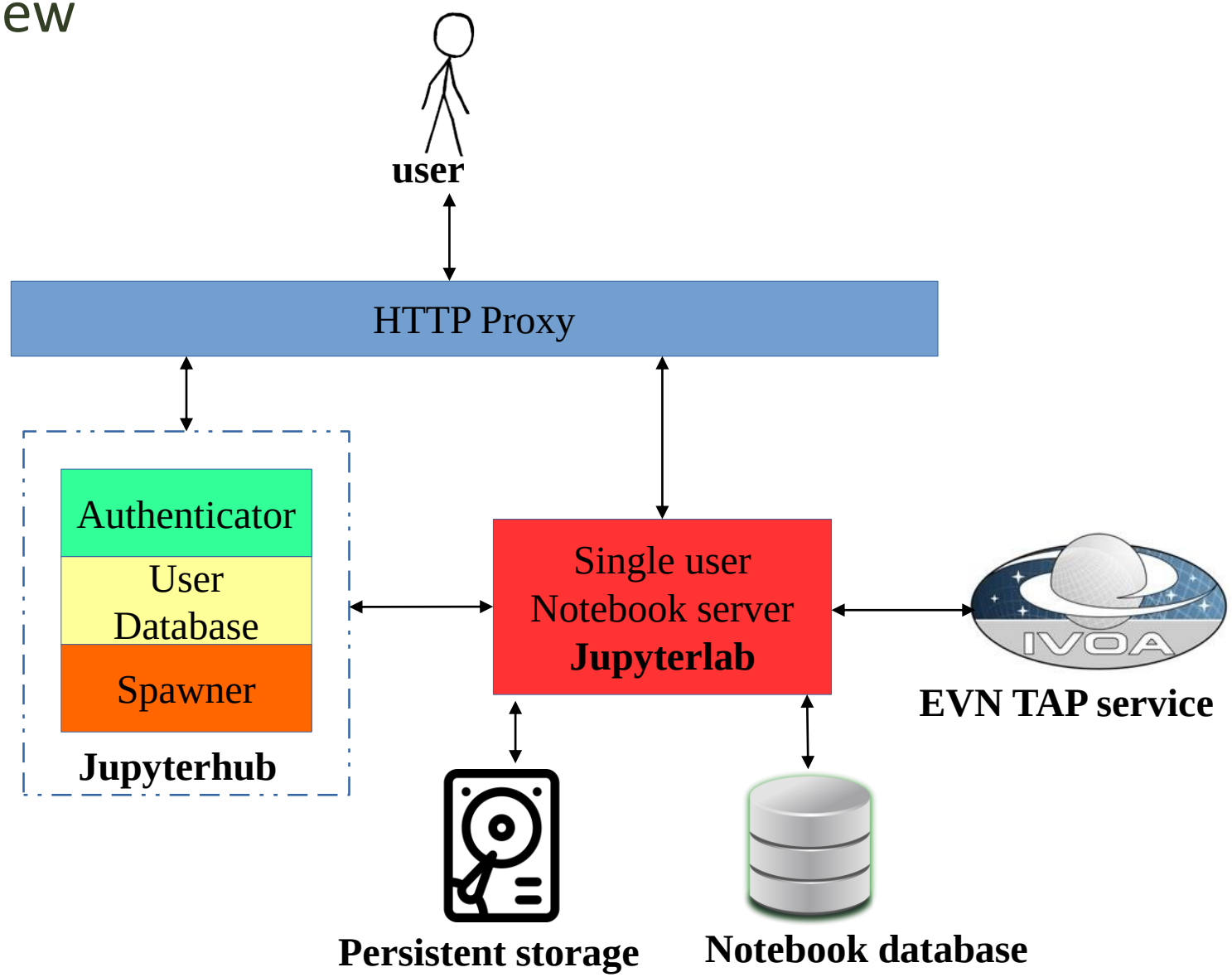
Overview



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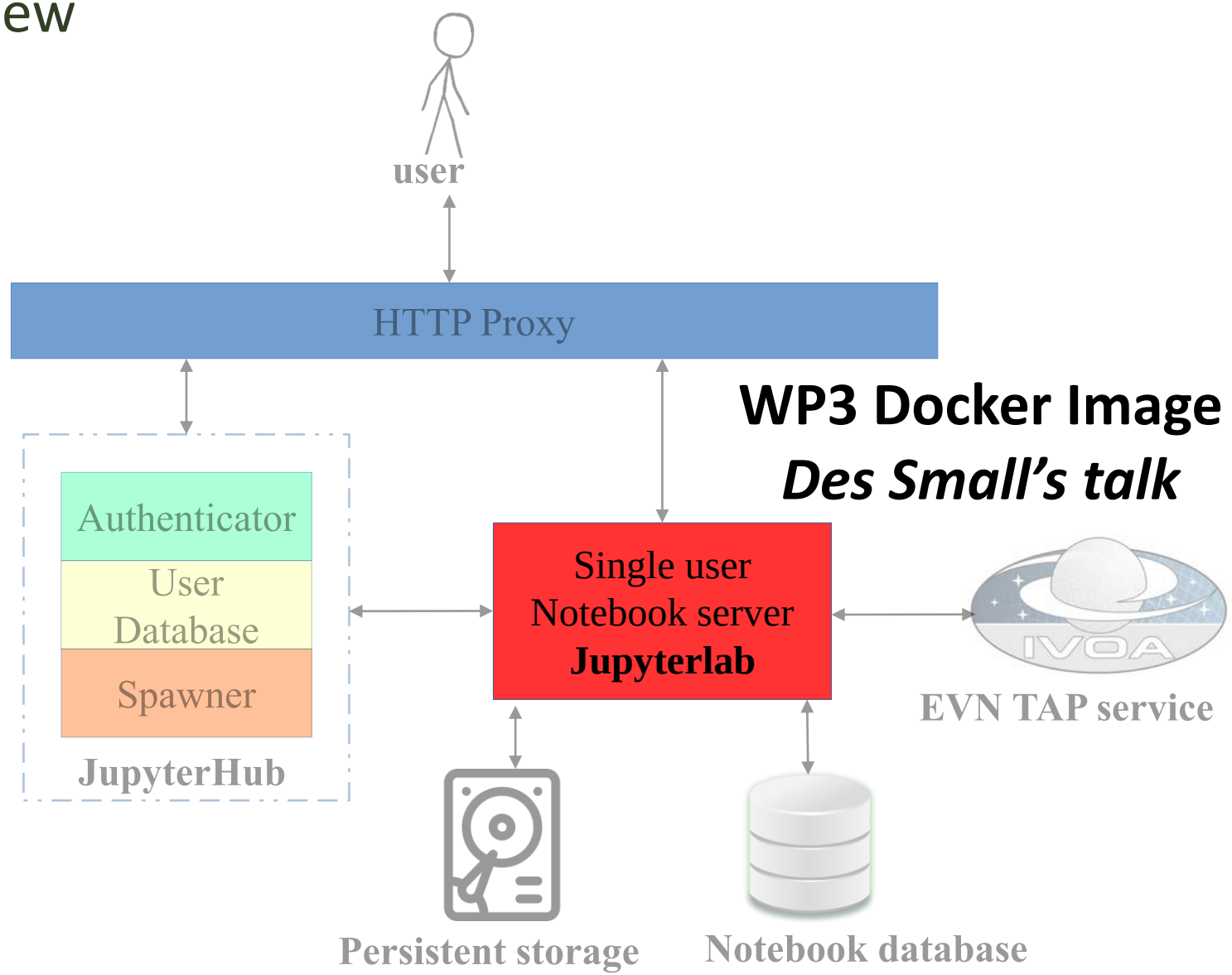
Overview



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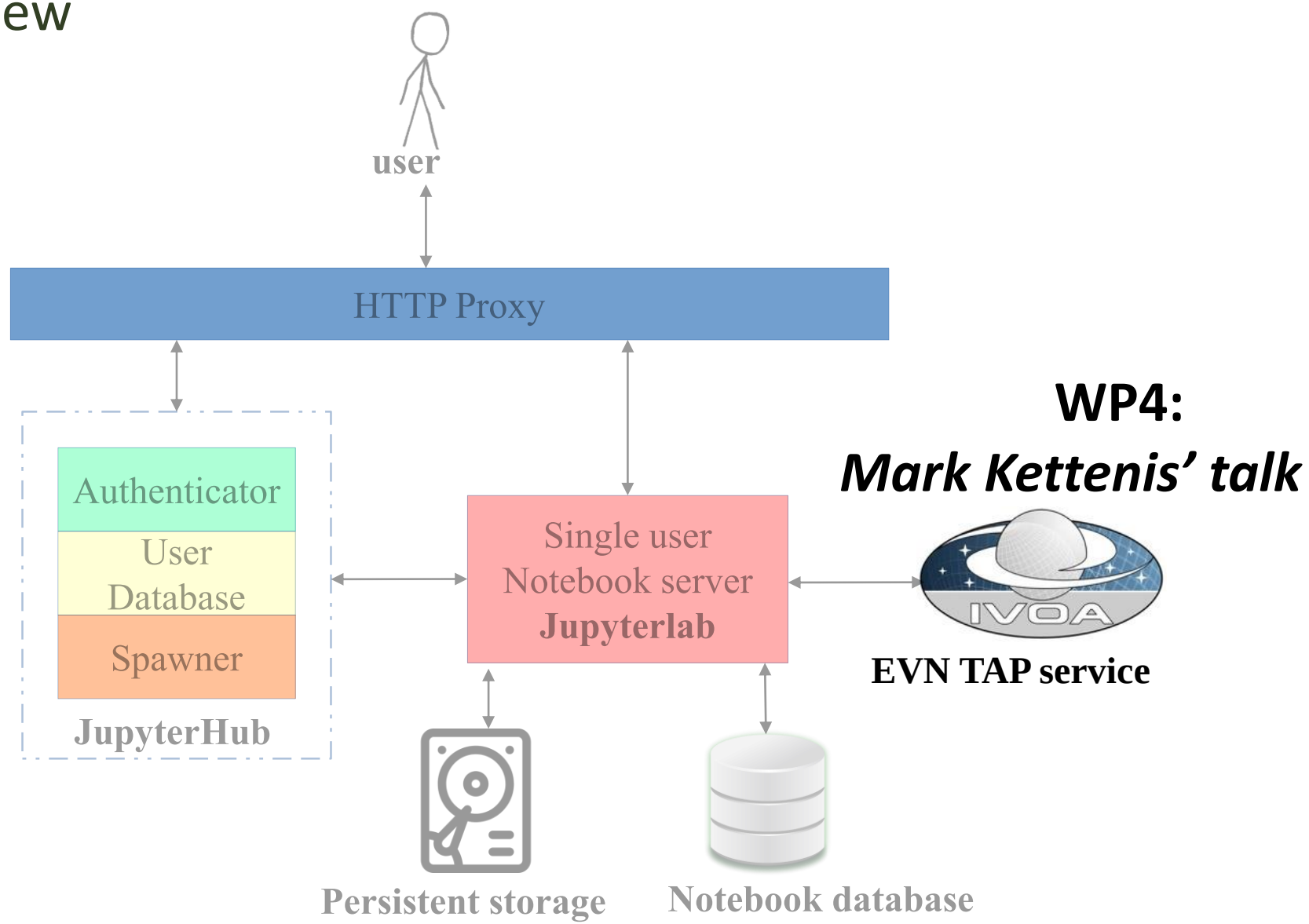
Overview



WP4:

Mark Kettenis' talk

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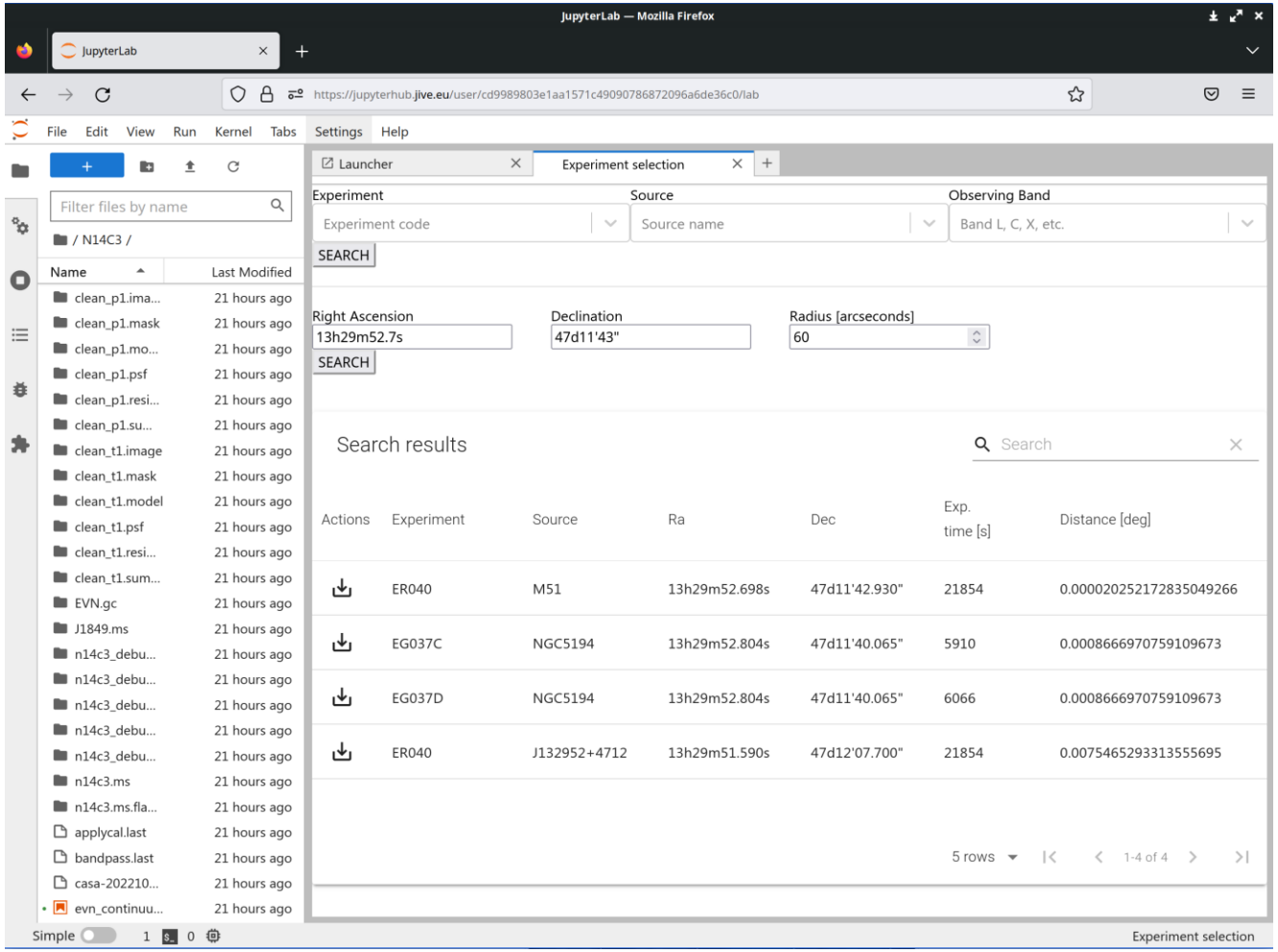
Data discovery

- Data discovery is through a JupyterLab plugin developed at JIVE
- The plugin executes queries using the EVN VO service
- The EVN VO contains the metadata pertaining to all public EVN observations
- Each search result has a Jupyter notebook associated with it



Cone search on the EVN archive

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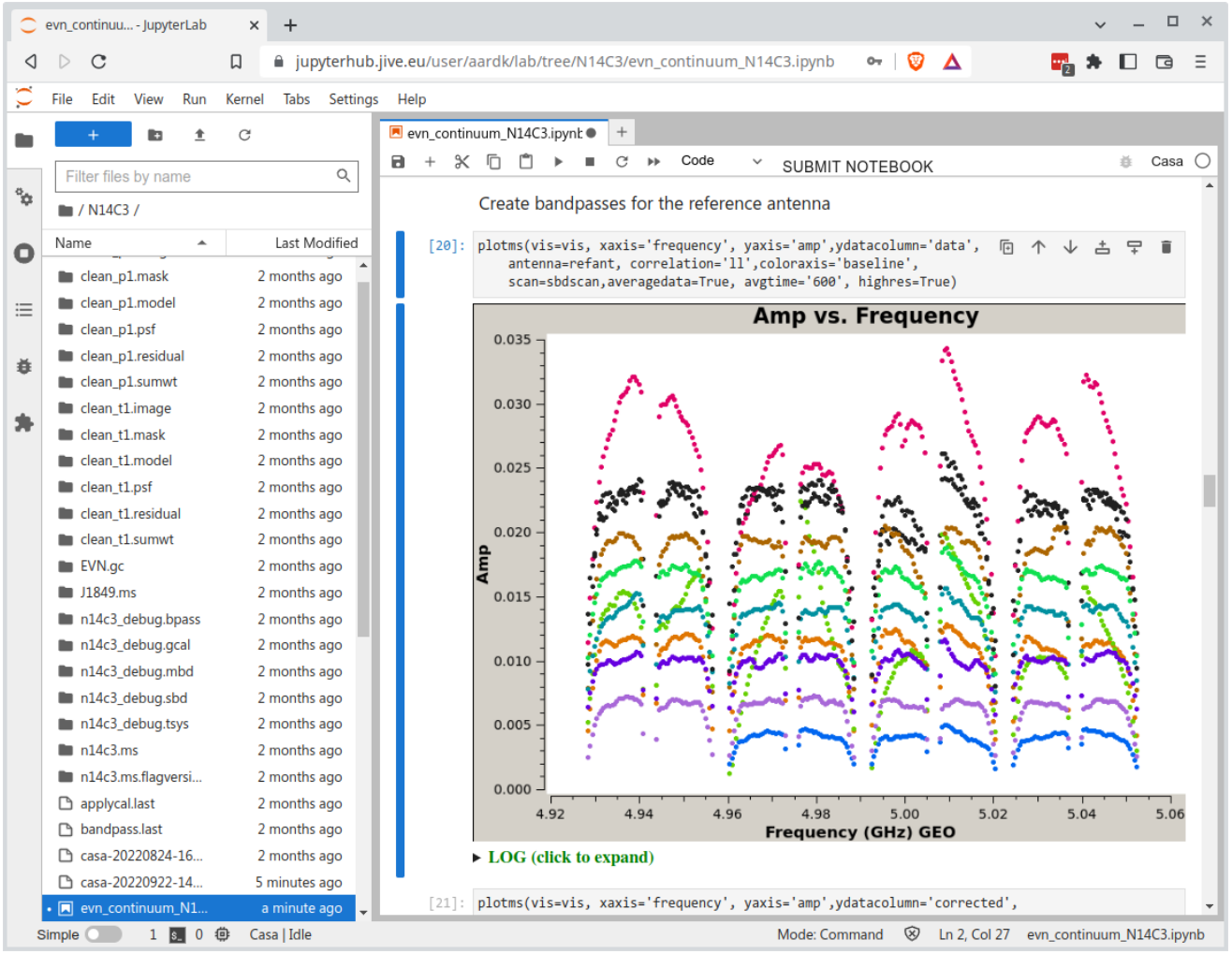
Jupyter-CASA docker image

- Astronomical data processing is based on the widely used CASA software
- The Docker image contains
  - CASA 6.5.1
  - WP3: The Jupyter-CASA kernel
  - WP3: CASA VLBI tools
  - EVN data discovery JupyterLab plugin
  - A collection of widely used radio astronomy packages



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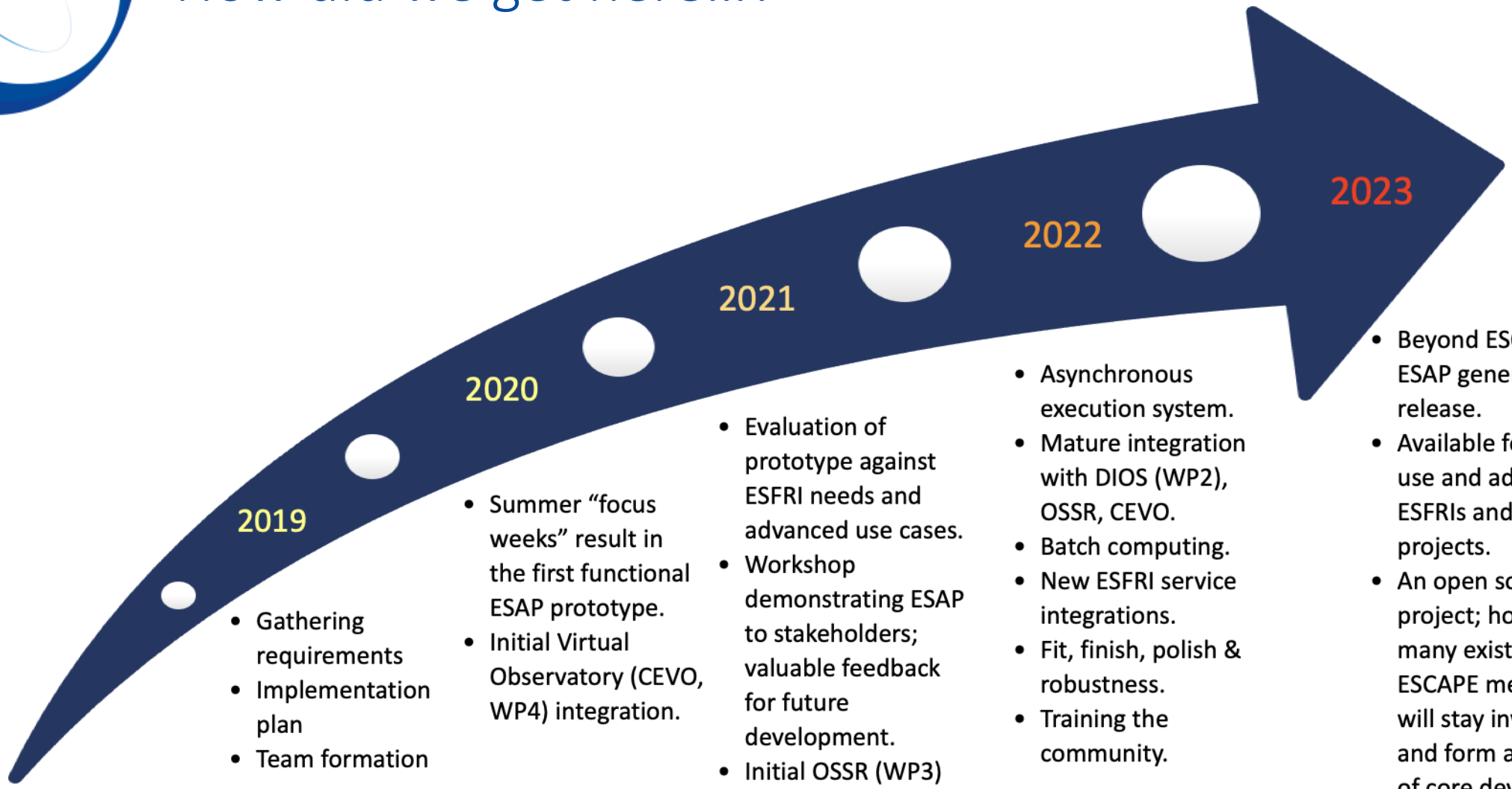
Thank you for your attention!

https://jupyterhub.jive.eu

How did we get here…?



- Gathering requirements
- Implementation plan
- Team formation

- Summer “focus weeks” result in the first functional ESAP prototype.
- Initial Virtual Observatory (CEVO, WP4) integration.

- Evaluation of prototype against ESFRI needs and advanced use cases.
- Workshop demonstrating ESAP to stakeholders; valuable feedback for future development.
- Initial OSSR (WP3) integration.

- Asynchronous execution system.
- Mature integration with DIOS (WP2), OSSR, CEVO.
- Batch computing.
- New ESFRI service integrations.
- Fit, finish, polish & robustness.
- Training the community.

- Beyond ESCAPE: ESAP general release.
- Available for general use and adoption by ESFRIs and other projects.
- An open source project; hoping many existing ESCAPE members will stay involved and form a nucleus of core developers.

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The ESAP Open Source Future

- *Technical Improvements*
  - Improved support for provenance and persistent identifiers.
  - Data sharing and collaborative workflows.
  - Persistent development environments.
  - Rich semantics for describing the relationships between data products, and between data products and compute/analysis software.
- *Sustainability*
  - Build out complete, ESFRI-focused virtual research environments using ESAP.
  - The ESAP open source core provides ongoing development and maintenance.
- *Common Standards*
  - A federated network of science platforms.
  - IVOA Execution Planner as a first step.

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