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A Scalable and Collaborative platform for Neutron science at ESS

- Computational infrastructure for scientific users

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03.09.2025 Data System & Technology (DST)

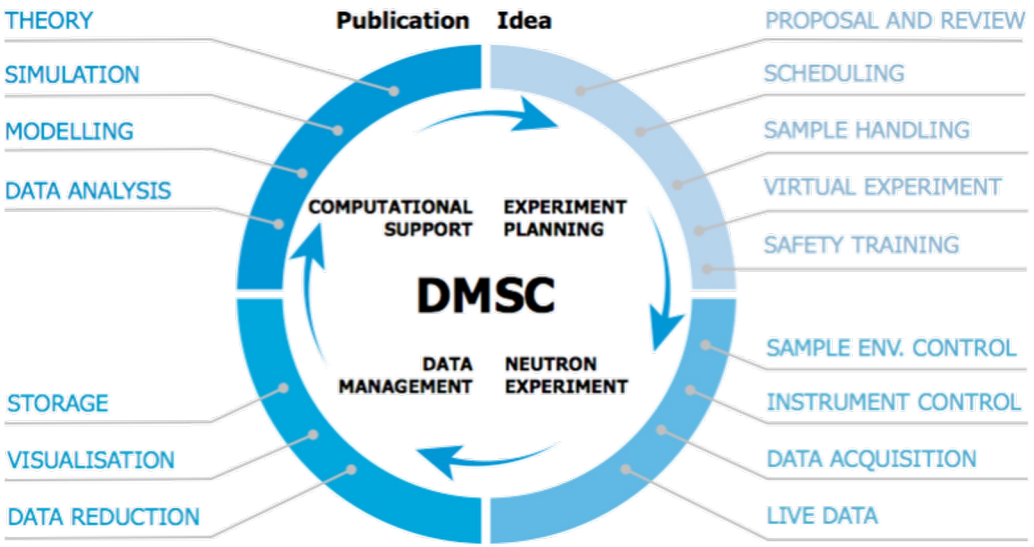
DMSC

Computational infrastructure for the scientific user program

Goal:

Provide computational infrastructure that supports the user-journey of the scientific user from **Idea** to **Publication**

- **Pre-Experiment**:
  - Simulations, modelling, virtual experiments
- **On-Experiment:**
  - Experiment control
  - Data acquisition / Live data / analysis
- **Post-Experiment:**
  - Data (re-)reduction and analysis
  - Simulation/modelling
  - Publication support



User-experience needs to be:

- Efficient
- Consistent
- User-friendly
- Powerful

In a way that supports:

- Collaboration
- FAIR principles
- Remote operations

VISA

Virtual **I**nfrastructure for **S**cientific **A**nalysis
- developed at ILL – funded by PANOSC

- **On-demand** desktop and JupyterLab environment for experiment users
- Available for users both **before**, **during** and **after** the experiment
- Sessions can be **shared** with collaborators (and local contacts / support)
- **Compute resources** are allocated based on experiment and instrument

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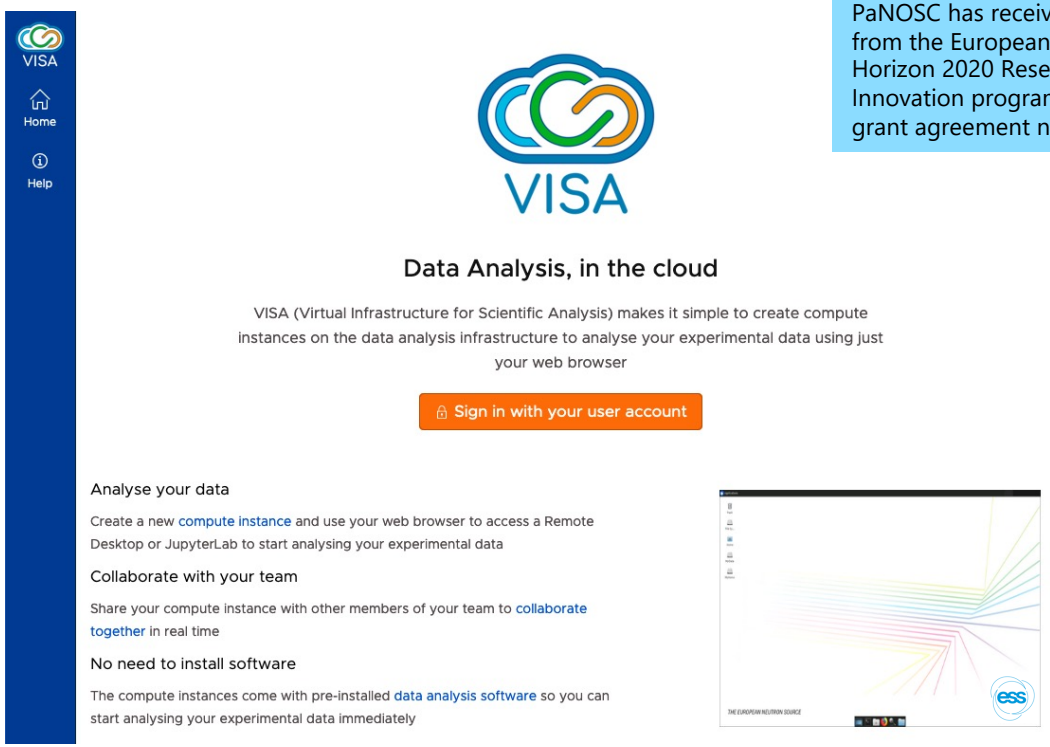

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VISA at ESS

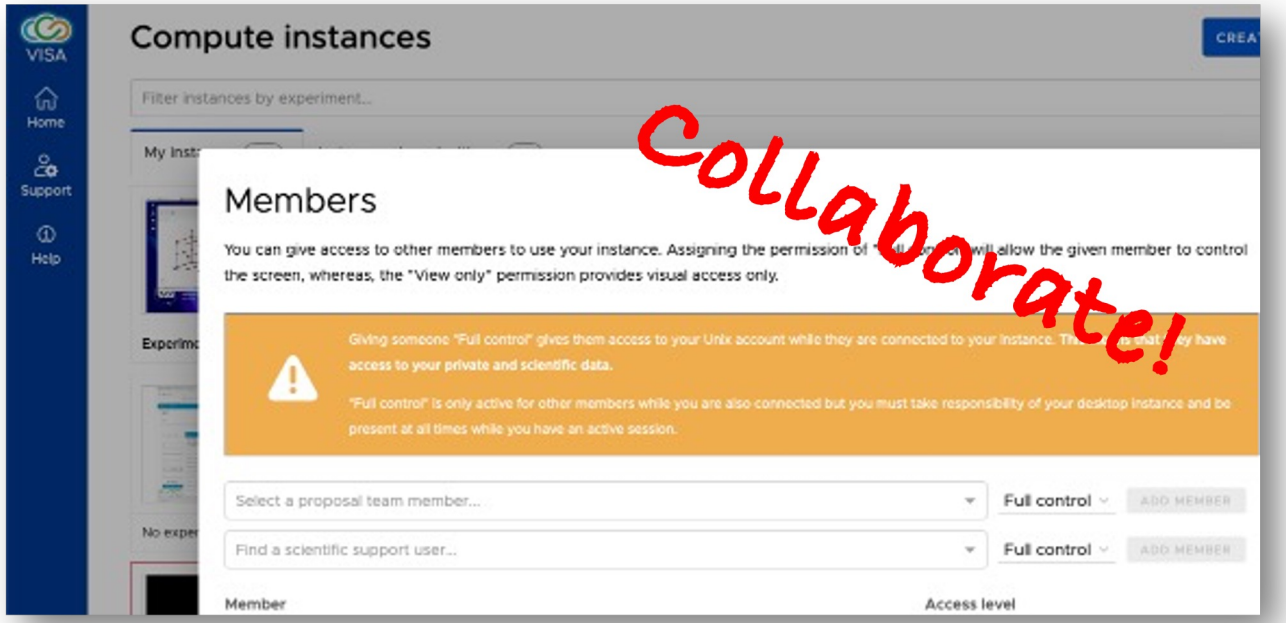
User-experience

- User-friendly:
  - Only local requirement for the user is a standard browser
- Efficient:
  - Low learning curve for new users through e.g. tutorials, templates and experiment preparation
  - All relevant tools, application and environments available for the user from the start
    - 45+ neutron science applications supported (and more coming)
  - Integrated jupyterLab-server with e.g. full support for scipp
- Consistent user-experience:
  - Same VISA experience in all phases of the experiment (before, during and after the experiment)

VISA at ESS

Collaboration

- Real-time collaboration tool for multi-institutional teams
  - Secure data-sharing (*/ess/data*)
  - Real-time support, incl. screen-sharing, from ess staff



- Collaborate with your team – easy screen- and data-sharing

VISA at ESS

Scalability

- ESS-based infrastructure:
  - enabling easy access to computational resources for large-scale datasets
  - HPC, GPU and storage
  - Available for users both on site and remotely

Interoperable

- Supports FAIR data-use (e.g. allows software versioning for re-producibility)
- Integration with SciCat data portal facilitates data re-discovery and re-exploitation
- Containerized (-based) scientific software mitigates dependency conflicts

VISA at ESS

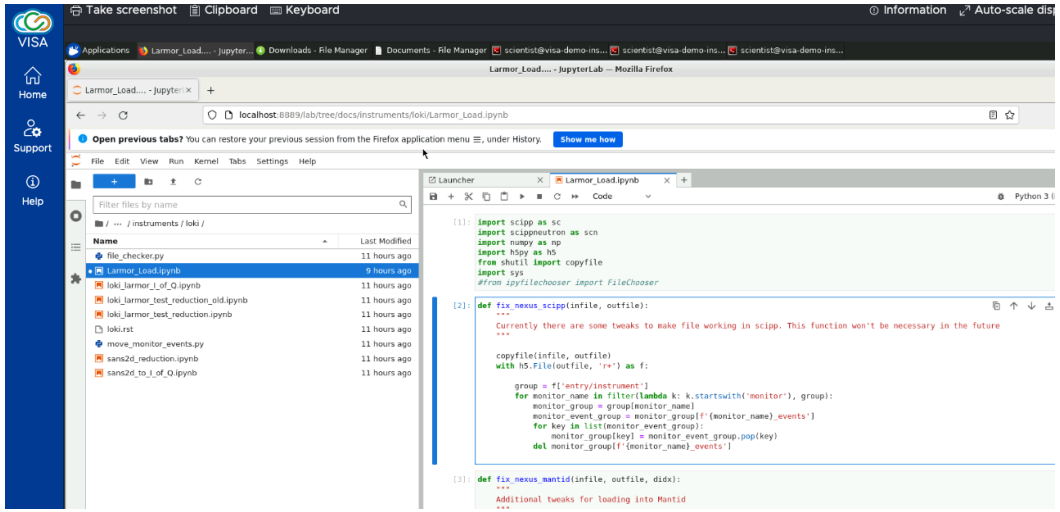
Scientific Applications

- Scientific applications (apps) in VISA will be made available through **apptainer containers**
- Containers allow for each app to **have its own environment** (which mitigates conflicts between different apps and versions)
- **Live updates to apps** (incl. hot-fixes in a support-situation) without the user needing to restart their instance

Apptainer

(formerly singularity project)

- docker-like containers without (most) of the security issues of docker. Provides a self-contained environment that can run independently of the host system and environment.



VISA at ESS

Scientific applications

- **Reproducibility** will be ensured as old versions of apps will still be available (and working) for users – also when redoing an analysis after many years – supporting **FAIR** data use

- **Flexibility** - as users can build and bring their own containers with applications, or download a container with the software used for a given proposal cycle to use on their own compute resources

- Work in progress:
  - SciCat integration
  - FAIR data use (third party)
  - BEAMLIME integration
  - Windows support

- Backend:
  - Openstack
  - Authentication through Keycloak / PingID
  - Authorization from UserOffice

VISA

Case study

- DMSC Summer School 2025
  - 20 external students
  - 5 days of training in Neutron science techniques and ESS software
  - Science User user-journey:
    - Sign up in Useroffice with ORCID as members of ‘Workshop’ proposal
    - Using VISA - juypyterlab

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VISA at ESS

2 min Demo

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Thank you

Questions?

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