



**EUROPEAN
SPALLATION
SOURCE**



Computational infrastructure for the scientific user program (VISA)

ESS DMSC meets DTU and UCPH, Workshop 2

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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:

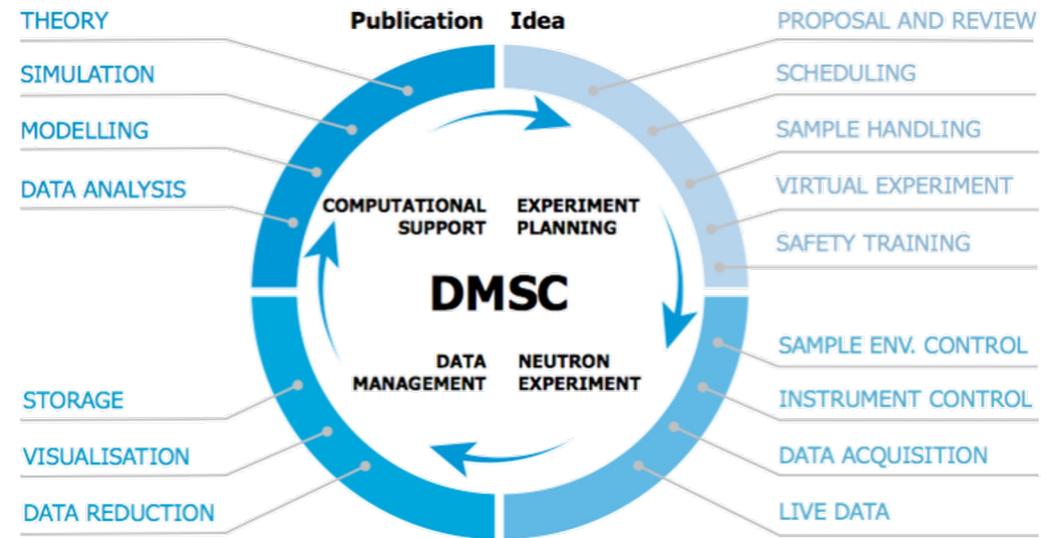
- Simulations, modelling, virtual experiments

– On-Experiment:

- Experiment control
- Data acquisition / Live data / analysis

– Post-Experiment:

- Data (re-)reduction and analysis
- Simulation/modelling



User-experience needs to be:

- Efficient
- Consistent
- User-friendly
- Powerful

In a way that supports:

- Collaboration
- FAIR principles
- Remote operations

VISA

Virtual Infrastructure for Scientific Analysis

- 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

<https://visa.readthedocs.io/>



Data Analysis, in the cloud

VISA (Virtual Infrastructure for Scientific Analysis) makes it simple to create compute instances on the data analysis infrastructure to analyse your experimental data using just your web browser

[Sign in with your user account](#)

Analyse your data

Create a new [compute instance](#) and use your web browser to access a Remote Desktop or JupyterLab to start analysing your experimental data

Collaborate with your team

Share your compute instance with other members of your team to [collaborate together](#) in real time

No need to install software

The compute instances come with pre-installed [data analysis software](#) so you can start analysing your experimental data immediately





VISA at ESS

Integration

- **Persistent storage/config** across sessions, instances and proposal cycles (though any given instance will have a limited lifetime, a new can just be started with the same settings)
- **Computing cluster integration** – to enable easy computing offload from e.g. JupyterLab/DASK to the DMSC HPC cluster



VISA at ESS

Scientific Applications



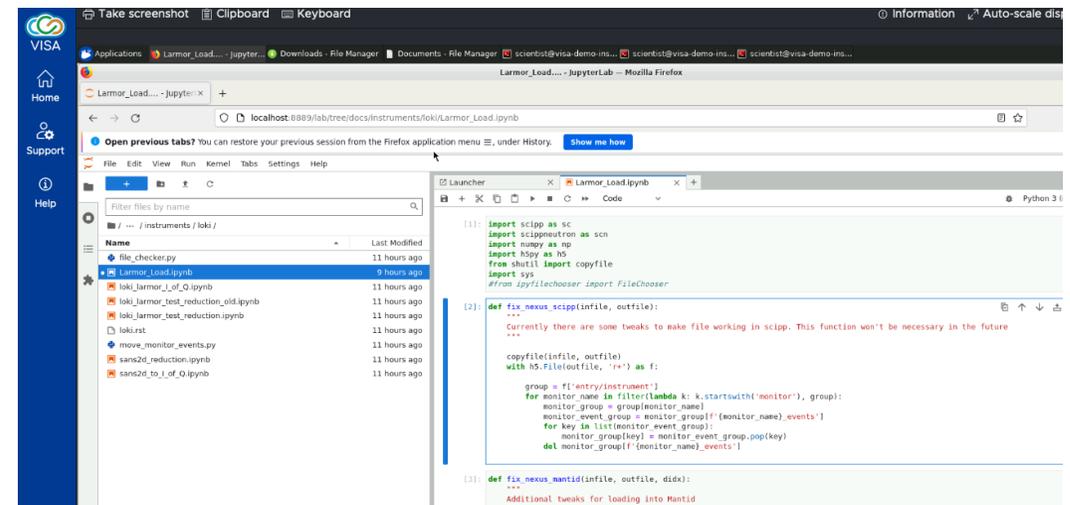
- Scientific applications (apps) in VISA will be made available through **apptainer containers**
- Containers allow for each app to **have its own environment** (which mitigates conflicts between different apps and versions)
- Live updates to apps** (incl. hot-fixes in a support-situation) without the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



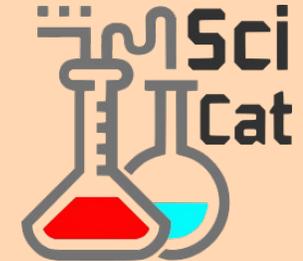


VISA at ESS

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

- Planned features:
 - SciCat integration
 - FAIR data use (third party)
 - Windows support



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





2 min Demo

<https://visa.readthedocs.io/>



Thank you

Questions?

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