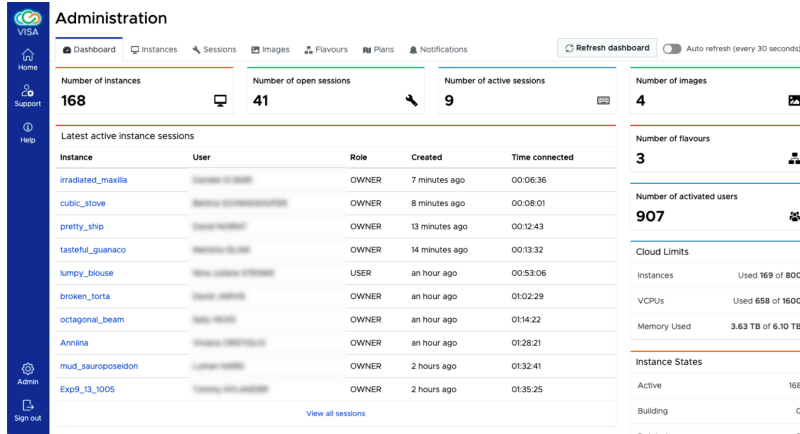


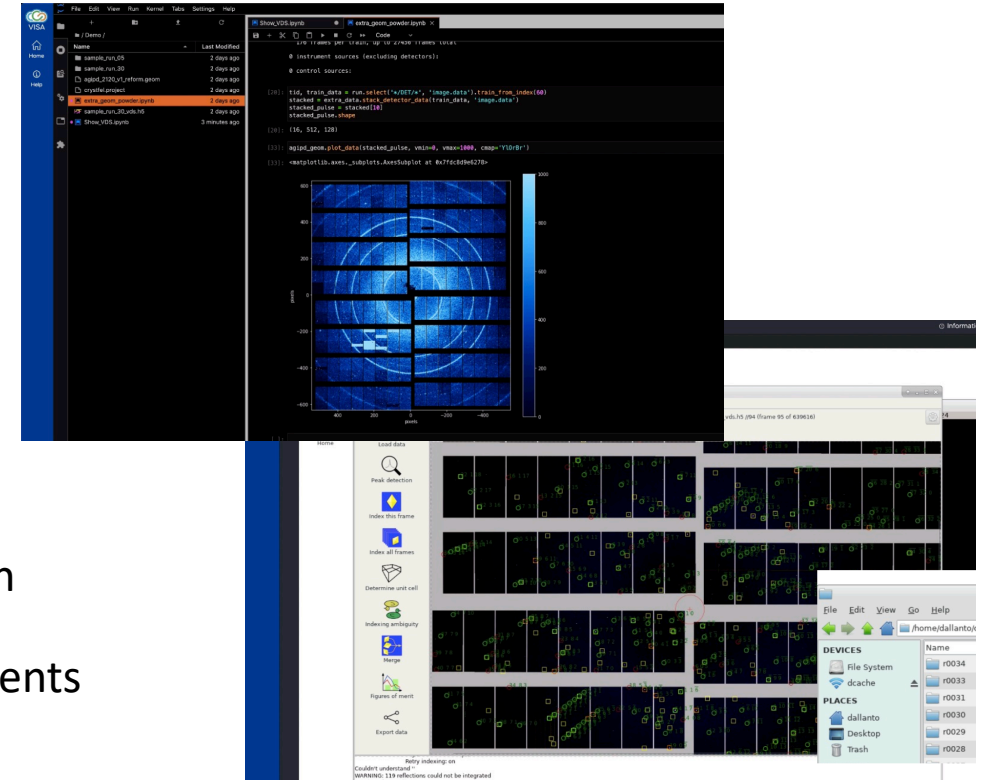
Lessons learned from conducting workshops and trainings using the VISA platform at the European XFEL



Visa - Virtual Infrastructure for Scientific Analysis



visa.readthedocs.io



“Abstract away” infrastructure and use case specific configuration

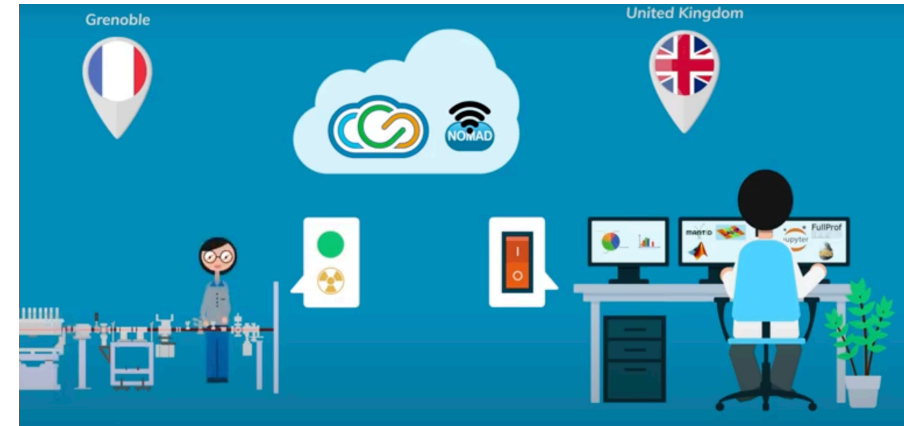
Facility integrates and scales generic data analysis environments

Jupyter Ecosystem

Linux remote desktop

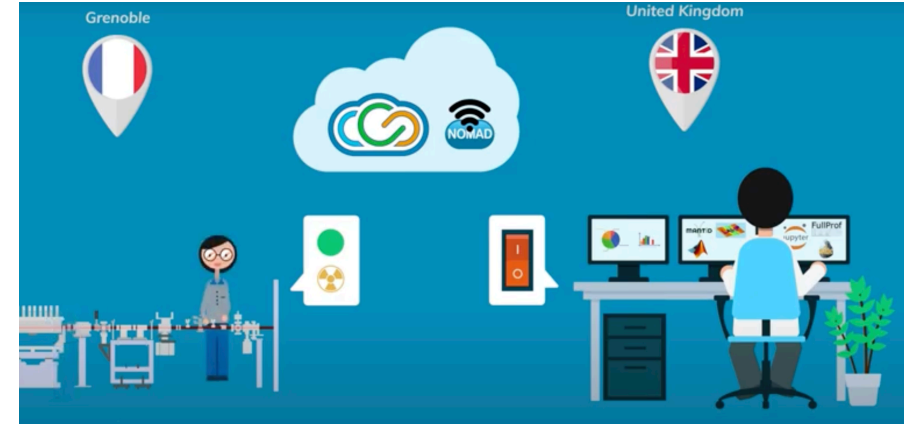
Use cases can provide specific data analysis environments, agnostic of the infrastructure

Visa - Virtual Infrastructure for Scientific Analysis



visa.ill.fr -> youtube.com/watch?v=EAVgbQXRldo

Visa - Virtual Infrastructure for Scientific Analysis

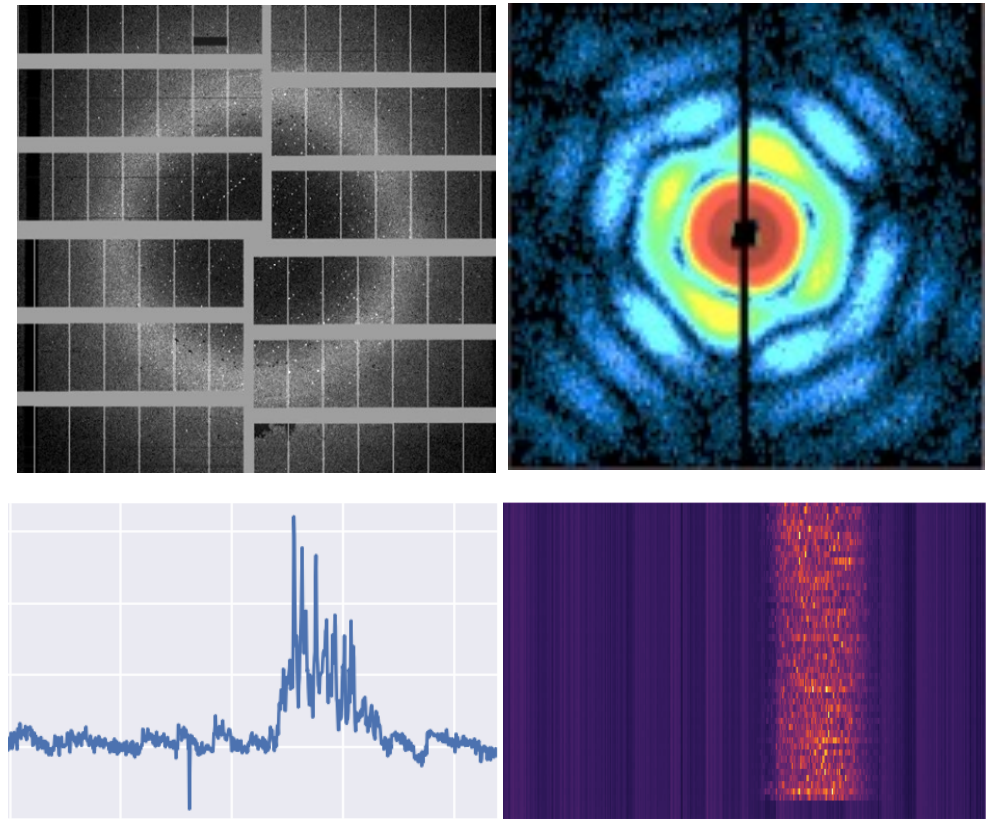
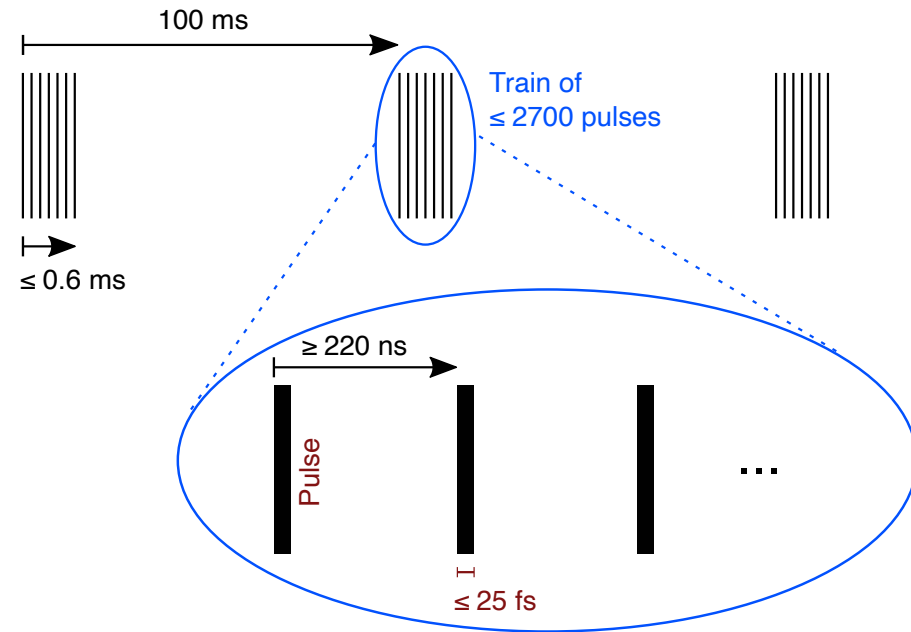


visa.ill.fr -> youtube.com/watch?v=EAVgbQXRldo

- Developed by ILL, project open sourced as part of the Photon and Neutron Open Science Cloud (PaNOSC)
- Remote data analysis, remote experiment control
- EuXFEL joined MoU on VISA Collaboration
- Provide users with access to open data, software, compute infrastructure and support (IT / scientific)

Use case 1 - open access to reference data and best practices

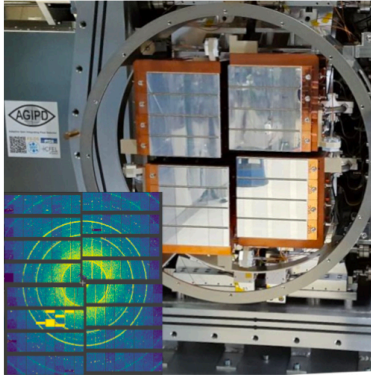
- Diffraction / scattering data from large area detectors
- Spectroscopic data from 1D detectors
- Digitisers, diagnostics devices, control data, ...
- High repetition rates at 4.5MHz



Source: Kirkwood et al. (2022) Nat. Sci. Data 9

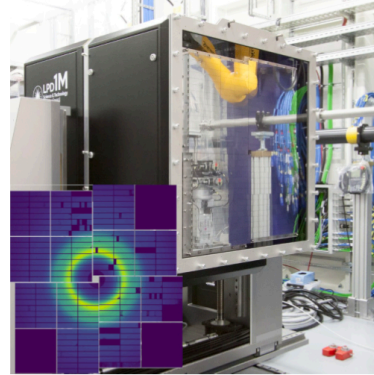
Use case 1 - open access to reference data and best practices

AGIPD-1M



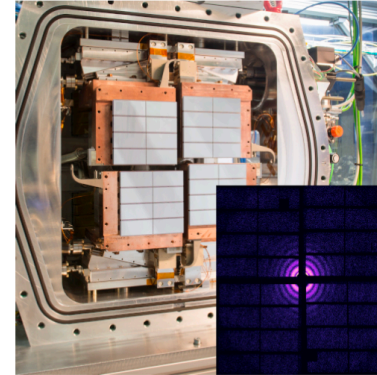
21 hours/PiB

LPD-1M



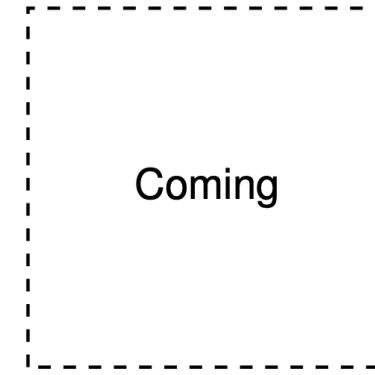
29 hours/PiB

DSSC-1M



19 hours/PiB

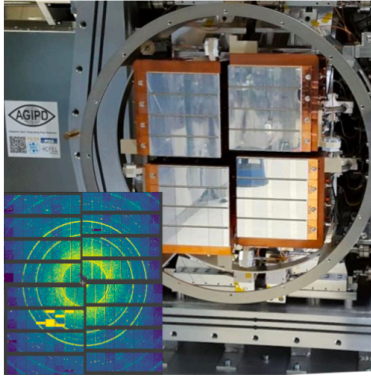
AGIPD-4M



6 hours/PiB

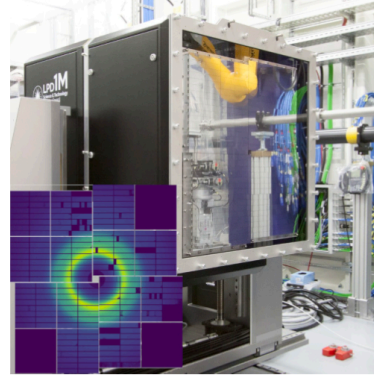
Use case 1 - open access to reference data and best practices

AGIPD-1M



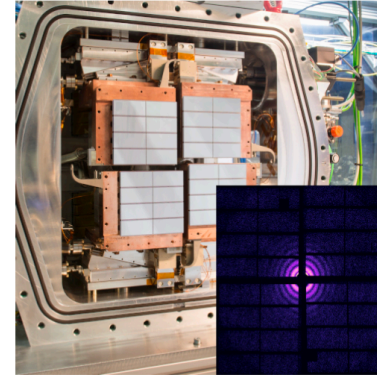
21 hours/PiB

LPD-1M



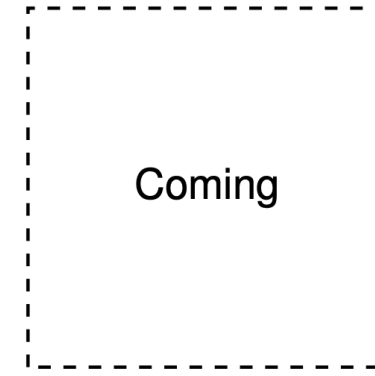
29 hours/PiB

DSSC-1M



19 hours/PiB

AGIPD-4M



6 hours/PiB

■ Data must be analysed and reduced at the facility

■ Time-limited access to compute infrastructure (allocated for a proposal / beam time)

■ Site specific authentication, authorisation, networking, software repositories, ...

Use case 1 - open access to reference data and best practices



The overall process of crystal structure determination

The first part of data analysis by SFX beamtime users ends with a unique set of crystallographic structure factors.

Interactive data analysis environment as additional service for readers of a scientific publication on automating photon science analysis pipeline

Data Availability Statement: Data sets used for the tutorial are freely accessible through [visa.xfel.eu] and, for European XFEL users, at [DOI: 10.22003/XFEL.EU-DATA-700000-00](https://doi.org/10.22003/XFEL.EU-DATA-700000-00)

A reduced data sample was prepared for this use case:
`frames_list="indexed_p700000_r0030.lst"`

EXtra-Xwiz: A Tool to Streamline Serial Femtosecond Crystallography Workflows at European XFEL

Article in *Crystals* · October 2023

DOI: 10.3390/cryst13111533

mdpi.com/2073-4352/13/11/1533

Use case 1 - open access to reference data and best practices



The screenshot shows the VISA interface with a sidebar on the left containing 'VISA', 'Home', and 'Help' icons. The main window displays a tutorial titled 'The overall process of crystal structure determination'. The process is shown as a sequence of four steps: 1. 'Diffraction image series' (a stack of images), 2. 'Image data processing' leading to a 'Reduced ("unique") data set of measured structure factor intensities' (a 3D cube of points), 3. 'Phasing' leading to 'Structure factors with phases added, Complete Fourier coefficients' (a 3D cube of points with colors), and 4. 'Reconstruction' leading to a 'Real space electron density map' (a 3D model of a crystal lattice). Below the diagram, it states: 'The first part of data analysis by SFX beamtime users ends with a unique set of crystallographic structure factors.'

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Use case 2 - Environments for trainings and tutorials on the Karabo control system

 <p>VISA_KARABO_WORKSHOP (0.2)</p>	 <p>EIROForum 2024 Summer School Automation tutorial (1)</p>	 <p>NOBUGS 2024 (1)</p>
<p>Image for Karabo Developer Workshop (Ubuntu 18 Bionic)</p>	<p>Image prepared to be used for the EIROForum 2024 Summer School Automation tutorial.</p>	<p>Image prepared to be used for the NOBUGS 2024 Karabo Workshop</p>

Foto: Steffen Hauf



- In-house developed open source system for Supervisory Control and Data Acquisition (SCADA)
- Karabo GUI is the main operator interface at EuXFEL
- Workshop participants interacting with Karabo through their web browser, using the remote desktop
- Image for a standalone Karabo installation, including auxiliary services: project database, message broker
- Workshop content updated outside of the image
 - Tasks implemented as git repo, users checkout tags
 - Resources imported from Nextcloud
 - Mar Internal at EuXFEL
 - May Summer school at EIROforum
 - Sep Satellite event at NOBUGS 2024

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Use case 2 - Environments for trainings and tutorials on the Karabo control system

The screenshot displays the Karabo GUI interface. On the left, a system topology tree shows the 'DEMO' environment. The main window features a 'Simulated Beam' plot with X and Y axes in pixels and a color scale. Below it, 'X and Y MOTORS' and 'X and Y MOTORS (FINE TUNE)' panels allow for target and actual position adjustments. A 'Beam on Sample' plot shows the beam's position on the sample with associated jitter and width parameters. A 'Start Here' panel provides a step-by-step guide for system initialization. A state graph shows the 'ON', 'OFF', and 'MOVING' states of the simulated motors over time. Annotations in yellow boxes provide detailed explanations of the beam position calculation, motor movement effects, and fine-tuning capabilities.

- Karabo GUI to build complex hierarchical scenes with Qt Widgets
- Use of labels to explain elements in great detail
- Runs with a simulated experiment, use case needs no data access
- Efficient real-time support by tutors leveraging the collaborative nature of the remote desktop service

Use case 3 - Empirical methods in Research Software Engineering (RSE)

```
xfel.eu data-reduction-recipe v1.0

- AgipdGain <exdf.data_reduction.builtins.AgipdGain>
rechunk-keys      SPB*AGIPD1M*:xtdf      image.data      (-1, 1, None, None)
subslice-keys     SPB*AGIPD1M*:xtdf      image.data      [0, :, :]

- ManualPattern <exdf.data_reduction.builtins.ManualPattern>
select-entries   SPB*AGIPD1M*:xtdf      image            by_id [10:60]

- SomeUserMethod <user.package.module>

...
```

Philipp Schmidt (IFDEPS 2024): Data reduction activities at European XFEL: early results

Domain Specific Language (DSL) for flexible data reduction pipelines

Extendable series of semantic expressions, generated by use case specific plug-ins

Operationalise rewriting of files (EXDF based on HDF5)

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```

```
- SomeUserMethod <user.package.module>
```

```
...
```

How do users interact with our data reduction tools

How are manual patterns achieved

Extend DSL with user supplied operations

Philipp Schmidt (IFDEPS 2024): Data reduction activities at European XFEL: early results

Domain Specific Language (DSL) for flexible data reduction pipelines

Extendable series of semantic expressions, generated by use case specific plug-ins

Operationalise rewriting of files (EXDF based on HDF5)

Wrap up

- Use case 1 - open access to reference data and best practices
 - Run data analysis software on sampled, reduced reference data
- Use case 2 - Environments for trainings and tutorials on the Karabo control system
 - Collaborative remote desktop sessions for real-time support from domain experts
- Use case 3 - Empirical research in Research Software Engineering (RSE)
 - Collaborative remote desktop sessions for interviewing users about data reduction recipes