

VISA @ European XFEL

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16th September 2022



Open data as training data @ EuXFEL

- Data file format @ EuXFEL is HDF5
- MHz Mpixel detectors create huge amounts of data, plus modular geometry, special data layout
- Training: selected XMPL runs = datasets from real experiments post-embargo (or commissioning)
- New users get access to "Maxwell" HPC cluster @ DESY, plus free-access folders on filesystem
- Typical environment for data analysis:
 - simple ssh for terminal and non-graphical command-line programs
 - JupyterHub at Maxwell sub-partition running JupyterLab servers, SLURM is underlying for distributed tasks
 - FastX remote desktop service to run graphical applications on "display nodes" of Maxwell



These projects have received funding from the *European Union's Horizon 2020 research and innovation programme* under grant agreements No 857641 and No 823852.



Proposal no. 700000

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Proposal Runs



- i** Automatically assess new runs (after being closed by DAQ) as: [To be evaluated manually](#) [Off](#)
- i** Automatically start run calibration after migration: [No](#)

| Run Number (alias) | Run type | Sample Name | Techniques | Start date | Run status | Data Assessment | Calibration | Run Comment | Edit |
|-----------------------|--------------------------------|----------------------------|--|---------------------------------|---------------|--------------------|----------------------|---|----------------------|
| 0034 | Single Particle Diffraction | Sucrose Solution 3% v/v | coherent diffraction imaging | 2021-06-01 02:25:08 +0200 | Closed | Good | Edit | View Add Edit | Edit |
| 0033 | scattering | Vycor | small angle x-ray scattering | 2021-04-10 14:48:20 +0200 | Closed | Good | Edit | View Add Edit | Edit |
| 0031 | Diffraction data | Lysozyme | serial femtosecond crystallography | 2021-04-15 10:48:26 +0200 | Closed | Good | Edit | View Add Edit | Edit |
| 0030 | Diffraction | Lysozyme | serial femtosecond crystallography | 2020-03-09 01:20:02 +0100 | Closed | Good | Edit | View Add Edit | Edit |
| 0029 | Diffraction | Lysozyme | serial femtosecond crystallography | 2020-03-09 01:07:51 +0100 | Closed | Good | Edit | View Add Edit | Edit |
| 0027 | scattering | Silica 50nm | small angle x-ray scattering | 2019-09-21 01:12:49 +0200 | Closed | Good | Edit | View Add Edit | Edit |

HIDE

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Open data as training data @ EuXFEL

- The established data analysis infrastructure & services work well for experienced EuXFEL users, working repeatedly on their own proposals
- For less experienced users, bringing together aspects of remote login, filesystem navigation, software environment setup and service usage poses a considerable barrier
- VISA integrates services, i. p. Jupyter and Remote desktop, to a user-friendly browser application with pre-built (or containerized / mounted) software and direct linkage to (open) data
- Streamlined data analysis procedures are enabled, the barrier lowered



<https://visa.xfel.eu>



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VISA login and creation of an instance



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New compute instance

Please fill in the details below to create a new compute instance. For information about VISA please checkout the [documentation](#).

Experiments

Select the experiments you wish to associate with your compute resource

Search for experiments

Search for your experiments using the filters below

Instrument All instruments between 2017 and sort by date (newest first)

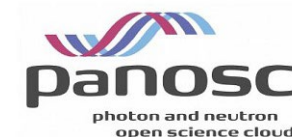
| Proposal | Title | Instrument | Start Date | End Date | |
|----------|--------------|------------|-------------|-------------|------------------------|
| p700000 | Example Data | XMPL | 01 Jun 2021 | 01 Jun 2021 | SELECT |
| p700000 | Example Data | XMPL | 15 Apr 2021 | 15 Apr 2021 | SELECT |
| p700000 | Example Data | XMPL | 10 Apr 2021 | 10 Apr 2021 | SELECT |
| p700000 | Example Data | XMPL | 14 Aug 2020 | 14 Aug 2020 | SELECT |
| p700000 | Example Data | XMPL | 14 Aug 2020 | 14 Aug 2020 | SELECT |
| p700000 | Example Data | XMPL | 14 Aug 2020 | 14 Aug 2020 | SELECT |
| p700000 | Example Data | XMPL | 14 Aug 2020 | 14 Aug 2020 | SELECT |
| p700000 | Example Data | XMPL | 09 Mar 2020 | 09 Mar 2020 | SELECT |

Results per page 50 1 - 39 of 39 experiments

Close



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VISA remote desktop and data browsing



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Take screenshot | Clipboard | Keyboard

Applications | r0030 - File Manager | [dallanto@visa-dev--108...]

r0030 - File Manager

File Edit View Go Help

/home/data/data/201750/p700000/proc/r0030/

DEVICES

- File System

PLACES

- dallanto
- Desktop
- Trash

NETWORK

- Browse Network

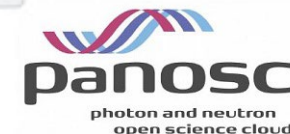
| Name | Size | Type | Date |
|-----------------------------|---------|---------------------|--------|
| agipd_2120_v1_reform.geom | 37.9 kB | plain text document | 06/12/ |
| CORR-R0097-AGIPD00-S00000.h | 16.8 GB | HDF document | 06/12/ |
| CORR-R0097-AGIPD00-S00001.h | 19.3 GB | HDF document | 06/12/ |
| CORR-R0097-AGIPD00-S00002.h | 19.3 GB | HDF document | 06/12/ |
| CORR-R0097-AGIPD00-S00003.h | 19.3 GB | HDF document | 06/12/ |
| CORR-R0097-AGIPD00-S00004.h | 19.3 GB | HDF document | 06/12/ |
| CORR-R0097-AGIPD00-S00005.h | 19.3 GB | HDF document | 06/12/ |
| CORR-R0097-AGIPD00-S00006.h | 19.3 GB | HDF document | 06/12/ |
| CORR-R0097-AGIPD00-S00007.h | 19.3 GB | HDF document | 06/12/ |
| CORR-R0097-AGIPD00-S00008.h | 19.3 GB | HDF document | 06/12/ |
| CORR-R0097-AGIPD00-S00009.h | 19.3 GB | HDF document | 06/12/ |
| CORR-R0097-AGIPD00-S00010.h | 19.3 GB | HDF document | 06/12/ |
| CORR-R0097-AGIPD00-S00011.h | 19.3 GB | HDF document | 06/12/ |
| CORR-R0097-AGIPD00-S00012.h | 19.3 GB | HDF document | 06/12/ |
| CORR-R0097-AGIPD00-S00013.h | 19.3 GB | HDF document | 06/12/ |
| CORR-R0097-AGIPD00-S00014.h | 19.3 GB | HDF document | 06/12/ |
| CORR-R0097-AGIPD00-S00015.h | 19.3 GB | HDF document | 06/12/ |
| CORR-R0097-AGIPD00-S00016.h | 19.3 GB | HDF document | 06/12/ |
| CORR-R0097-AGIPD00-S00017.h | 19.3 GB | HDF document | 06/12/ |
| CORR-R0097-AGIPD00-S00018.h | 19.3 GB | HDF document | 06/12/ |
| CORR-R0097-AGIPD00-S00019.h | 12.7 GB | HDF document | 06/12/ |
| CORR-R0097-AGIPD01-S00000.h | 16.8 GB | HDF document | 06/12/ |
| CORR-R0097-AGIPD01-S00001.h | 19.3 GB | HDF document | 06/12/ |
| CORR-R0097-AGIPD01-S00002.h | 19.3 GB | HDF document | 06/12/ |
| CORR-R0097-AGIPD01-S00003.h | 19.3 GB | HDF document | 06/12/ |

VISA

00:00,00



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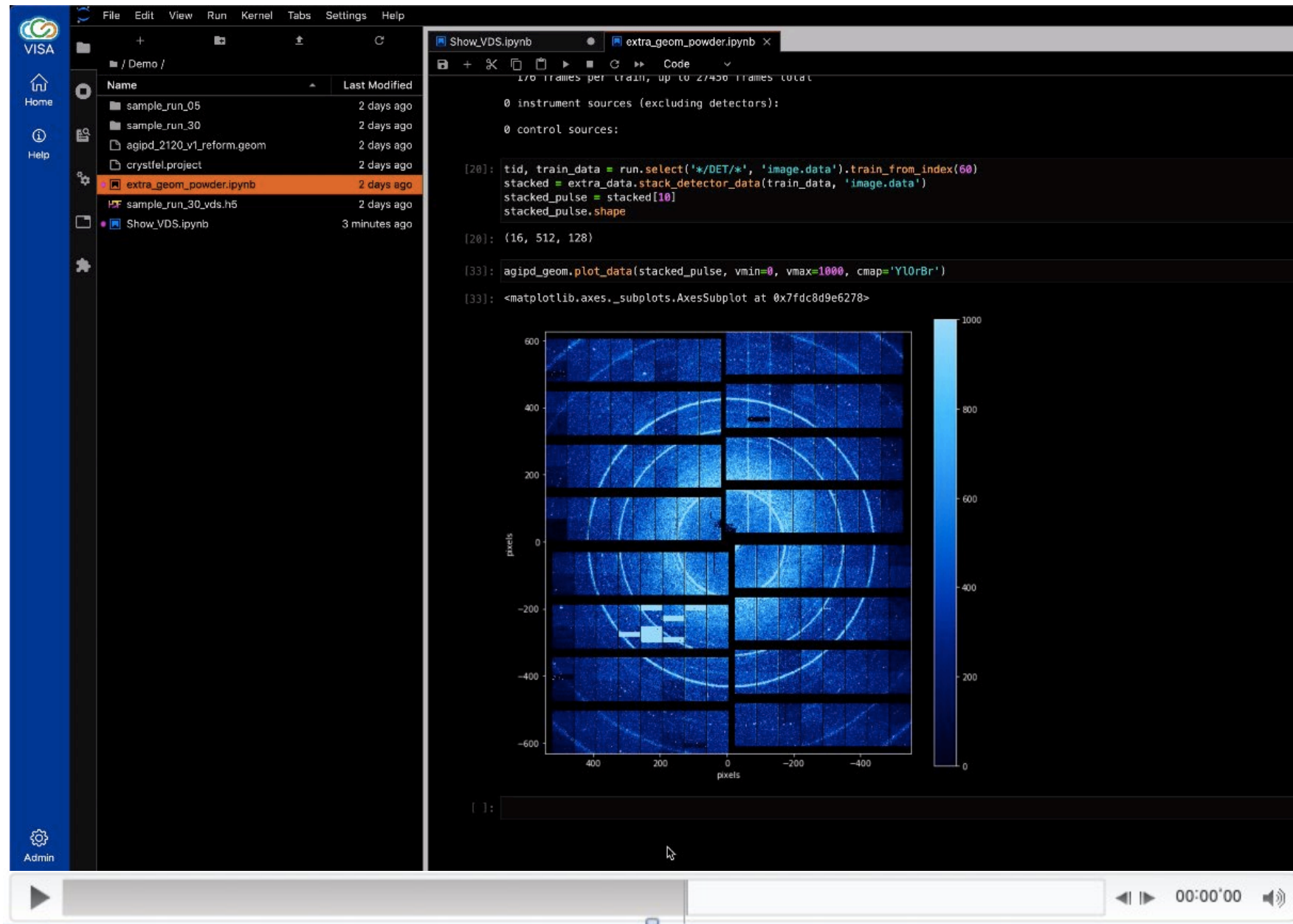


Jupyter and detector data/geometry inspection in VISA



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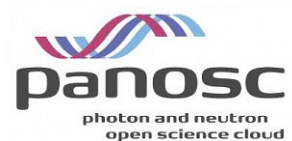


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CrystFEL-GUI in the VISA remote desktop

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Take screenshot | Clipboard | Keyboard | Information | Auto-scale

VISA

Home

Help

Applications | CrystFEL

Trash

File System

Home

CrystFEL

File View Tools Help

/home/dallanto/Demo/sample_run_30_vds.h5 //94 (frame 95 of 639616)

Show results from: Calculations within GUI

Load data

Peak detection

Index this frame

Index all frames

Determine unit cell

Indexing ambiguity

Merge

Figures of merit

Export data

Retry indexing: on

Couldn't understand "

WARNING: 119 reflections could not be integrated

Number of crystals: 1

triclinic, right handed.

| a | b | c | alpha | beta | gamma |
|-------|-------|---------|-------|-------|-----------|
| 79.80 | 79.89 | 38.09 Å | 89.94 | 90.03 | 90.03 deg |

Admin

00:00,00



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