LEAPS-IT Working Group 3 Workshop on "IT Solutions to address Operational Challenges during Covid-19"

Workflow at DESY Photon Science and selected actions taken at PETRA III to the pandemic

A. Rothkirch DESY Photon Science, FS-EC

and many colleagues from FS-EC, DESY Central IT and the beamlines



HELMHOLTZ RESEARCH FOR GRAND CHALLENGES

DESY.

Outline/brief overview

- Experiment/data life cycle
- Digital User Office
- Managed storage system Start/Stop a Beamtime
- gamma-portal
- Data access and analysis environment
- Response/changes to pandemic (selection)
- Remote control at P11

PETRA III as of May 6

- No new users since March 13th 2020
- Stand-by of PETRA III at noon on March 20th, 2020 with ability to restart operation within ~24 h for fast-track access Corona-relevant experiments
- Corona-relevant experiments done at P03, P10, P11, P13, P14 since March 30
- PETRA III operation resumed on May 04 in reduced mode (german users and mail-in experiments)

HELMHOLTZ RESEARCH FOR GRAND CHALLENGES



DESY.

Experiment/data life cycle

Apply for an experiment

Experiment preparation

• Integrate brought in equipment

Start of the experiment

- access to the storage space
- access for functional account & users
- configure exports and endpoints

Data acquisition

- 0D, 1D, 2D, 3D data
- variety of formats and sizes

Activities during the experiment

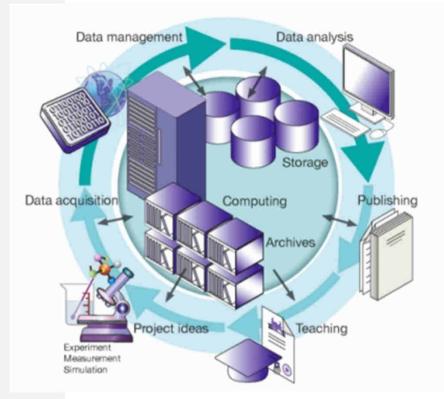
End of the experiment

• Data not accessible for next user group

Data access past the experiment

• Offline analysis on- and off-site

Data archival

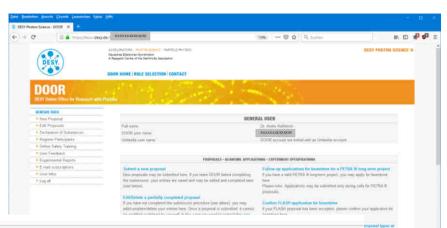


Digital User Office

J.P. Kurz (EC), D. Unger (PS), U. Lindemann (IT)

The Digital User Office DOOR facilitates

- Proposal submission
- Peer reviews
- Beamtime scheduling
- Declaration of substances/ List of participants
- Miscellaneous administrative tasks.
- DOOR is based on DUO (PSI).
 It is a common activity between the FS department and central IT
- Generation of unique ID per BT "Beamtime Application ID"



PROPOSALS - BEAMTIME APPLICATIONS - EXPERIM

Submit a new proposal

New proposals may be submitted here. If you leave DOOR before completing the submission, your entries are saved and may be edited and completed later (see below).

Edit/Delete a partially completed proposal

Follow-up a PETRA III Io If you have a you may app Please note: during calls f

If you have not completed the submission procedure (see above), you may edit/complete

Confirm FL

If your FLAS

PROPOSALS LIST

SEARCH	

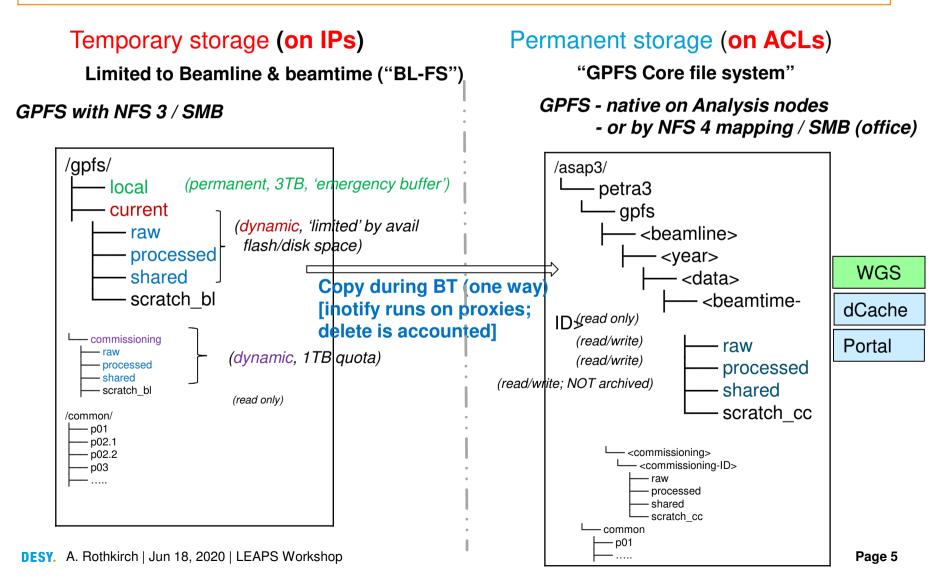
	Proposal	Title	Submitted on
Details	I-20191502	Neolithic Gold and Medieval Silver: Cast or beaten out ?	02-Sep-2019
Details	1-20191458	Strain analysis of Neolithic bronze Axes	02-Sep-2019
Details	I-20190660	Deformation strain mapping of archaeological Iron	01-Mar-2019
Details	I-20190601	Non invasive authenticity test for prehistoric gold objects	01-Mar-2019

The DOOR user portal

Start/Stop a Beamtime

Predefined directory toplevel structure and rules/constraints

[psana001.desy.de]\$ startBeamtime --beamtimeId <beamtimeID> --beamline <beamline>



Gamma-Portal (htts://gamma-portal.desy.de)

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Documentation	Browse data Here you can browse data from your experiments. This function allows searching within the archive or filesystem, viewing properties/details of a dataset and staging of data. Staging means to copy datasets from tape to DESY disk space for further access.	 Different views depending on role 			
	Download via FTP A FTP server provides interactive access for DOOR users to beamtime directories using the FTP protocol. It allows you to browse and download beam time data using any suitable FTP	data stage from duache			
	client. Access is granted according to the working group definitions in the Gamma Portal. Please note that you must select a beamtime in the portal before you can access it via FTP. Use Menu FTP Registration to do this. As we are using a secure implementation of the FTP protocol, your might have to configure your client. Detailed description please refer to Documentation				
	Staging status Staging status This function provides an overview of staged datasets. It displays the current	(currently data before 2015 by user otherwise via FS-EC)			
	staging status (running, finished, or error) as well as where to find the data (path).	 Project leader & applicant can manage ACLs 			
y	Note: data download v	ia a dlobus is also			

DESY. A. Rothkirch | Jun 18, 2020 | LEAPS Workshop possible and implies scientific account

Data access and analysis environment

(located @ Computer Center)

- Invention of Scientific accounts (i.e. DESY accounts for external users ('external' ≠ industry/commercial) with own namespace 'psx'
- Provision of interactive resources max-fsc/max-fsg
- Creation of specific batch resources for PS managed by SLURM
 - Slurm partition ps (inhouse)
 - Slurm partition psx (external [noncommercial] users or use cases)
- Invention of display-servers for processing involving GUI
- Remote access (firewall/tunnel or Web-Browser)

Erstellen

Q

Suchen

Seiten / Computing @ DESY

Resources

Frank Schluenzen posted on 20. Apr. 2015 09:07h - last edited by Frank Schluenzen on 20. Jun. 2016 17:03h

Compute resources & background information

DESY IT offers a number of compute resources with varying capabilities. We collected a rough overview and some background information about available platforms. For more details please consult the official IT pages.

DESY hosts a number of large scale compute infrastructures, check the related sites for details.

Related sites

- Batch computing: BIRD
- Grid computing: GRID
 High Performance
- Computing: Maxwell

Search the compute space

- Linux@DESY
 Software Downloads (DESY
- credentials) • Windows@DESY





- Running Jobs on Maxwell gestern um Sep 05. 2019 14:36 • aktualisie von Andre Rothkirch • Änderung anzeigen
- Visualization Aug 26, 2019 14:23 • aktualisiert von Fran Schluenzen • Änderung anzeigen
- Tools
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- Simulation
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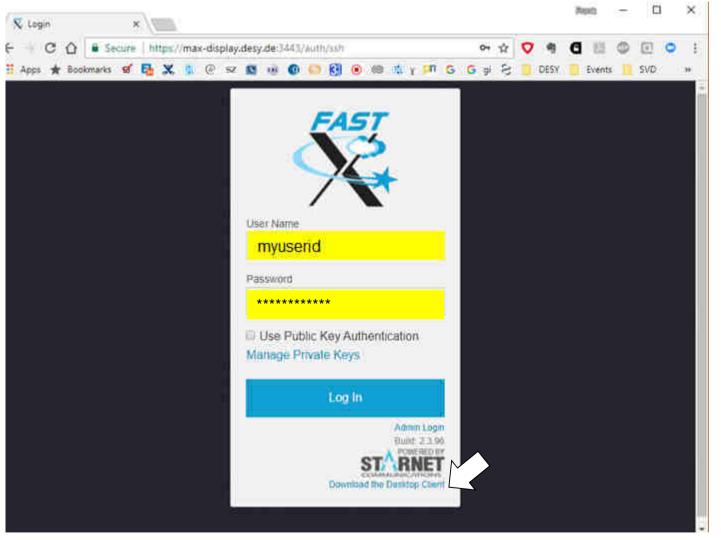
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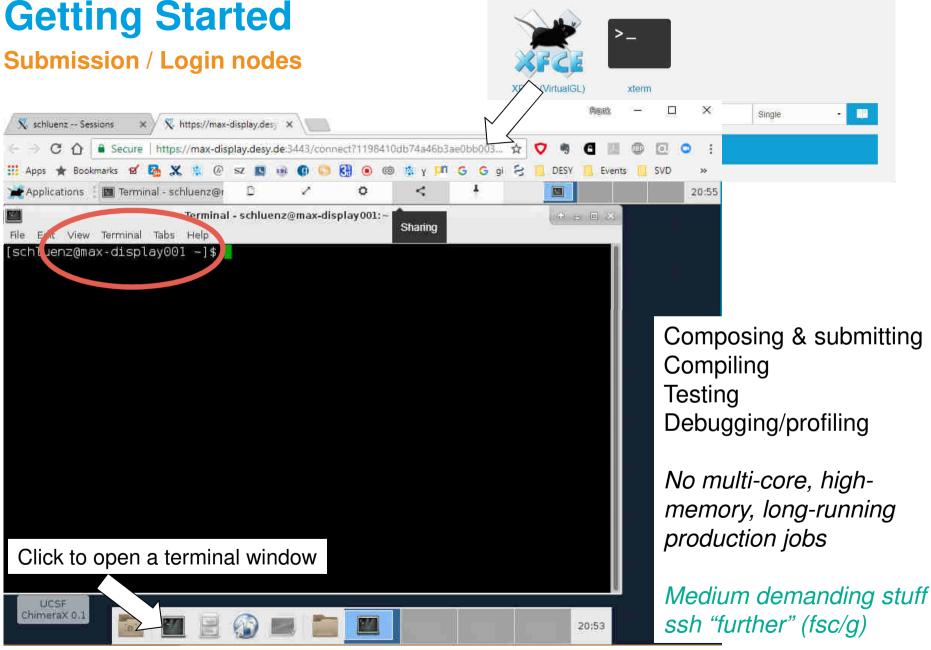
Batch (Maxwell cluster)

- Exclusive resources usage for jobs managed by SLURM
- Efficient resource usage (batch queue, resource definitions, optimize costs etc.)
- Homogeneous/common environment for 'all groups', e.g. rules, IB, GPFS ...

Getting Started

Submission / Login nodes - max-display [from everywhere by Browser]





Response/changes to pandemic (selection)

- Pushing implementation of remote control at P11, handover to/allow (selected) users
- Mail-in offered by beamlines which never did it before (9 beamlines in total)
- Likely no increase in unattended operation of experiments (depending on what's meant, it's already daily business at the BIs [and some have to run supervised/attended due to e.g. safety or instrument complexity])

Some future plans in response to COVID 19

- Improvements / further development of remote control & communication at P11
- Implementation/adaption of remote concept at other beamlines, P02.1 next/to come soon
- Increase amount of Mail-in beamtimes (more an "orga"-challenge)

Remote access/control P11

Prerequisites

What was wanted and what was needed

P11, FS-EC and IT

- Beamline control through one user exclusively
- Do not expose any functionality which is not needed
- Eliminate abuse
- Ability to monitor the user actions
- Take back control at any time
- No special hardware, software or OS dependencies for the users
- Possibility to forward control to between legitimized users

D5 and User Office

- Authentication against a personalized account
- Make remote access dependent on safety instructions, Door account, etc.
- Introduce additional safety instructions
 for remote users
- Log remote access to database for statistical purposes
- Remote access has to be requested in DOOR

Technical Implementation

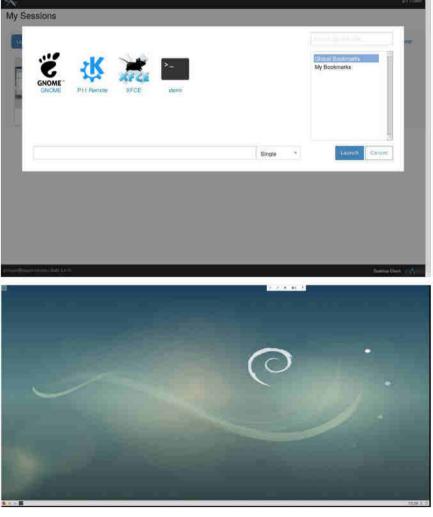
Make it working

FastX

- Commercial software, license available
- Already in use for Maxwell access
- X server in a browser
- Sessions can be shared
- Running on a dedicated host

Tailored X session

- Kiosk mode KDE
- Experiment control GUI
- Beam position monitor / feedback
- Browser (results, cameras, wiki)
- No terminal!



Formal Arrangements

Make it legal

Safety Requirements

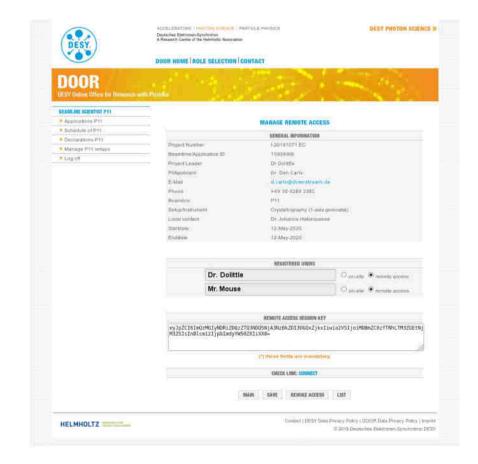
- Currently as onsite, but shutter permission
- One user with onsite experience
- Additional online instructions in the near future

Door

- Grant online access per beamtime and user
- Save FastX session key

Proxy Node

Authenticate against Door

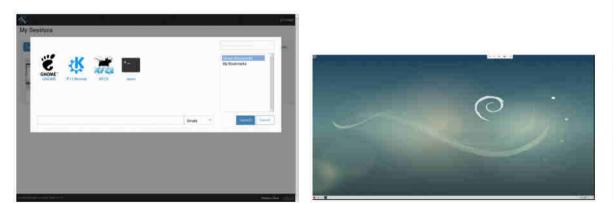


Handling

How things work from the staff perspective

Start

- Prepare beamline, load samples, etc. •
- Open beamtime .
- Open FastX session and share it ٠
- Save shared session key in door ٠
- Contact users by video chat or phone •



Stop

- Close FastX session
- Unload samples
- ...

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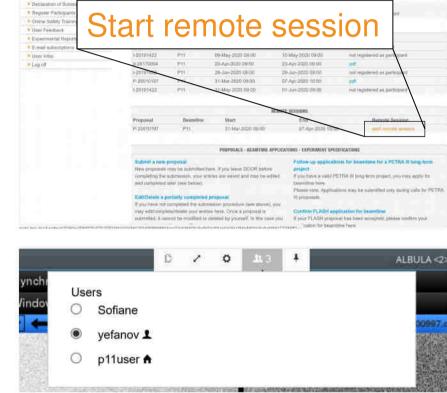
How things work from the users perspective

Start

- Log in to Door, it presents you a link to the remote session
- Take control
- Adjust screen size
- Go on like normal

Stop

- Log out from Door
- Close browser window





What it looks like

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First Experiences – *it works :-)*

• Stable – first session was running for more than a week in large collaboration

Compound target screening of the Covid-19 main protease, A. Meents et al. (DESY, CFEL, Uni HH [CUI], EMBL, TU HH, CIT, SLAC, DLS,)

Statistics		
Luca Gelisio posted on 18. May. 2020 21:16h - last edited by Luca Gelisio on 16. Jun. 2020 18:30h		
Number of crystals : 7857 Crystals screened: 7857 Number of unique compounds : 4036 Unique targets : SARS-CoV-2 Main Protease Number of diffraction data sets marked as <i>success</i> : 6637	P11	8,000 7,000 6,000 5,000 4,000 3,000
 This page is automatically generated (last update Tue Jun 16 18:30:01 2020) Database: SARS_COV_2_v2 on cfeld-vm04.desy.de 	P13 P14 ■ P11 (5,900 - 89%) ■ P13 (221 - 3%) ■ P14 (493 - 7%)	Crystals/day Crystals Diffraction experiments/day Diffraction experiments Source: Luca Gelisio, private copy

- Responsiveness depends on the network connection
- Screen size is an issue
- Communication is another
- Handover of control between users during the experiment is a big advantage
- · Remove possibilities to break the interlock from GUI

Environment

Other things to think about

- Sample shipping, delivery, handling, loading, ...
- Coordinate which sample is loaded where
- How to deal with new users, how to train them in remote control?
- There might be problems coming from the connection or the user computer
- Communication between local contact and controlling user
- Make people locally aware of ongoing remote activities



Backup slide

Maxwell cluster batch resource (by IT)

What is the Maxwell cluster?

- A large number of powerful computers (named max-<something>)
 - All connected through a fast low latency network (56Gb EDR/FDR)
 - All connected to Petra3 GPFS storage (and CFEL, EXFEL, CSSB storage)
 - All connected to dCache ("on demand")
 - All equipped with 256GB up to 1.5TB of memory per node
 - Quite a number of nodes with 1-4 Nvidia P100 GPUs
 - · Lots of software pre-installed
- Main purpose
 - High Performance Computing
 - Offline Data Analysis
 - · Simulations of all kind
 - Remote Visualization
 - Any application which can make use of the special features of Maxwell!

E.g. Ansys, Comsol, Fdmnes (MPI version), Matlab, OpenFOAM, Orca, Quantum espresso, Tensorflow, Xds, Xmimsim, XRT

E.g. <u>Conuss</u> less well suited (single threaded/few mem.)

All jobs are scheduled by the SLURM scheduler (via submission hosts)!

- Usually jobs don't have to wait very long
- · But it depends on the jobs requirements
- and there is no VIP fast lane ...
- max-p3a* aka max-fsc, max-fsg, desy-ps-cpu, desy-ps-gpu are NOT part of SLURM

DESY. A. Rothkirch | Dec 10, 2019 | ESRF

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Overview

