Serving Photon Science and HEP at the same Facility

27th Conference on Computing in High Energy and Nuclear Physics

Christian Voß on behalf of DESY-IT
Krakow, 24th October 2024

DESY as a Laboratory

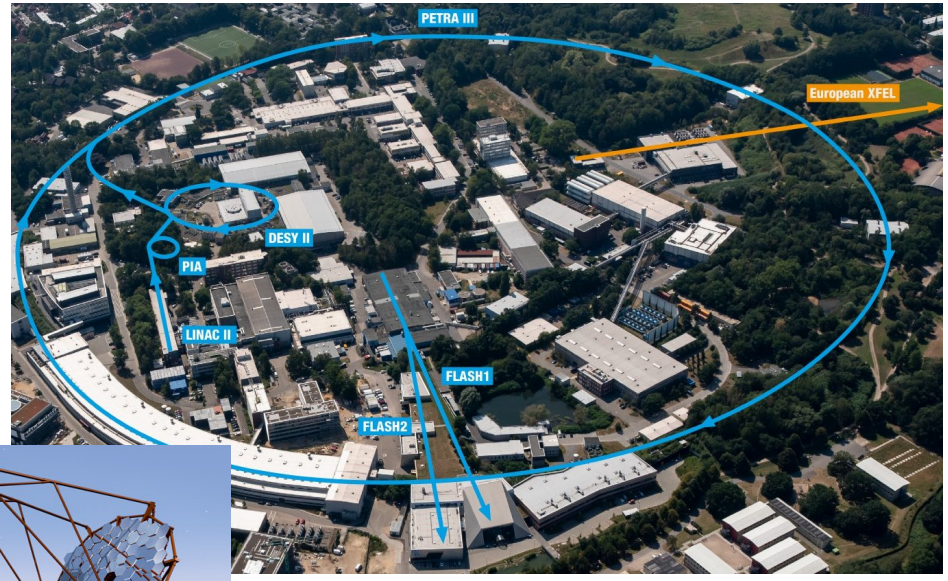
Origins and Overview

DESY-Hamburg historically centered on Particle Physics together with strong accelerator division:

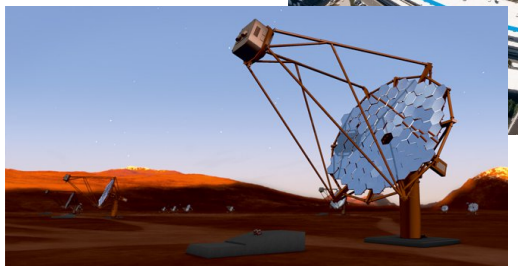
- HERA and original PETRA accelerator, DORIS with ARGUS
- Discoveries: Gluon and B-mixing

Accelerated transition to an accelerator laboratory with

- Large photon science user facilities
- Large local particle physics groups
- Small on-site particle physics experimental groups



And a strong Astro-Particle physics community at DESY-Zeuthen



DESY as a Laboratory and Data Analysis Facility

Supported Communities

- **Accelerator Data**

FLASH. Free-Electron Laser FLASH

European XFEL

FF

- **Accelerator Development Data**

SINBAD

- **HPC simulations**
- **Test-beam data**

Detector and Accelerator R&D

- **Facility User Data**

European XFEL

PETRA III

FLASH. Free-Electron Laser FLASH

- **Data of external Partners**

CFEL SCIENCE

CSSB Centre for Structural Systems Biology

EMBL

Helmholtz-Zentrum hereon

Research with Photons

- **Particle Physics Data**

CMS

ATLAS EXPERIMENT

LHCb

ilc international linear collider

Belle II

MADMAX

ALPS

IAXO

- **Astro-Particle Data**

IceCube

H.E.S.S.

cta cherenkov telescope array

Astro- Particle Physics

DESY as Site for the Large HEP Experiments

Commitments for WLCG, Belle II, ILC and the Preserved HERA Data

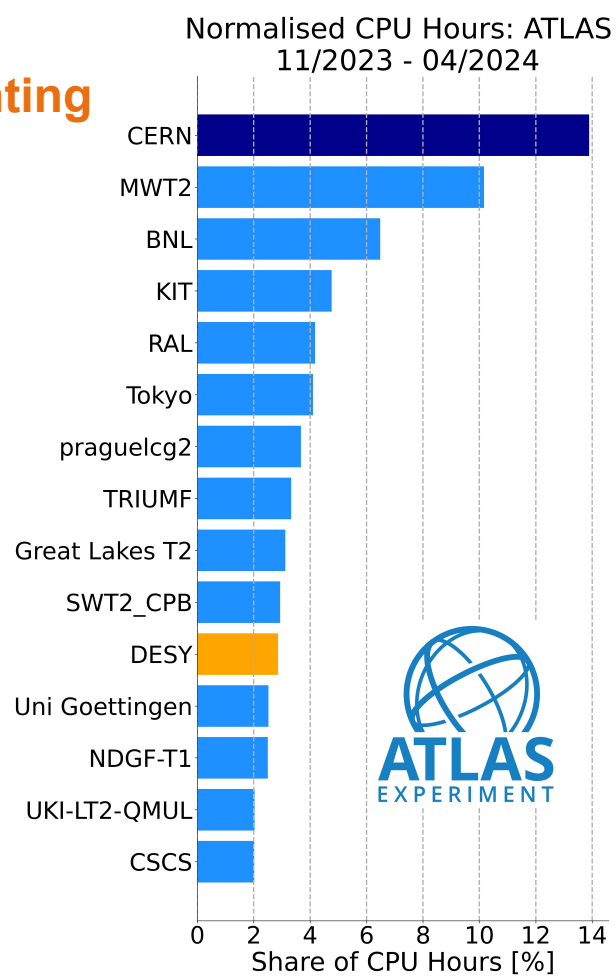
- DESY is historically a multi-VO site given that e.g. HERA hosted several experiments
  ➜ Commitment to keep the unique HERA data ready to support further analyses
- DESY has large local ATLAS and CMS groups, close collaboration with CMS group of the University of Hamburg
  - DESY is a major Tier-2 for ATLAS and CMS and a Tier-2 for LHCb (compute only)
  - DESY offers National Analysis Facility (NAF) as Tier-3 for the whole German LHC community
- DESY Belle II group is one of the largest in Belle II
  - DESY is a RAW Data Centre (similar to the Tier-1)
  - NAF is open to all Belle II scientists as an analysis facility
  - Collaborative services and tools
- DESY as a major contributor to Future Collider R&D

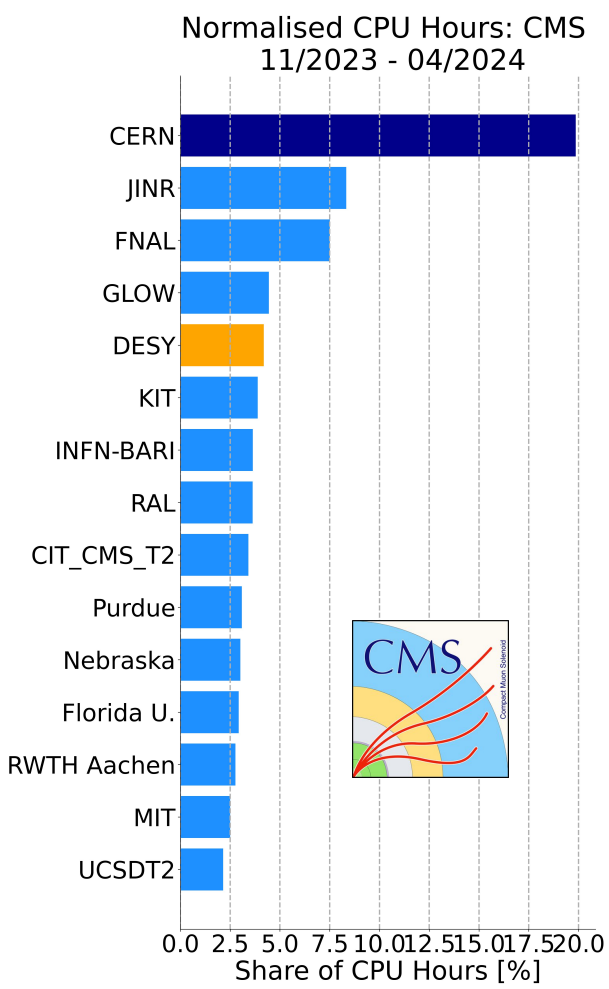
Position of DESY with WLCG and the Belle II Computing

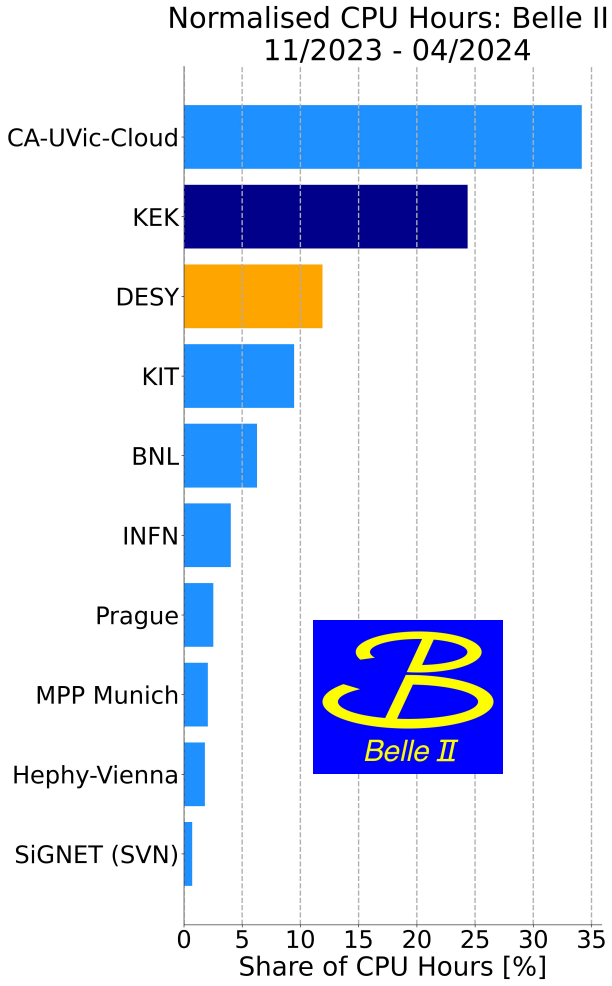
Quick Overview of offered CPU Hours

- DESY as a multi-VO site with a Grid Compute cluster of 26k Cores and 415 kHS23

EGI Accounting

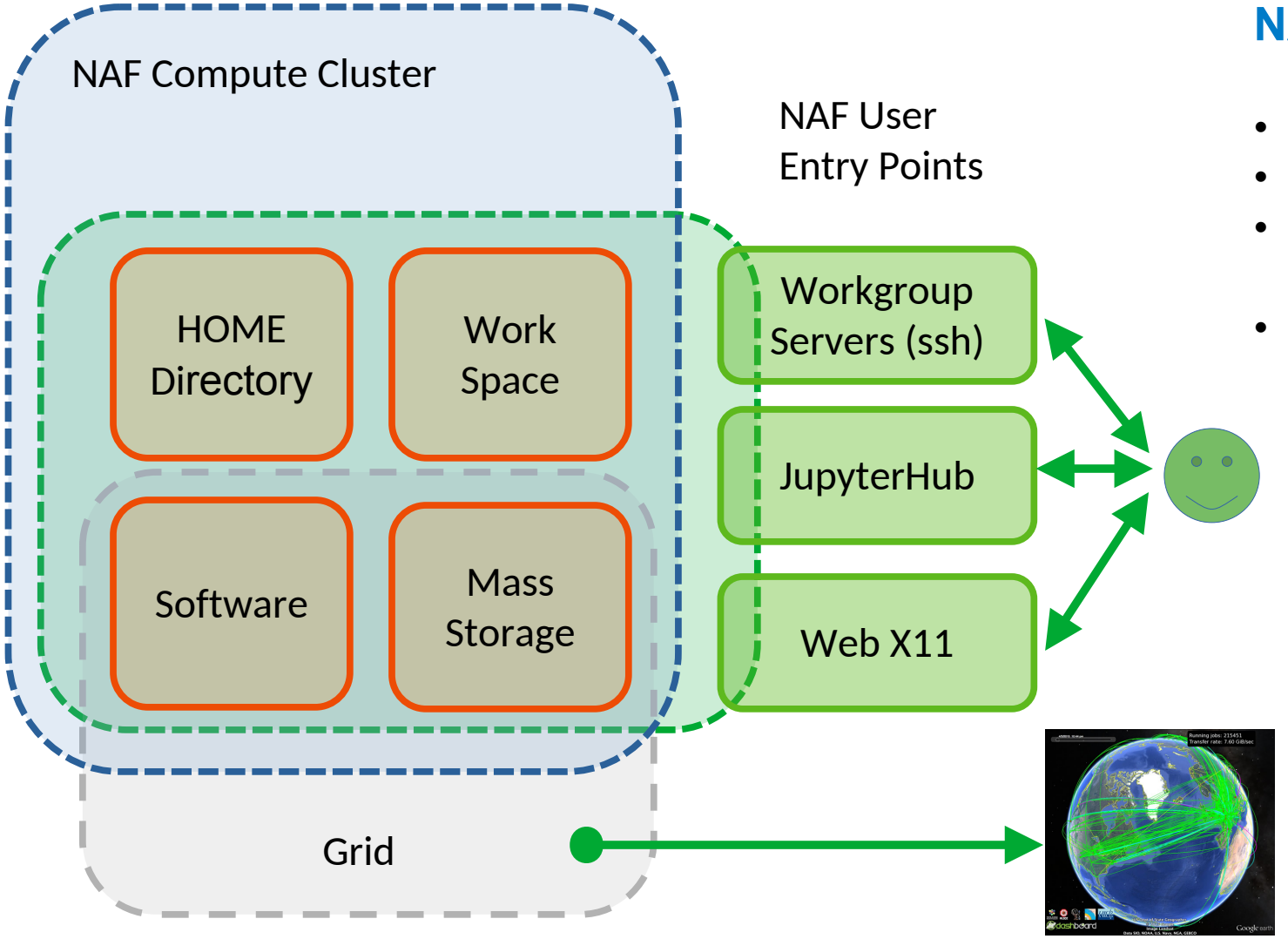






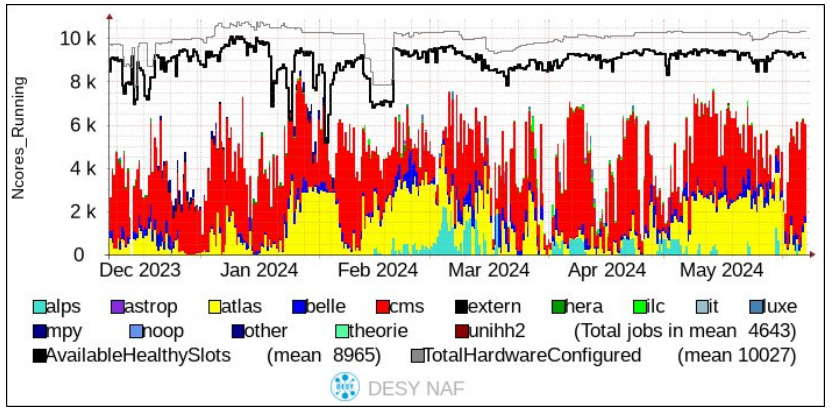
National Analysis Facility

HTC cluster (~300 kHS23) based on HTCondor in Production since 2007



NAF Setup

- Offer fast turnaround times
- Grant access to the full Grid SEs
- Use central data-management of experiments to store data at DESY
- Dedicated mass storage for NAF users as part of the Grid SEs



Leave enough free cycles for short turnarounds

Software for HEP: dCache Development at DESY

Providing one of the Fundamental Building Blocks of HEP Computing

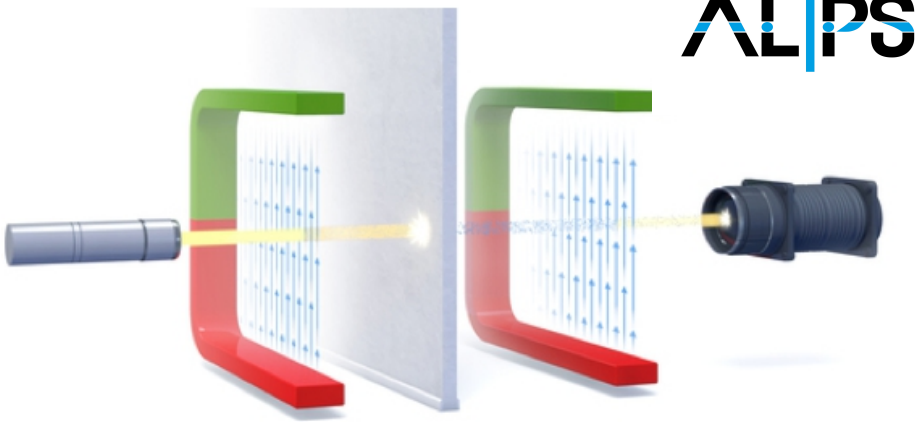
- Central element in overall storage strategy
- Collaborative development under open source licence by
  - DESY
  - Fermilab
  - Nordic e-Infrastructure Collaboration (unofficially NDGF)
- Particle Physics in general
  - In production at 9 WLCG Tier-1 centres
  - In use at over 60 Tier-2 sites worldwide
  - 75% of all remote LHC data stored on dCache
  - In addition: Tevatron and HERA data
  - All smaller DESY experiments store data in dCache
- Photon Science
  - Raw data for all DESY light sources
  - Long-term archival

dCache.org

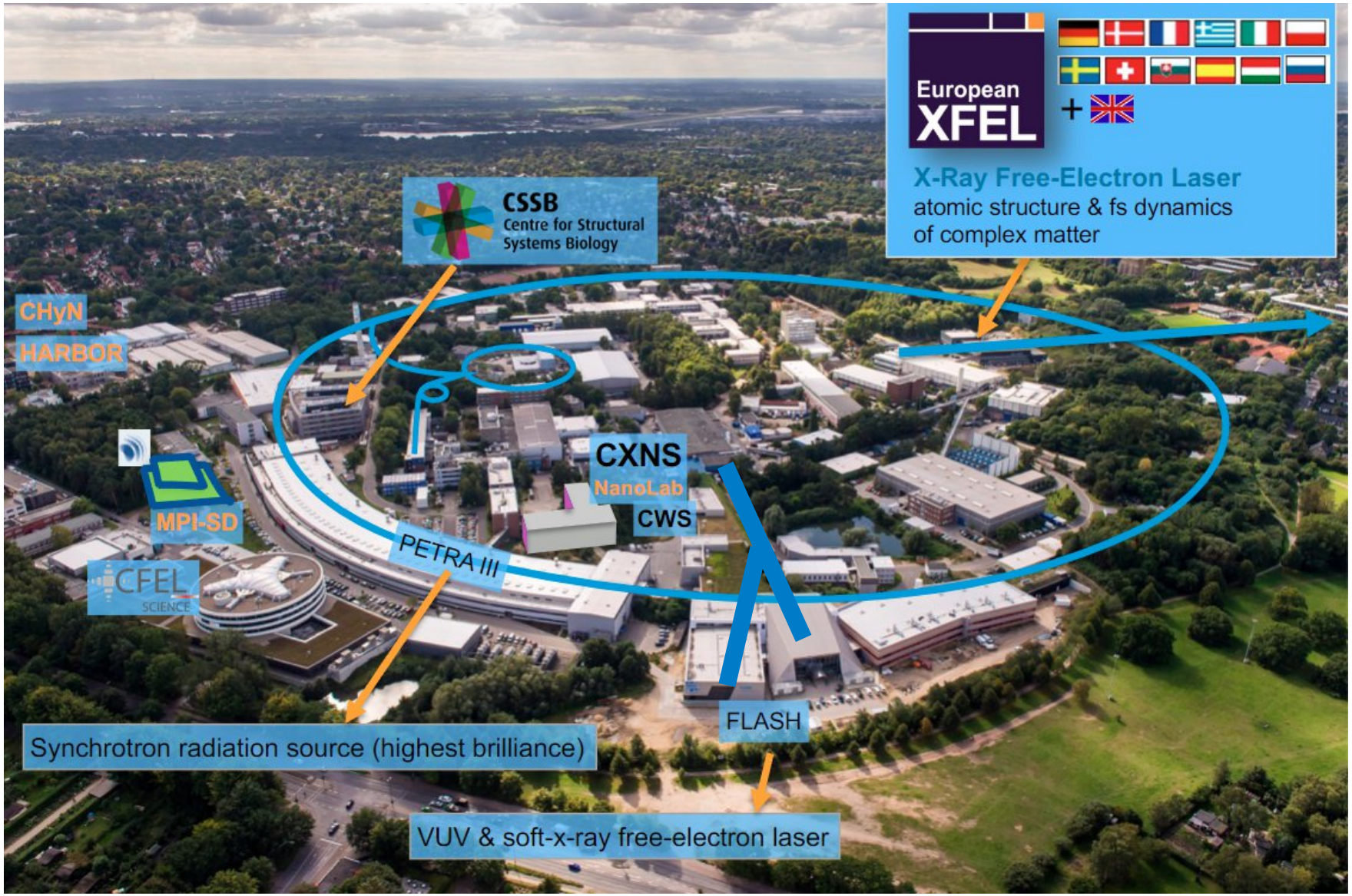
Small On-Site Particle Physics Experiments

New and Upcoming Dark Matter Searches

- Recently a number of smaller Particle Physics experiments started/are about to start taking data
- Dark Matter search experiments (mostly for Axions-Photon conversions **using light through a wall**)
- Produced data are relatively limited in size and rate
- Experiments are organised on dedicated albeit small collaborations similar to our HEP community
- Less than 100 collaborators mostly without a background in computing
- ALPS II data taking completely integrated into the DAQ system of the machine division, data stored and analysed on the Nation Analysis Facility **making use of as many already existing workflows as possible**



Photon Science — New Facilities and Partners



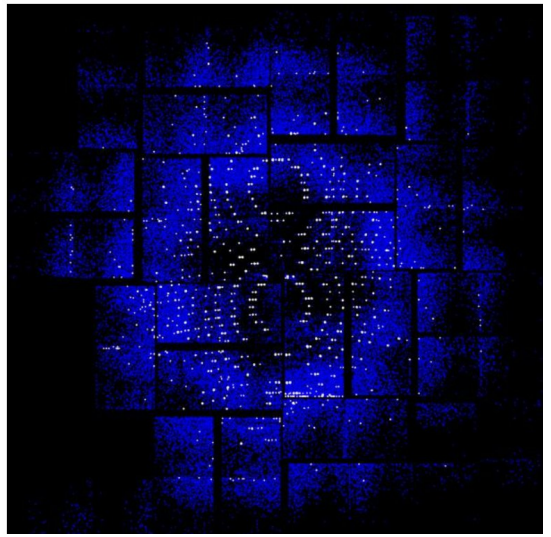
Introduction to Photon Science Users

Communities Collected under the Umbrella of Photon Science

- What is Photon Science? Naively you would think about laser physics on non-linear optics
- Here: umbrella term for basically anything that is not (astro-)particle physics and includes
  - Material sciences from fundamental research to commercial applications
  - Chemistry: studies on catalytics, solvation processes, inorganic molecules for quantum technologies
  - Biology: molecular and cellular biology, complex protein structures and interactions
  - Medicine: Corona research in 2020, e.g. BioNTech had beamtimes at PETRA III in 2020
  - Non-linear optics and high density field lasers
  - Studies towards novel applications of free electron lasers

Diverse field, uses a lot of different experimental techniques

- Mostly different flavor of diffraction experiments
- But many targets (a stream of molecules randomly oriented in space)



Tools Needed Beyond Computing to Enable Photon Science

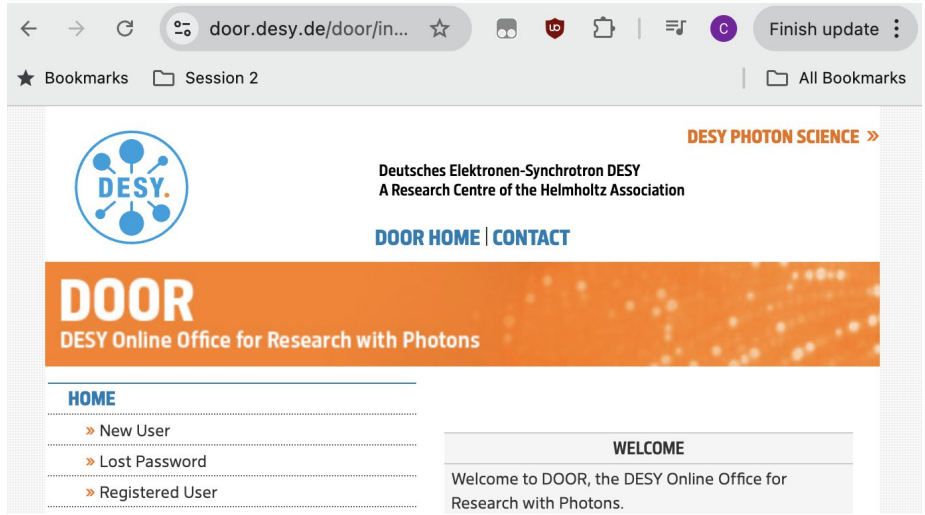
Managing Proposals, Users and Meta-Data

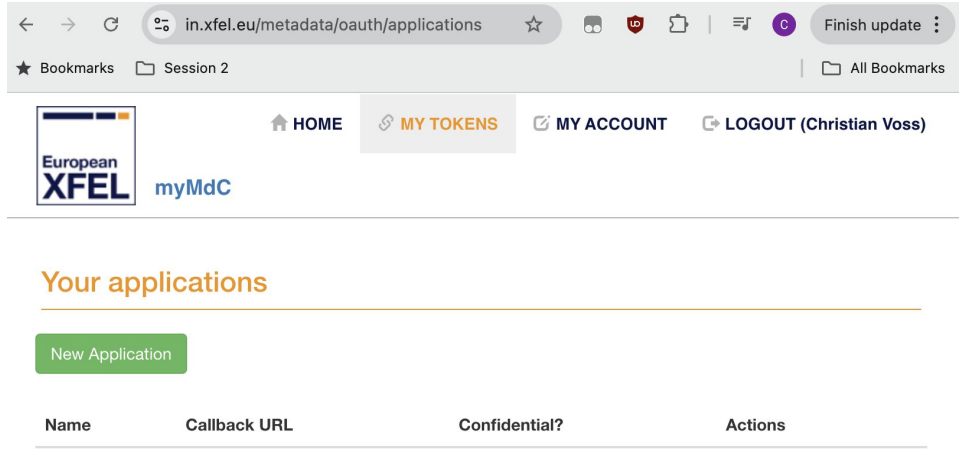
- External scientists apply for beamtimes at photon facilities
  ➜ Need a proposal system to register without DESY credentials
- Need for an electronic log-book suited for all kinds of experiments
- Need for a meta-data catalogue with a common scheme
  ➜ EuXFEL has developed `myMDC` as meta data catalogue
  ➜ For PETRA III and FLASH proposed to use `SciCat`
- Need a standardized file format describing the instruments
  ➜ `NeXus` flavour of `HDF5` files as standard through many labs
- Community analysis tools that can be of general use for certain experiments:

NeXus

SciCat

CrystFEL
data processing for FEL crystallography

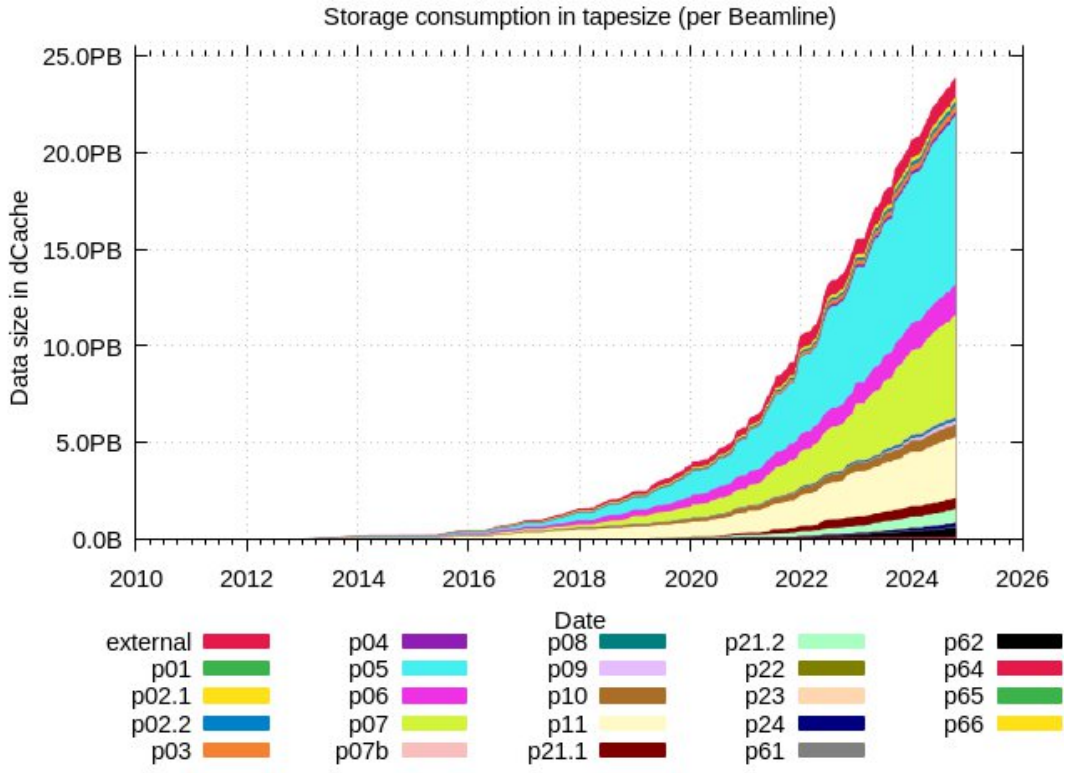


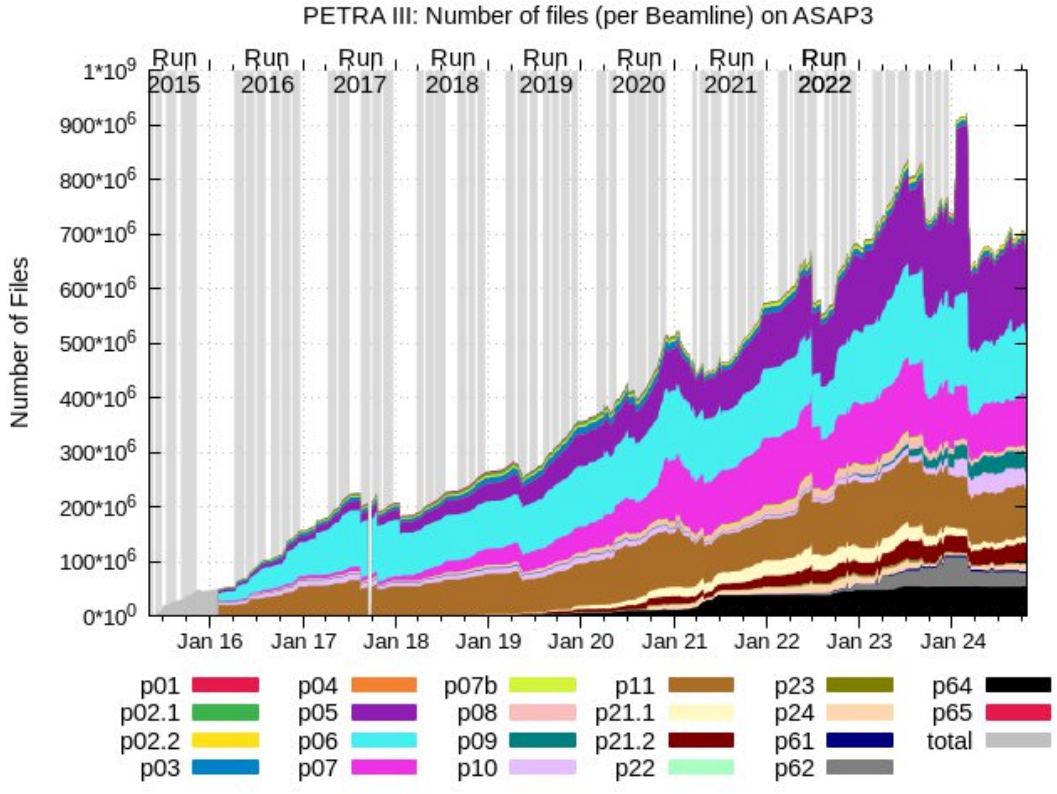


DESY Infrastructure for Photon Science — PETRA III

Third Generation Synchrotron Facility

- Synchrotron radiation for 25 beamlines supporting specific experimental methods
- Habit of users to **write large number of small files** (imagine root files with a single entry)
  ➜ need to provide a packing service before archival
- Wide range of **Heterogenic** custom/commercial detectors ➜ From Windows PCs to data streaming pipelines





Infrastructure for Photon Science — Free Electron Lasers

FLASH (Part of DESY) and European XFEL (Independent Facility with DESY participation)

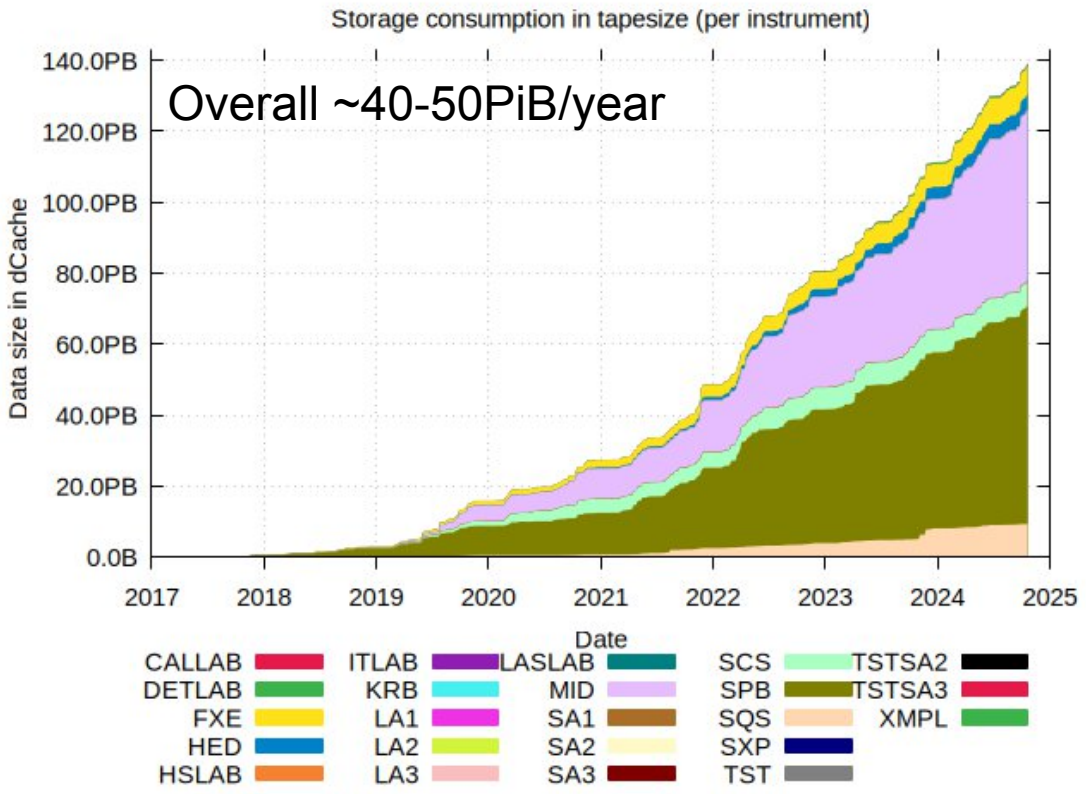
- Operate in the soft (FLASH) and hard (EuXFEL) X-ray regime (FLASH is run similarly to PETRA III)
- EuXFEL is a multinational (12 partner countries) company with DESY as main shareholder
- EuXFEL has dedicated data analysis team providing data calibration and user support
- EuXFEL staffed in part by former HERA scientists ➜ More HEP-like thinking compared to PETRA III
- EuXFEL detectors built by collaborations similar to HEP detectors
  ➜ Detectors produce HDF5 files with a custom but defined data structure
  ➜ Largest detectors produce ~5PiB/beamtime (a few days)
- Different detectors produce very different amounts of data depending on experimental methods

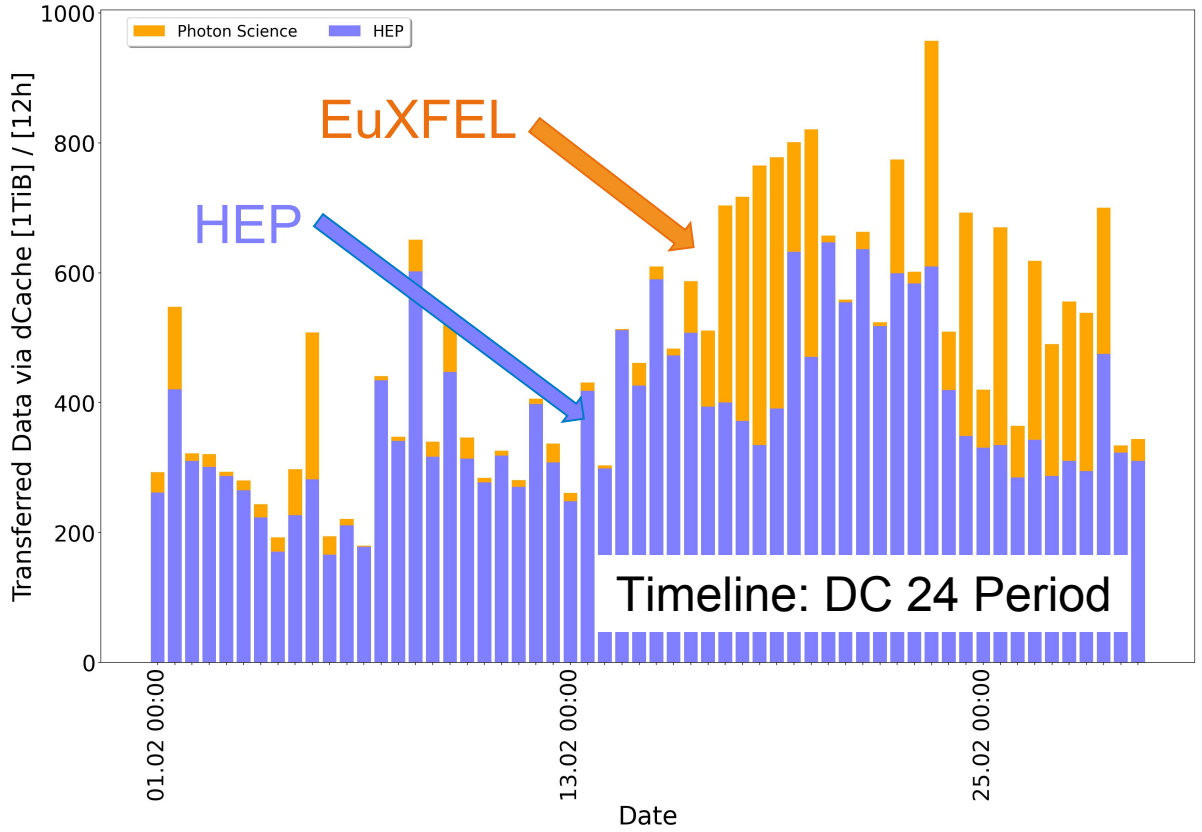
Distance of 3.4km

Large Data Rates — European XFEL

Growth of Data Taken by European XFEL

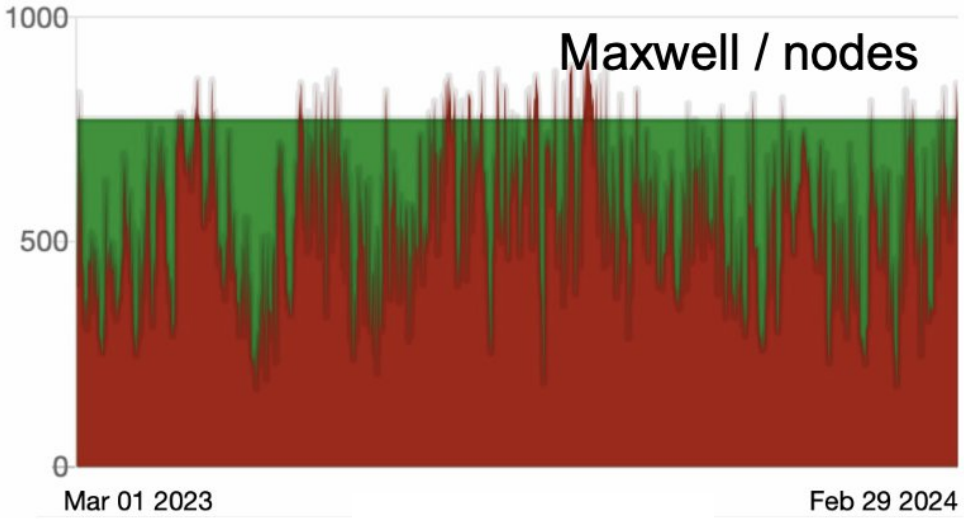
- Two 4Mpixel detectors produce >80% of all data ➜ ~5PiB/proposal raw and additional 5PiB PROC data
- Amount of data depends on skill of experimentalists and issues with samples/accelerator
- Data ingress in unpredictable bursts instead of steady data ingest like at HEP experiments





DESY Infrastructure for Photon Science — Computing

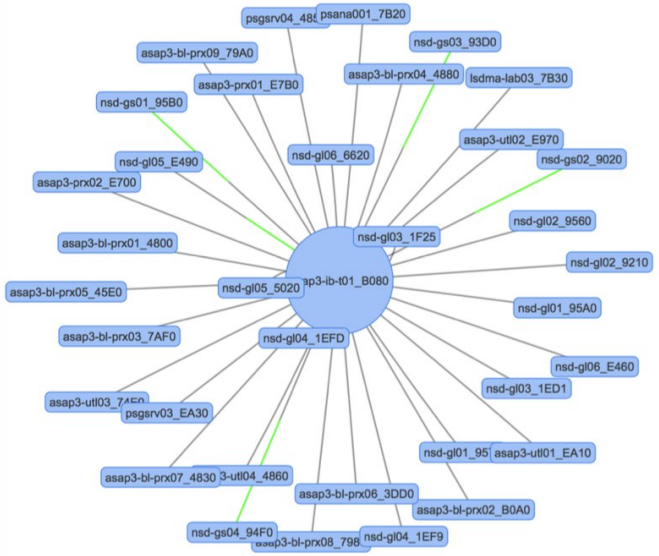
HPC-Like System with Fast Infiniband Interconnect to Fast and Low Latency Storage



- Reminder: DESY operates two HTC compute clusters: Grid&NAF
  ➜ ~30k Core, 20 PiB dCache and 3.1 PiB GPFS based scratch
  ➜ Networking based on Ethernet (10GE/worker node)
- Not talked about Photon Science when introducing NAF&Grid
  ➜ Photon Science and other communities run on ‘HPC’ system
- Photon Science is supported on the Maxwell cluster
  ➜ **~50k Cores/250 GPUs**
  ➜ Dedicated storage for each customer:

  PETRA III/FLASH: 17 PiB GPFS and 1 PiB dCache
  European XFEL: 64 PiB GPFS and 120 PiB dCache

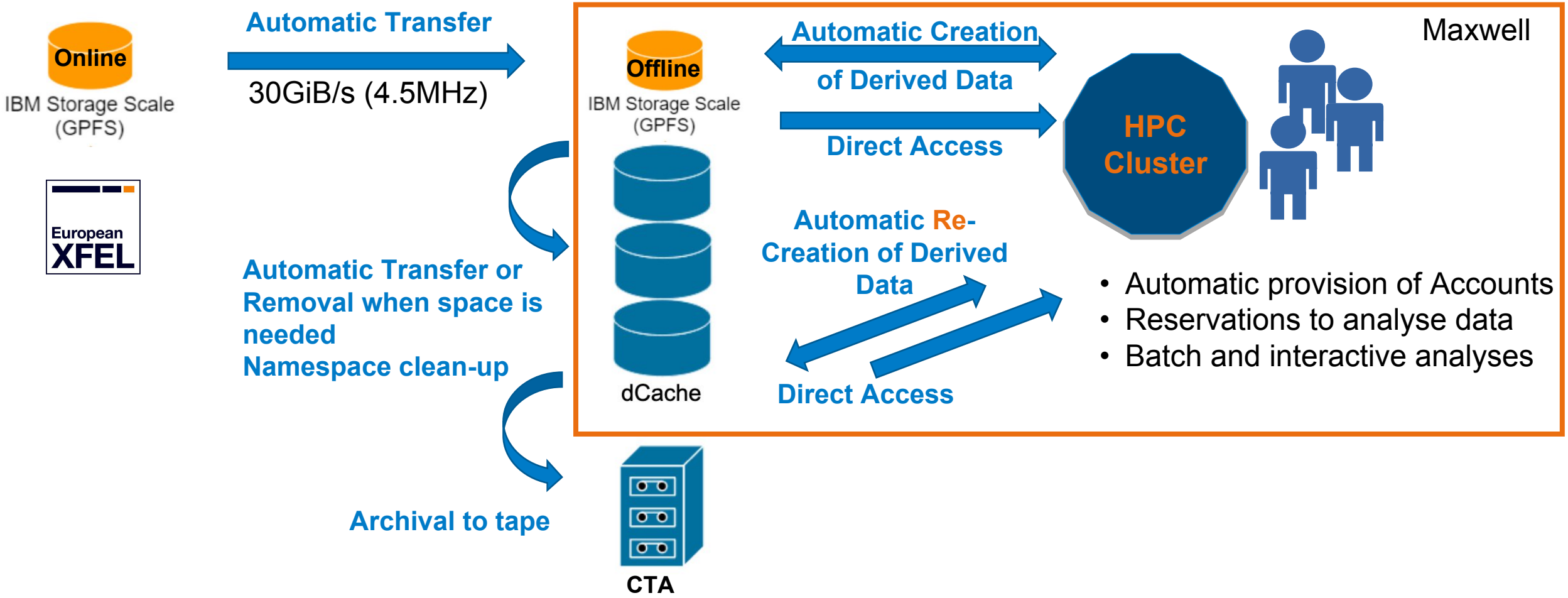
  ➜ Fast interconnect based on Infiniband (up to 200GB/s) to GPFS
  ➜ Access to dCache: Ethernet (10GE/worker node)
- Single node scheduling to partition compute for beamtimes (SLURM)



Photon Science — From Online to Offline

Example: Workflow for European XFEL

- After data transferred to DESY computing centre ➜ automatic calibration of runs applied on reserved nodes
- Analysis during data taking is supported on dedicated resources to further refine measurements



Analysis Workflow

Interactive and Batch Compute with Fast, Low-Latency Storage w.r.t. Classical HTC Workflows in HEP

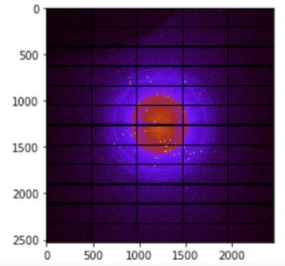
- A lot of demand for interactive analysis also in Offline compute
  ➜ See heavy usage of Jupyter and its challenge of scheduling
- Offer ready-to-start analysis setups for some Photon Science use cases
- Heavy use of GPUs beyond AI/ML applications due to
  ➜ 3D rendering of images done with graphical applications
  ➜ Reaction movies or structure analysis relies on series of images that are not independent
- Access to data: GPFS with POSIX and elaborated ACLs
  ➜ Read and write groups; beamline scientists are members of all groups
  ➜ Certain propriety software supporting local-file only

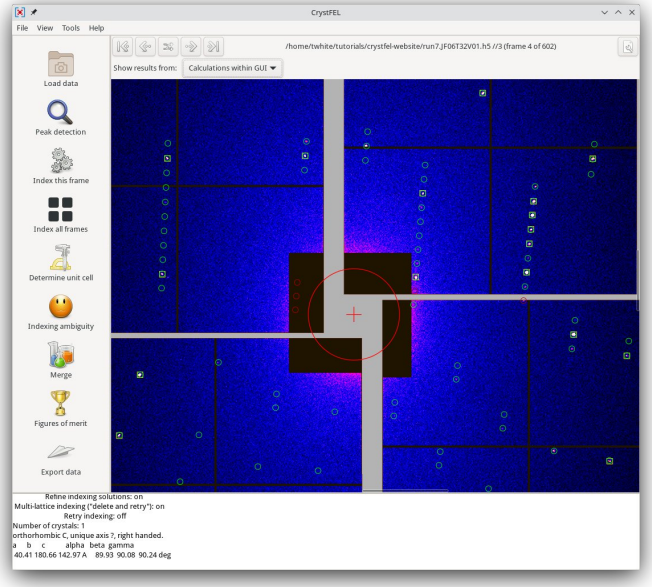
```
In [2]: %matplotlib inline

In [3]: import asapo_worker
        import numpy as np
        import matplotlib.pyplot as plt
        import tempfile
        import cbf

        broker, err = asapo_worker.create_server_broker("asapo-server:8400",

In [4]: data, meta, err = broker.get_last(meta_only=False)
        plt.imshow(data, cmap='gnuplot', vmax=500)
        plt.show()
```



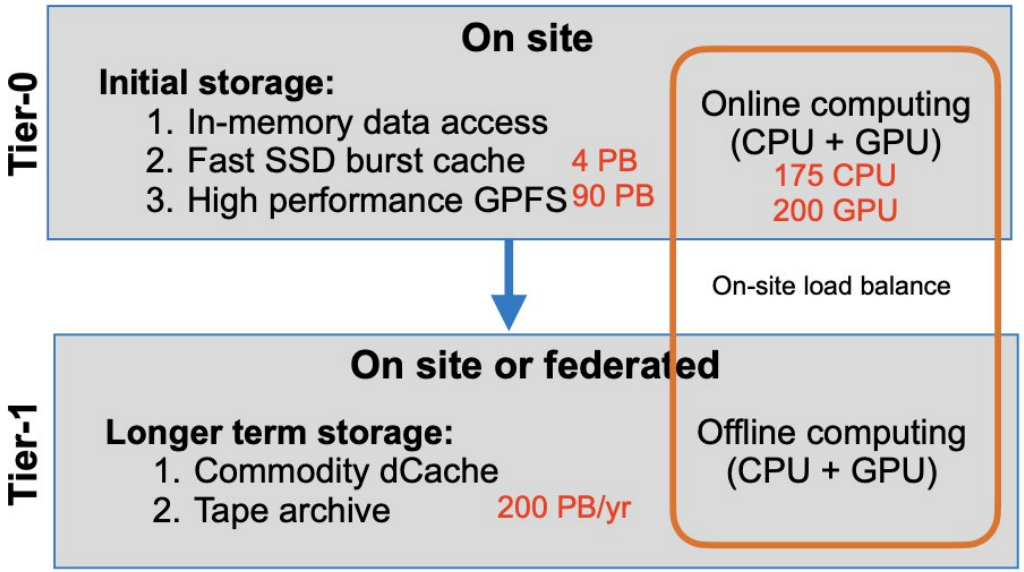


Outlook into the 2030s — PETRA IV

Photon Science at a New Scale

- On a parallel timeframe to HL-LHC DESY is planning to build a 4th generation Photon Source — PETRA IV
- Multi-Bend-Achromat technology decreases beam diameter, increasing brightness by 10^3, coherence to 25%
- Higher brightness and better resolution allow supporting detector with larger data rates: 4-5x of EuXFEL now
- Idea to provide **Photon Science as a Service**
- Deliver **Science-Ready Data**
- **Strong focus on commercial users**

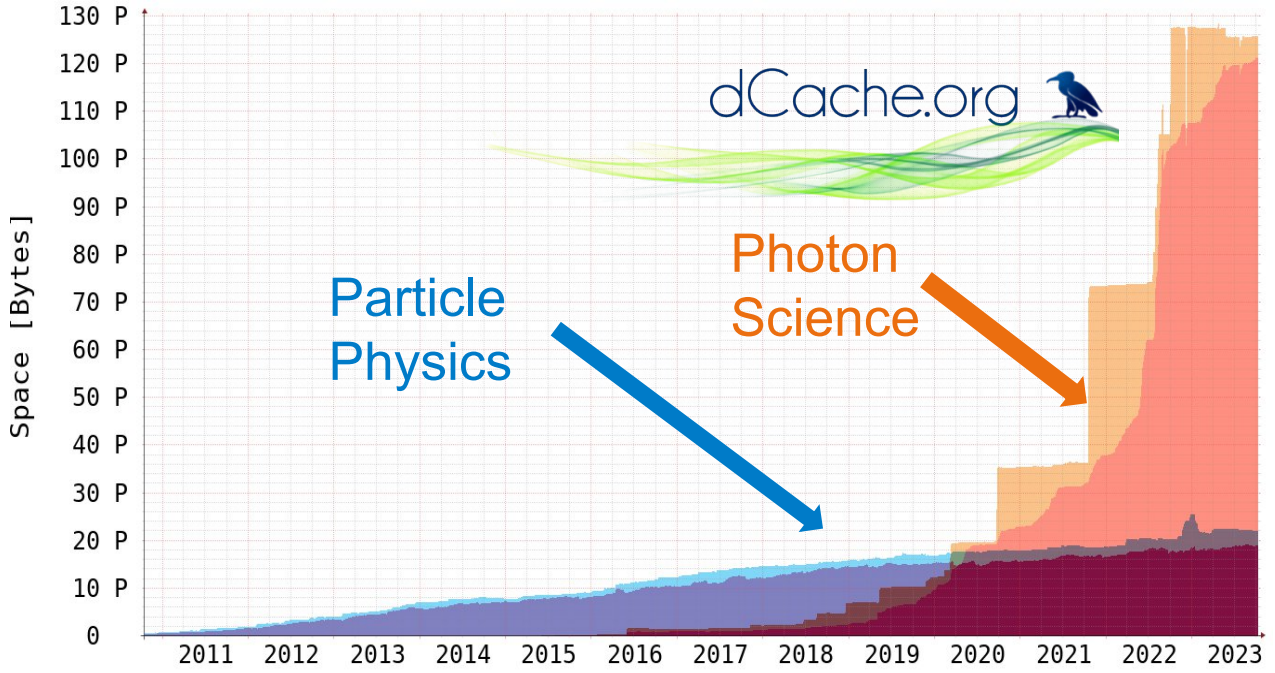
Numbers by Anton Barty (DESY-FS)

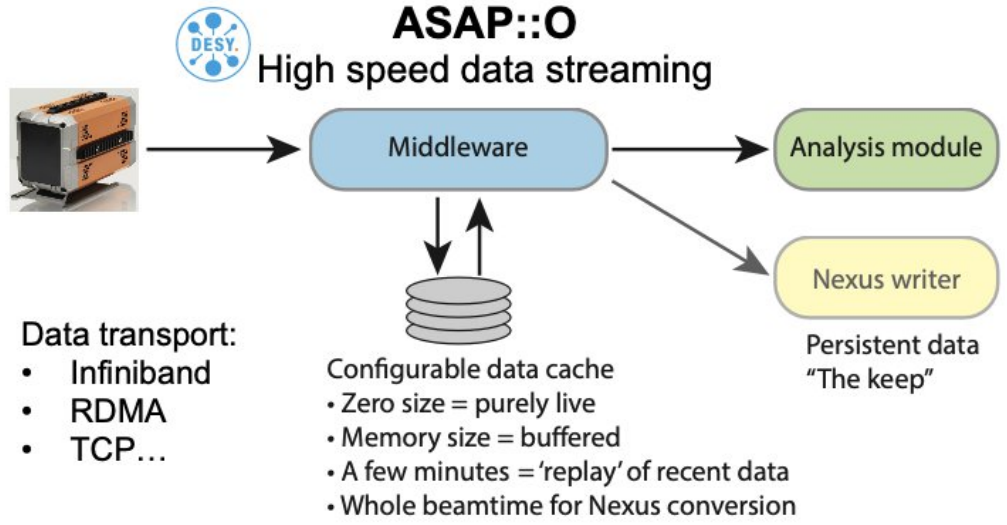


Data Reduction and Trigger

Novel Constraints for Photon Science

- So far we hardly spoke about triggers
- Simple reason: **there are none how HEP understands it**
- Idea of ‘losing’ data alien to photon scientists
- Diversity makes triggering difficult (AI/ML efforts)
- XFEL decided to enforce data reduction after storing
  ➜ After three months users are allowed to keep 10%
- Plan for PETRA IV:
  Reduce data before storing (through near-realtime analysis)
  ➜ Use the new data acquisition framework developed
  ➜ In production at a data intensive PETRA III beamline





Role of DESY in Particle Physics in the Future

Analysis Facilities — Generic Solution for All

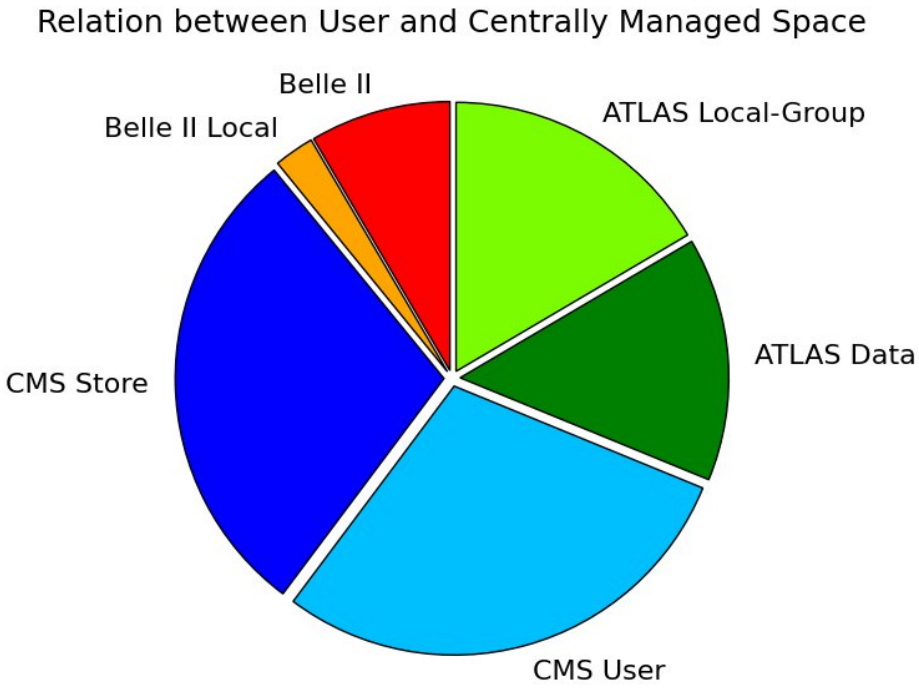
Using a Single Analysis Facility for all of our Communities

- DESY is a multi-VO and interdisciplinary laboratory
- DESY provides access to two Analysis Facilities we'd like to consolidate
- HSF discussions on Analysis Facilities very interesting to DESY
- Certain Tools already in use by Photon Science
  ➜ `Jupyter` notebooks in widespread use
  ➜ Python `Dask` deployed by some groups to scale out of notebooks
- Strong preference to stick to generic and vanilla solutions:
  - Stick to native `numpy`, `pandas` and `dask` solutions, no extra dependencies
  - No dedicated solutions for ATLAS and CMS ➜ hard to support as single site
  - No reliance on HEP-specific protocols for data access like `XRootD`
- Need to reserve resources exclusively for Photon Science Online Compute
- Observation: all our users stick to/depend on and prefer POSIX

Role of DESY Going into the HL-LHC Era

Commitment for dCache and Existing Tier-2 Status

- DESY committed to support the dCache development
- DESY committed to be a major Tier-2 for ATLAS, CMS and LHCb into the HL-LHC era and as a Raw Data Centre for Belle II
- DESY will continue to provide compute and storage resources as agreed upon with the LHC experiments (process of negotiating extended federal funding together with GridKa and GSI)
- DESY is committed to provide our communities with a user analysis facility
- DESY is committed to provide the corresponding storage and compute resources necessary for HL-LHC analyses
- DESY began to provide limited tape resources to ATLAS&CMS
  ➜ willing to extend the volume but DESY will not become a Tier-1



Role of DESY in the Shifting German WLCG Environment

Overview of the Changes

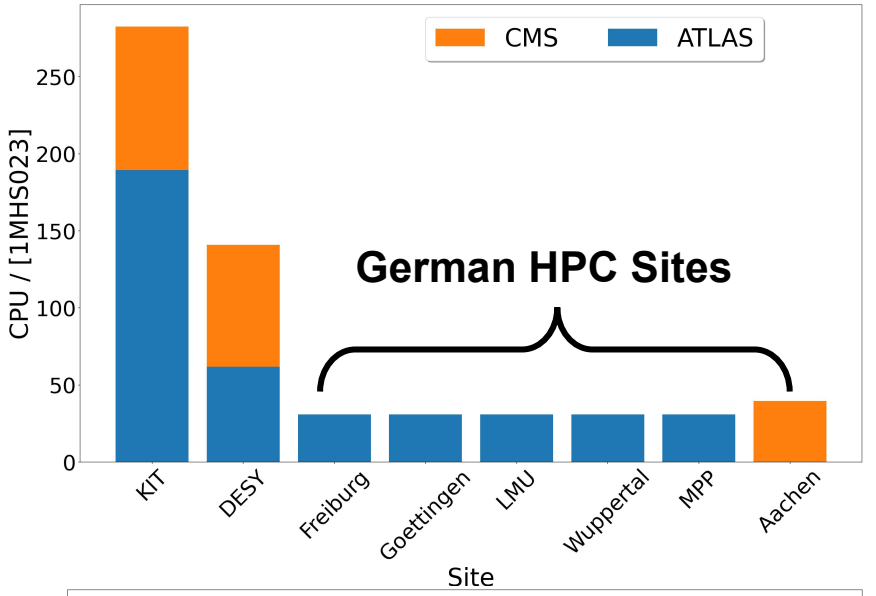
Change in future for the LHC computing:

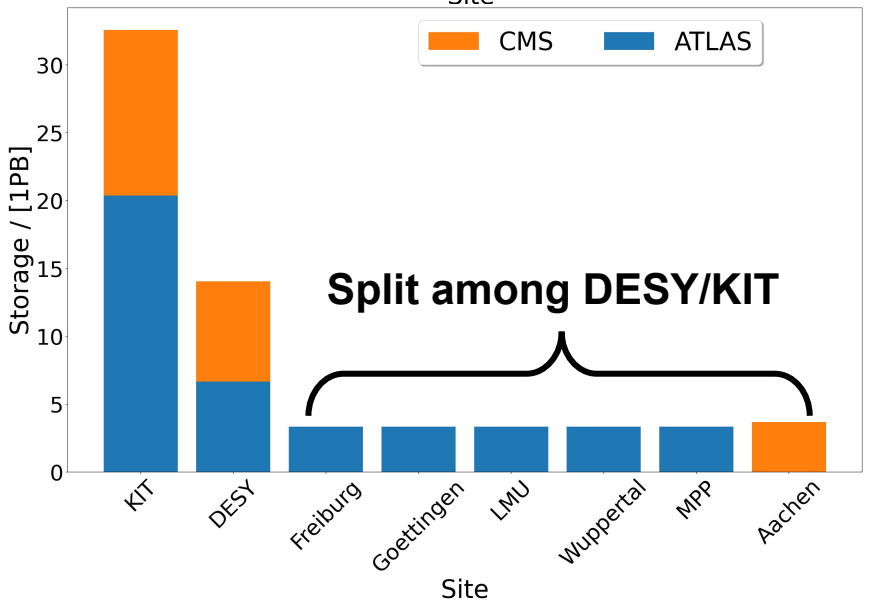
- Next to DESY&GSI several German universities operate Tier-2s
- Compute for universities moving to National HPC centres (NHR)
- Due to the federal funding ➜ incentive to retire the Uni Tier-2s
- Gradual replacement towards the HL-LHC

How will the new computing look like

- Several large German HPC sites will take over the CPU share
- Helmholtz sites DESY/KIT will take over the storage shares
- Process will start in 2025
  - Annual ramp down of 20% of the University shares
  - Increase of the storage pledges taken over by DESY&KIT

German LHC Compute Pledges 2024

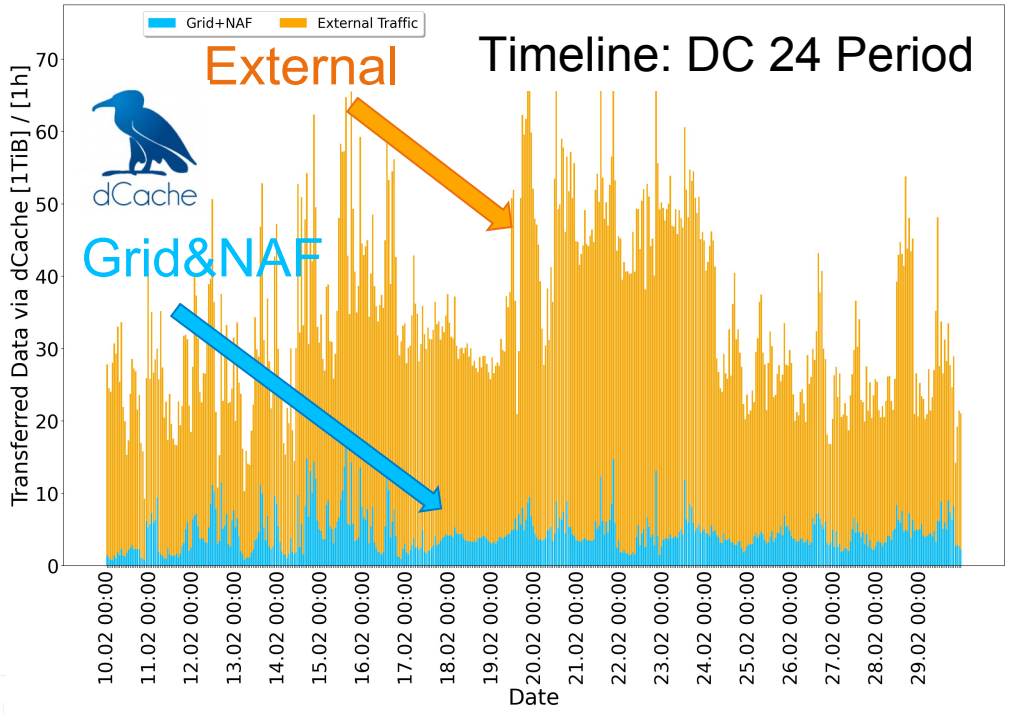


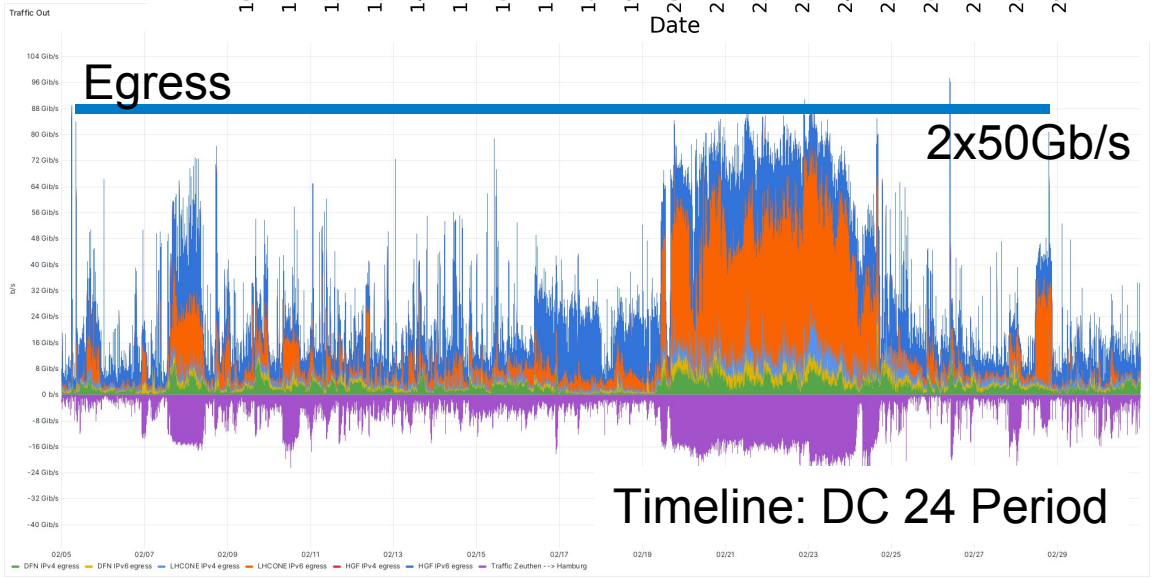


Role of DESY in the Shifting German WLCG Environment

Risks and How DESY will Position Itself in the New Scheme

- Connecting between CPUs at HPC sites and storage at DESY not yet finalised ➜ most likely caching at the NHR
- Remote read will put further strain on our limited network connection (2x50Gb/s) ➜ network-limited during DC'24
- DESY willing to help develop and provide a caching solution taking a leading role in an upcoming project call
  - Utilise a dCache-based solution similar to Nordic Tier-1 ➜ treat the NHRs as satellite sites providing disk only, becoming a part of the hosting site, e.g. DESY
  - Goal is to make the deployment and configuration easier
  - Adapt existing tape workflows to 'warm-up' the caches at the NHR sites
  - Consider employing a similar idea to support Uni Tier-3s





Summary

DESY as an Interdisciplinary Accelerator Laboratory

- DESY is an interdisciplinary laboratory providing user facilities to take and analyze data
- Support full data life cycle different communities use different steps
- DESY-HH operates a grid cluster and two analysis facilities for HEP and Photon Science/machine group
- Interdisciplinary nature makes generic solutions highly desirable (move to a single analysis facility)

- Photon Science profits from collaborating with HEP community to adapt using HEP tools like Rucio and FTS (Automate data transition inside the Photon Science ecosystem using FTS, HEPiX watch-groups)
- Photon Science would profit from the HEP experience in distributed computing if necessity arises

- European XFEL data rates per year comparable to an LHC experiment and PETRA IV is on the horizon
- DESY is committed to contribute significantly to the HL-LHC scientific and computational endeavors

Thank you, any Questions?

Further Related Talks at CHEP 2024

Robin Hofsaess: First Deployment of XCache for Workflow and Efficiency Optimizations on Opportunistic HPC Resources in Germany

Thomas Hartmann: Evolution and Broadening of the National Analysis Facility at DESY

Uday Saidev Polisetty: Integration of the Goettingen HPC cluster Emmy to the WLCG Tier-2 centre GoeGrid and performance tests