# The DAPHNE4NFD project

Anton Barty FS Scientific Computing



HELMHOLTZ





Brings together:

- Large-scale photon and neutron research facilities
- Universities
- KFS and KFN
- Research institutions
- Wider community



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Lead institution: DESY Speakers: Anton Barty, Bridget Murphy 7 German large scale facilities + 11 Universities €3.3M/year, 5 years, €16.7M (with overhead) October 2021 to October 2026





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#### Funded partners **11 Universities** 7 Large scale facilities CAU UNIVERSITÄT Christian-Albrechts-Universitätics K XFEL пп Fechnische Universität Müncher JÜLICH EBERHARD KARLS UNIVERSI TUBINGEN Zentrum Berlin BERGISCHE Universität TRIEDRICH-ALEIANDER JHEVENDICKT ERLANGER-NÜRNBORG EMBL MU Heimholtz-Zentrum Geesthacht GEORG-AUGUST-UNIVERSITÄT hereor Centre for Materials and Coastal Research GÖTTINGEN



What is the economic value of data? Who pays?



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- Academic tradition
- · 'Good scientific practice'
- Sometimes mandated by law (USA)?
- Typically archive all 'raw' data for 10 years
- · Including data known to be 'dud'
- A 'nice to have' or 'must have'?

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Economic reality:

What is the economic value of data? Who pays?

How much are we willing to spend to retain data? What data gives best value for money? What are we keeping it for?

> Most samples and experiments are replaceable at some cost in time and money







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Economic reality:

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How much (limited) money do we spend on old data vs new outcomes?

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Economic reality:

# Data production and retention at PETRA-III today

### A snapshot of the status quo

- Current data retention policy
  - Data on disk for 180 days after measurement
    - (was: 180 days after last access)
  - All data migrated to tape after 180 days
    - retention on site (dCache), dual tape copy
    - 4.5 PB ingested to GPFS in past 12 months
    - 6 PB/year archived to tape
    - 12 PB tapes/yr with dual copy (€20K/PB/10YR)
- Usage highly variable between instruments
- Time to analyse data often limits publication rate
  - ~2 years from measurement to publication
- Hardware typically has a 5 year lifetime
  - Budget for regular replacement



### Data generation easily exceeds 1PB per day across the facility

Continuing "business as usual" at PETRA-IV will:

- Use over 500PB of disk space to keep data for 180 days, and up to 1EB of tape storage per year
- Cost > €150M for disks, plus > €50M per year for consumables and upkeep
- Consume between 1-2 MW of power and exceed the current data centre space
- Swamp users with complicated data further increasing time on disk and slowing science output
  - Performance metric is publications and citations (re-use) not PB on disk

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Peak facility daily data generation today can easily exceed 1PB per day

 Actual peak data generation from 2021 GPFS usage mapped to new P-IV instruments

By 2028, detectors will be larger and faster:

- Planned 130 kHz detector with a frame size of 10 MP and dynamical range of 2 Bytes, would produce **2.5 TB/s**
- Some individual instruments will produce >1PB per day
  - Luckily, not at all instruments are data volcanoes

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Actual peak TB generated in 24 hours by equivalent PETRA-III instruments in 2021

#### Reality check:

- Some single instruments at ESRF already produce 1 PB per day
- In 2022, EuXFEL operating only 3 instruments simultaneously has produced 7 PB in a week (=364 PB/yr)
- 1 PB/day \* 5 flagship big data instruments \* 180 days = 900 PB

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  - Who pays?
  - Who are we keeping it for?
  - Is it worth the cost?

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- · Persistent availability of data requires persistent funding
  - What happens at the end of a 5 or 10 year funding cycle?























Accelerate the path to science outcomes



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- Maximise information density of preserved data



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- · 'Safety net' to catch errors or the unexpected
## The definition of raw data is subjective



- Accelerate the path to science outcomes
- Maximise information density of preserved data
- Potentially a significant reduction in archived data volumes
- · 'Safety net' to catch errors or the unexpected
- Already done in other fields (eg: Square Kilometre Array telescope)

'Raw data' is typically the input to the user's own data analysis pipeline or the limit of their expertise



Graphic: Patrick Fuhrmann DESY









### Key products:

Electronic log books



**Evaluate** 

Graphic: Patrick Fuhrmann DESY

**TA1: Managing data production** 

### Key products:

Electronic log books

Data formats

Storage

Metadata

- SampleID database
- Integration to instrumentation



Save

Store and Archive

Metadata & Data 0

Papers

Findable Accessible

What does FAIR provide?

(FAIR data is not always open data)

### TA2: Data repositories and catalogues

Open rep Key products:

Search • Repositories of raw data and

Interline processed data linked to publications

Federa • Searchable federated catalogues

or destroy

Graphic: Patrick Fuhrmann DESY

Proposal

**TA1: Managing data production** 

### Key products:

Electronic log books

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Storage

Metadata

- SampleID database
- Integration to instrumentation



### **TA3: Infrastructure for evaluation and reuse**

Key products:

Curate, Store and Archive

> Metadata & Data

- Sustainable and reusable software ecosystem
- Power user software deployed on facility infrastructure

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Proposal

Enabling re-use and repeatability of results, ideally searchable

### **Before experiment**

### Proposal

- Proposal number (ID)
- Science motivation
- Experiment concept
- Technique(s)
- Sample(s)
- Sample environment
- Instrumentation
- Science team

### Facility

- Which facility?
- Beam parameters
- Instrumentation
- Detectors

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### **Digital Sample ID**

- 'DOI for samples'
- (MX has sample QR codes)
- Cross link to other consortia

## **During experiment**

### **Facility logs**

- Experiment ID (directory)
- Beam parameters
- Motor positions
- Instrument configuration
- Sample environment
- Detector calibration

### +

### User record of experiment

- Instrumentation configuration
- Actual samples used
  - Ideally a digital sample ID
- Actual sample environment
- Changes to original plan
- What happened when
- Run log (data lookup table)
- Currently: Paper logbooks, google
  - sheets, confluence, and more

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## After experiment

### Analysis

- Data Data analysis steps
- can be Not all data is useful (runs)
- 750 TB Intermediate data, code, scripts



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# Data - Data analysis steps Can be - Not all data is useful (runs) 750 TB - Intermediate data, code, scripts Publication - Findable and searchable - Should describe what was done - Citation, DOI reference

- Sometimes data is deposited (PDB, CXIDB)
- May use a subset of data, or data from many experiments

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### **Re-use**

- Check and verify results
- Improve the analysis
- Re-use code for new work
- Build on past data

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## Daphne is introducing unique sample identifiers

### Tracking samples from creation through to data and publication

- Uniquely identify samples so that they can be tracked through logbooks and datasets
- Identifier should be unique and persistent even though samples themselves may not always persistent
- Must be simple, easy to use, minimal paperwork overhead

### The IGSN<sup>\*</sup> system has been developed for other disciplines IGSN is a globally unique and persistent identifier for material samples.





https://www.igsn.org/

https://ardc.edu.au/services

International Geo Generic Sample Number





In September 2021, IGSN e.V. and DataCite entered a partnership under which DataCite will provide the IGSN ID registration services and supporting technology to enable the ongoing sustainability of the IGSN PID infrastructure.

### **Researchers**

## **DAPHNE** is using SciCat as a catalogue foundation

DESY is in the process of deploying and developing SciCat as the FS data catalogue

Discover data via WebUI									User specific data
					Arch	Archive			? Help 👔 About
Sparch	💻 Clear	My Data Public Data All Archivable Retriev	able Work In Progress System Error	User Error		lace	ltems per p	age: 25 🔻	F Add to Cart
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Location	Faaat	Name	Source Folder	Size	Start Time	Туре	Proposal ID	Group	Data Status
Group	racel	029_estaillades1_q01_fw085_ss	1_fw085_ss	1 TB	2020-12-23 Wed 00:05	derived		p17614	
p18788   2300	search	020_estaillades1_q01_fw085_us	1_fw085_us	729 GB	2020-12-23 Wed 00:05	derived		p17614	▲ retrievable
p18762   10		019_estaillades1_q01_fw085_us	1_fw085_us	376 GB	2020-12-23 Wed 00:05	derived		p17614	🖍 retrievable
p18761   49		018_estaillades1_q01_fw085_us	1_fw085_us	376 GB	2020-12-23 Wed 00:05	derived		p17614	▲ retrievable
p18748   147		031_estaillades1_q01_fw085_ss	1_fw085_ss	4 TB	2020-12-22 Tue 22:02	derived		p17614	▲ retrievable
p18675   18		20201214_ANAXAM/11_360_	AM/11_360_	47 GB	2020-12-14 Mon 20:59	raw	unknown	p17896	archivable
		20201214_ANAXAM/10_360_	AM/10_360_	47 GB	2020-12-14 Mon 20:37	raw	unknown	p17896	archivable
		09_360/09_360_513_	9_360_513_	47 GB	2020-12-14 Mon 20:09	raw	unknown	p17896	archivable
		09_360/09_360_512_	9_360_512_	47 GB	2020-12-14 Mon 20:03	raw	unknown	p17896	archivable
		09_360/09_360_511_	9_360_511_	47 GB	2020-12-14 Mon 19:57	raw	unknown	p17896	archivable
		09_360/09_360_510_	9_360_S10_	47 GB	2020-12-14 Mon 19:52	raw	unknown	p17896	archivable
		09_360/09_360_509_	9_360_509_	47 GB	2020-12-14 Mon 19:46	raw	unknown	p17896	archivable
		09_360/09_360_508_	9_360_508_	47 GB	2020-12-14 Mon 19:40	raw	unknown	p17896	archivable
		09_360/09_360_507_	9_360_507_	47 GB	2020-12-14 Mon 19:35	raw	unknown	p17896	archivable
		09_360/09_360_506_	9_360_506_	47 GB	2020-12-14 Mon 19:29	raw	unknown	p17896	archivable

Initial development by





### Some features:

- Data browsing
- Data search
- Data download
- Access control
- Federated login
- Metadata management
- Online logbooks
- Online chat session
- DataDOI generation
- Archive interface
- Catalogue harvesting
- Data previews
- 'Data lake' for
  - reference datasets
  - simulations
  - LK-I data



## Harmonising ontologies and semantic interoperability

### **Standard file formats**

- Nexus adoption is a starting point
- What about downstream data?

## Standard metadata

- Community languages
- Essential for interoperable catalogues

### **Interoperability validators and libraries**

• eg: PDB check

Daphne brings communities and facilities together

## **Task areas 3: Sustainable software development**

EYCLOAK

OpenID<sup>®</sup>

Drawing on experience in professional IT at the facilities, eg:

dCache.org

Strike a balance between agile user-focussed design with sustainability and integration as critical infrastructure



AAI infrastructure: UmbrelaID + Keycloak





('login with facebook' for researchers)

### Teach and practice sustainable research software

# The DAPHNE work program targets data management resources for photon and neutron science



**Cross-cutting interdisciplinary synergies and strategic opportunities for joint engagement** 

• Federated storage and computing

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- AAI and access management for large scale collaborations

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