Diffraction data reuse: the good, the bad and the challenging

Managing and curating data flows at PETRA-IV

Don’t become storage or compute limited within a reasonable budget envelope
Keeping data has economic consequences

What is the economic value of data? Who pays?
Keeping data has economic consequences

What is the economic value of data? Who pays?

- 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’?
Keeping data has economic consequences

What is the economic value of data? Who pays?

- 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’?

Economic reality:
Keeping raw data costs significant money (M€) and energy (MW)
Keeping all data for lots of experiments becomes expensive very quickly
Facility cost or user’s own cost?
Keeping data has economic consequences

What is the economic value of data? Who pays?

• 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’?

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

Economic reality:
Keeping raw data costs significant money (M€) and energy (MW)
Keeping all data for lots of experiments becomes expensive very quickly
Facility cost or user’s own cost?
Keeping data has economic consequences

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

- 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'?

Economic reality:
Keeping raw data costs significant money (M€) and energy (MW)
Keeping all data for lots of experiments becomes expensive very quickly
Facility cost or user's own cost?
Keeping data has economic consequences

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?

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

- 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'?

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

Economic reality:
Keeping raw data costs significant money (M€) and energy (MW)
Keeping all data for lots of experiments becomes expensive very quickly
Facility cost or user's own cost?
The Petra-IV upgrade project

A new ring and an updated operation model serving as a national analytic facility

- A rebuilt low emittance ring
- 28-30 instruments
- A completely new hall to the west
- Ready for operation 2028 (or so)
The Petra-IV upgrade project
A new ring and an updated operation model serving as a national analytic facility

- A rebuilt low emittance ring
- 28-30 instruments
- A completely new hall to the west
- Ready for operation 2028 (or so)
The Petra-IV upgrade project
A new ring and an updated operation model serving as a national analytic facility

From basic science to broad application

- A rebuilt low emittance ring
- 28-30 instruments
- A completely new hall to the west
- Ready for operation 2028 (or so)

- Support for non-expert users
- Faster turnaround from proposal to measurement
- Increased use of automation
- Deliver outcomes rather than data on disk
Data production and retention at PETRA-III today

A snapshot of the status quo

• Data policy
  • Data on disk for 180 days after measurement
    • (was: 180 days after last access)

  • 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
Projection for PETRA-IV operation in 2028

PETRA-IV science output should not be storage or compute limited

Peak total daily data generation will exceed **1PB per day** based on actual peak 2021 GPFS usage
- Operation of any one instrument should not jeopardise operation of other 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
  - Increase inevitable **almost regardless of PETRA-IV project**

Numbers are the **actual peak TB generated in 24 hours** by the comparable PETRA-III instrument in 2021
Projection for PETRA-IV operation in 2028
PETRA-IV science output should not be storage or compute limited

Peak total daily data generation will exceed 1PB per day based on actual peak 2021 GPFS usage
• Operation of any one instrument should not jeopardise operation of other 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
• Increase inevitable almost regardless of PETRA-IV project

Reality check:
• Some 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 big data instruments * 180 days = 900 PB
In the future, retaining all data for 10 years is unaffordable

This problem will exist regardless of PETRA-IV

Continuing “business as usual” will:

- 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
In the future, retaining all data for 10 years is unaffordable

This problem will exist regardless of PETRA-IV

<table>
<thead>
<tr>
<th>Continuing “business as usual” will:</th>
</tr>
</thead>
<tbody>
<tr>
<td>• Over 500PB of disk space to keep data for 180 days, and up to 1EB of tape storage per year</td>
</tr>
<tr>
<td>• Cost &gt; €150M for disks, plus &gt; €50M per year for consumables and upkeep</td>
</tr>
<tr>
<td>• Consume between 1-2 MW of power and exceed the current data centre space</td>
</tr>
<tr>
<td>• Swamp users with complicated data further increasing time on disk and slowing science output</td>
</tr>
<tr>
<td>• Performance metric is publications and citations (re-use) not PB on disk</td>
</tr>
</tbody>
</table>

Reality check:

• Some 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 instruments * 180 days = 900 PB
In the future, retaining all data for 10 years is unaffordable
This problem will exist regardless of PETRA-IV

Continuing “business as usual” will:
• 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

Cost driver
• PB of data generated (per instrument per day)
• PB of data saved to disk (reduction, veto or quotas)
• Number of high data rate instruments
• Number of days of operation
• Efficiency of data collection (and automation)

• Data reduction/compression ratios
• All data on GPFS for 180 days
• Efficiency of analysis (time on disk)
• Archive all data for 10 years

Reality check:
• Some 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 instruments * 180 days = 900 PB
In the future, retaining all data for 10 years is unaffordable

This problem will exist regardless of PETRA-IV

Continuing “business as usual” will:
• 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

Cost driver
• PB of data generated (per instrument per day)
• PB of data saved to disk (reduction, veto or quotas)
• Number of high data rate instruments
• Number of days of operation
• Efficiency of data collection (and automation)
• Data reduction/compression ratios
• All data on GPFS for 180 days
• Efficiency of analysis (time on disk)
• Archive all data for 10 years

Remedial action
• Smaller, slower detectors; shorter measurement time
• Enforce limited data quotas (eg: 1PB/week)
• High data instruments are mostly the flagships
• Reduce user hours (ie: measurement time)
• Operate inefficiently (eg: manual alignment…)

Reality check:
• Some 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 instruments * 180 days = 900 PB
In the future, retaining all data for 10 years is unaffordable
This problem will exist regardless of PETRA-IV

Continuing “business as usual” will:
- 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

Cost driver
- PB of data generated (per instrument per day)
- PB of data saved to disk (reduction, veto or quotas)
- Number of high data rate instruments
- Number of days of operation
- Efficiency of data collection (and automation)
- Data reduction/compression ratios
- All data on GPFS for 180 days
- Efficiency of analysis (time on disk)
- Archive all data for 10 years

Remedial action
- Smaller, slower detectors; shorter measurement time
- Enforce limited data quotas (eg: 1PB/week)
- High data instruments are mostly the flagships
- Reduce user hours (ie: measurement time)
- Operate inefficiently (eg: manual alignment…)
- Will do this anyway (lossless ~4x, lossy varies a lot)
- Data stays on GPFS for ~30 days (6x reduction)
- Optimised pipelines, particularly for measurements
- Redefine what gets kept after 30 days

Reality check:
- Some 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 instruments * 180 days = 900 PB
The definition of raw data depends on your starting point
The definition of raw data depends on your starting point

Instrumentation → Trusted processing steps → Raw data → User competence → Result
The definition of raw data depends on your starting point

I need the raw detector data

Here it is in ADU

Can you give me the photons per pixel?

User competence

Raw data

Trusted processing steps

Instrumentation
The definition of raw data depends on your starting point

- Instrumentation
- Trusted processing steps
- Raw data
- User competence

I need the raw detector data
Here it is in ADU
Can I have the raw data?
Sure, here are the images
Can you give me the photons per pixel?
I need the 1D powder pattern
The definition of raw data depends on your starting point

0. Instrumentation
1. Trusted processing steps
2. Raw data
3. User competence

I need the raw detector data

Here it is in ADU

Can you give me the photons per pixel?

Can I have the raw data?

Sure, here are the images

I need the 1D powder pattern

Can I have the raw data?

Sure, here are the H5 files

Can I have the raw data?

Sure, here are the images

I need the 1D powder pattern

No, I mean the MTZ file
The definition of raw data depends on your starting point

Instrumentation $\rightarrow$ Trusted processing steps $\rightarrow$ Raw data $\rightarrow$ User competence

- I need the raw detector data
  - Here it is in ADU
- Can I have the raw data?
  - Sure, here are the images
- I need the 1D powder pattern
  - Can you give me the photons per pixel?
- Can I have the raw data?
  - Sure, here are the H5 files
- Can I have the raw fluorescence data?
  - The event stream from the detector is here
- Can I have the chemical concentration?
  - No, I mean the MTZ file
The definition of raw data depends on your starting point

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

1. I need the raw detector data
   - Here it is in ADU
   - Can you give me the photons per pixel?

2. Can I have the raw data?
   - Sure, here are the images

3. I need the 1D powder pattern
   - Can I have the raw data?
   - Sure, here are the H5 files

4. Can I have the raw data?
   - Sure, here are the H5 files
   - I need the 1D powder pattern
   - No, I mean the MTZ file

5. Can I have the raw fluorescence data?
   - The event stream from the detector is here

6. Can I have the chemical concentration?
PETRA-IV requires a different approach to data retention

Provide results to users and retain low-level data for only 30 days

Instrumentation → Trusted processing steps → Raw data → User competence

Keep for <30 days

Archive after 30 days
PETRA-IV requires a different approach to data retention

Provide results to users and retain low-level data for only 30 days

Aim to **maximise science content of stored data:**
1) Develop trusted and validated processing pipelines to efficiently deliver results to users
2) Processing output is the product we give to the users,
3) Keep instrument data for 30 days during which time processing problems can be corrected
4) Develop a data weeding strategy (policy for discarding data), including (maybe) deleting raw data
PETRA-IV requires a different approach to data retention

Provide results to users and retain low-level data for only 30 days

Aim to **maximise science content of stored data:**

1) Develop trusted and validated processing pipelines to efficiently deliver results to users
2) Processing output is the product we give to the users,
3) Keep instrument data for 30 days during which time processing problems can be corrected
4) Develop a data weeding strategy (policy for discarding data), including (maybe) deleting raw data
PETRA-IV requires a different approach to data retention

Provide results to users and retain low-level data for only 30 days

Aim to **maximise science content of stored data:**
1) Develop trusted and validated processing pipelines to efficiently deliver results to users
2) Processing output is the product we give to the users,
3) Keep instrument data for 30 days during which time processing problems can be corrected
4) Develop a data weeding strategy (policy for discarding data), including (maybe) deleting raw data

Data processing vs analysis:
- **Data analysis** is where researchers turn processed data into scientific knowledge
  - Domain specialists interpret processed data to answer their science question(s)
- **Processed data** is in a form suitable for the non-expert user to continue with their analysis
  - Processing is often generic and deterministic; optimised pipelines can be provided
  - Calibration, geometry and masking procedures must be standardised, minimise parameter tweaking
  - Often highly reduced data volumes (at worst, avoid data duplication)
PETRA-IV requires a different approach to data retention

Provide results to users and retain low-level data for only 30 days

Aim to maximise science content of stored data:
1) Develop trusted and validated processing pipelines to efficiently deliver results to users
2) Processing output is the product we give to the users,
3) Keep instrument data for 30 days during which time processing problems can be corrected
4) Develop a data weeding strategy (policy for discarding data), including (maybe) deleting raw data

Data processing vs analysis:
- **Data analysis** is where researchers turn processed data into scientific knowledge
  - Domain specialists interpret processed data to answer their science question(s)

- **Processed data** is in a form suitable for the non-expert user to continue with their analysis
  - Processing is often generic and deterministic; optimised pipelines can be provided
  - Calibration, geometry and masking procedures must be standardised, minimise parameter tweaking
  - Often highly reduced data volumes (at worst, avoid data duplication)

Not all instruments or samples are equal - policies must be implemented sensibly
The human factor: trust is a big issue

Confidence that initial processing is correct must be ensured
The human factor: trust is a big issue
Confidence that initial processing is correct must be ensured

Online analysis may be 80% good enough, but I need 95%-100% for my paper
The human factor: trust is a big issue
Confidence that initial processing is correct must be ensured

Online analysis may be 80% good enough, but I need 95%-100% for my paper

Detector location needs to be refined from the data (experiment geometry)

The detector response is not properly calibrated

Beam centre may move, I need to refine it from the data

Can't trust the metadata (detector distance, wavelength)

ROI adjustment, eg: unexpected bad regions on the detectors (shadows)
The human factor: trust is a big issue
Confidence that initial processing is correct must be ensured

- The detector response is not properly calibrated
- Beam centre may move, I need to refine it from the data
- Detector location needs to be refined from the data (experiment geometry)
- Can't trust the metadata (detector distance, wavelength)
- ROI adjustment, eg: unexpected bad regions on the detectors (shadows)
- Online analysis may be 80% good enough, but I need 95%-100% for my paper
- I need to convert file formats
- PhD student needs to do the analysis / write the code
- My analysis only works using files
- There are parameters/thresholds to tweak
- Just in case... I need to check it's right myself
We move data to the central data centre as soon as possible

Exploit large scale shared infrastructure

Dedicated 96x 400GE fibre per instrument
We move data to the central data centre as soon as possible

Exploit large scale shared infrastructure

Dedicated 96x 400GE fibre per instrument

**ASAP::O**

High speed data streaming

---

**Data transport:**
- Infiniband
- RDMA
- TCP...

**Configurable data cache**
- Zero size = purely live
- Memory size = buffered
- A few minutes = ‘replay’ of recent data
- Whole beamtime for Nexus conversion

**Middleware**

**Analysis module**

**Nexus writer**

**Persistent data “The keep”**

---

**Producer:**
- create producer (beamtimeID, data source)
- send data raw(scan name, index)
- send data array(scan name, index) (same but hides serialisation)
- send data(/monitor) (monitoring mode)
- end scan(nframes)

**Consumer:**
- create consumer (beamtimeID, data source)
- get data(scan name, index)
- get next(scan name)
- get latest() [monitoring mode - no need for scan name]

---

**Copy files from detector PC to GPFS**

---

**Primary data store**

All data saved in ASAP::O message format forever

“The keep” of data

---

**Temporary data cache**

- Zero size = purely live
- Memory size = buffered
- A few minutes = ‘replay’ of recent data
- Whole beamtime for Nexus conversion

Data here eventually gets deleted

---

**File transfer (HiDRA replacement)**

---

**Nexus writer**

**Middleware**

**Analysis module**

---

**Data transport:**
- Infiniband
- RDMA
- TCP…
We move data to the central data centre as soon as possible

Exploit large scale shared infrastructure

Dedicated 96x 400GE fibre per instrument

Initial storage:
1. In-memory data access
2. Fast SSD burst cache
3. High performance GPFS

Online computing (CPU + GPU)

Tier-0

- Replace HiDRA with system based on ASAP::O
- Re-read data once saved in HDF5 format
- Dashboard to control all producers and analysis modules, monitor health and status

Note:
Control system controls the experiment and data taking, indexes the data, and tells the producer whether to save or monitor.
In this sense ASAP::O is not the same as a classic DAQ which takes care of timestamping, synchronisation and event building.

To do:
• get latest function for monitoring
• send array function to hide serialisation
• Swap easily between monitoring and saving modes
- Save permanently or cache messages
- Wait for consumer or drop

Producer:
- create producer (beamtimeID, data source)
- send data raw(scan name, index)
- send data array(scan name, index) (same but hides serialisation)
- send data(/monitor) (monitoring mode)
- end scan(nframes)

Consumer:
- create consumer (beamtimeID, data source)
- get data(scan name, index)
- get next(scan name)
- get latest() [monitoring mode - no need for scan name]

Data flow control: does producer wait for consumer to be ready, cache/save intermediate results, or drop data?

Data transport:
• Infiniband
• RDMA
• TCP...

Nexus writer
Middleware
Analysis module
Persistent data “The keep”

Producer
Consumer
Middleware
ASAP::O
High speed data streaming

Configurable data cache
• Zero size = purely live
• Memory size = buffered
• A few minutes = ‘replay’ of recent data
• Whole beamtime for Nexus conversion

Copy files from detector PC to GPFS

2. Temporary data cache
• Zero size = purely live
• Memory size = buffered
• A few minutes = ‘replay’ of recent data
• Whole beamtime for Nexus conversion

Copy files from detector PC to GPFS

3. File transfer (HiDRA replacement)
We move data to the central data centre as soon as possible

Exploit large scale shared infrastructure

Dedicated 96x 400GE fibre per instrument

ASAP::O
High speed data streaming

Data transport:
• Infiniband
• RDMA
• TCP...

Middleware

Analysis module

Nexus writer

Persistent data “The keep”

Configurable data cache
• Zero size = purely live
• Memory size = buffered
• A few minutes = ‘replay’ of recent data
• Whole beamtime for Nexus conversion

Initial storage:
1. In-memory data access
2. Fast SSD burst cache
3. High performance GPFS

Online computing (CPU + GPU)

Tier-0

On site

On site or federated

Longer term storage:
1. Commodity dCache
2. Tape archive

Offline computing (CPU + GPU)

Tier-1
We move data to the central data centre as soon as possible

Exploit large scale shared infrastructure

Dedicated 96x 400GE fibre per instrument

ASAP::O
High speed data streaming

Middleware
Analysis module
Nexus writer

Data transport:
- Infiniband
- RDMA
- TCP...

Configurable data cache
- Zero size = purely live
- Memory size = buffered
- A few minutes = ‘replay’ of recent data
- Whole beamtime for Nexus conversion

Persistant data “The keep”

On site

Initial storage:
1. In-memory data access
2. Fast SSD burst cache
3. High performance GPFS

Online computing (CPU + GPU)
On-site load balance

On site or federated

Longer term storage:
1. Commodity dCache
2. Tape archive

Offline computing (CPU + GPU)
We already process and reduce data before it is saved to disk

Real time serial crystallography at P11 using central compute resources

1. Description of actual experiment:

We performed the first test of real-time data processing for serial crystallography, with – in principle – no requirement to store the raw image data. Physically, the experiment was performed as planned, using the tape drive serial crystallography setup with liquid mixing injector, and crystals of lysozyme and SARS-CoV-2 main protease. On the data processing side, an almost completely new setup was used (see diagram). In the standard P11 setup, the Dectris software writes data files directly to disk. In our setup, the Dectris streaming interface was used to send data over the network into the ASAP::O framework. Two pieces of analysis software were attached to the ASAP::O data stream: OM (OnDA-Monitor), which provided real-time feedback on the crystal “hit rate” (the fraction of detector frames containing true crystal diffraction), and CrystFEL, which indexed and integrated each diffraction pattern to produce a set of unmerged Bragg intensity measurements ready for merging.

The experiment was very successful. Even on this first attempt, we were able to process the entire data stream at the maximum frame rate of the detector (133 frames per second). The computing requirements vary in proportion to the hit rate, because blank frames can be quickly skipped over. Between 300 and 1800 CPUs were required, a small fraction of the resources available in the Maxwell cluster. The real-time data processing system was able to cope even in the “worst case scenario” where every frame contained diffraction. We were therefore able to establish “boundary conditions” on the amount of computing power needed for a certain data rate.

2. Difficulties encountered:

No problems were encountered on the experimental side. The main purpose of this experiment was to discover what difficulties would occur on the data processing side, and indeed several technical difficulties were encountered concerning the performance of the software, network topology and other aspects of the computing system. Workarounds or solutions were implemented for these, or they were noted as improvements to be made in time for the next experiment. Feedback has been collected and already discussed with DESY IT and FS-SC, who were closely involved with all stages of the experiment.

3. Alterations made:

No alterations were made compared to the submitted proposal.

4. Aims achieved:

The aims of this first step were achieved. No changes are necessary to the objectives and milestones. The concept of real-time data processing will be refined and stabilised in the future beamtimes.

5. Sufficiency for publication:

Given the excitement in the community about real-time processing for serial crystallography, the developments are already sufficient for presentation at conferences. In fact, an abstract has already been submitted to SRI 2021 (14th International Conference on Synchrotron Radiation Instrumentation). DESY staff, in particular from the P11, FS-SC, IT and FS-CFEL groups, are included as co-authors and will also be included in future publications. A formal journal publication is not yet appropriate, but can be expected once the system has been refined and stabilised.

Tom White, et.al. DESY

More details in Alexandra’s talk later today

• Average 200 ms per frame (5 frames per second per CPU) when working on the full 16 megapixel frames from Eiger (16 bits per pixel).
• Uses two dedicated computers (2x 192 CPUs) running CrystFEL plus other parts of the pipeline (NeXus writer, OM, OM GUI, binning worker)
• ASAP::O handles high speed data transfer, bookkeeping, etc; always performed after a similar experiment for which the calibrations exist

Real-time data processing at the max. Eiger2 16M frame rate of 133 frames per second
PETRA-IV will offer services for the complete data life cycle

Data management by the facility for the non expert user community

What does FAIR provide?
- Findable
- Accessible
- Interoperable
- Reusable

Open data
- Impact Research
- Reviews
- Teaching

Metadata
- Plan
  - Proposal
  - Data formats
  - Storage Sources
  - Metadata
- Create
  - Experiment Measurements
  - Collect Metadata
- Process
  - Store Data
  - Validate Data
  - Visualize Data
- Analysis
  - Integrate Data
  - Create Output
  - Publish Results

Reuse
- Impact Research
- Reviews
- Teaching

Curate or destroy
- Save
  - Curate, Store and Archive
  - Metadata & Data
- Access
  - Share Data
  - Open Access
  - Access rules and control

Evaluate
- Publish
- Papers

User portal

(FAIR data is not always open data)
PETRA-IV will offer services for the complete data life cycle

Data management by the facility for the non-expert user community

- **Collect**
  - Dedicated 96x 400GE fibre + SSD fast cache

- **Plan**
  - Data formats
  - Storage sources
  - Metadata

- **Create**
  - Experiment measurements
  - Collect metadata

- **Process**
  - Store data
  - Validate data
  - Visualize data

- **Analysis**
  - Integrate data
  - Create output
  - Publish results

- **Evaluate**
  - Curate or destroy

- **Save**
  - Curate, store and archive metadata & data

- **Access**
  - Share data
  - Open access
  - Access rules and control

- **Reuse**
  - Impact research
  - Reviews
  - Teaching

- **Open data**

What does FAIR provide?

- **F**indable
- **A**ccessible
- **I**nteroperable
- **R**eusable

(FAIR data is not always open data)

- **User portal**

- **Proposal**
  - Metadata

- **Curate**

- **Publish**
  - Papers

**Graphic:** Patrick Fuhrmann DESY
PETRA-IV will offer services for the complete data life cycle

Data management by the facility for the a non expert user community

Plan
- Data formats
- Storage sources
- Metadata

Collect
- Dedicated 96x 400GE fibre + SSD fast cache

Create
- Experiment measurements
- Collect metadata

Process
- Store data
- Validate data
- Visualize data

Analysis
- Integrate data
- Create output
- Publish results

Save
- Curate, store and archive
- Metadata & data

Access
- Share data
- Open access
- Access rules and control

Curate or destroy

Reuse
- Impact research
- Reviews
- Teaching

Evaluate
- Tiered central computing model
  - Tier-0: On-site computing (near real time processing)
  - Tier-1: On site and/or federated (analysis after experiment)

Open data

What does FAIR provide?
- Findable
- Accessible
- Interoperable
- Reusable

(FAIR data is not always open data)

Graphic: Patrick Fuhrmann DESY
PETRA-IV will offer services for the complete data life cycle

Data management by the facility for the a non expert user community

Open repositories
- Searchable
- Interlinked
- Federated
- Reused

User portal

Open data
- Reuse
  - Impact Research
  - Reviews
  - Teaching

Metadata
- Proposal
  - Plan
    - Data formats
    - Storage
    - Sources
    - Metadata
  - Collect Metadata
- Create
  - Experiment
  - Measurements
- Process
  - Store Data
  - Validate Data
  - Visualize Data
- Analysis
  - Integrate Data
  - Create Output
  - Publish Results

Evaluate
- Tiered central computing model
- Tier-0: On-site computing (near real time processing)
- Tier-1: On site and/or federated (analysis after experiment)

Graphic: Patrick Fuhrmann DESY
PETRA-IV will offer complete data life cycle services

Data management for the non expert user community

**What does FAIR provide?**

- **F**: Findable
- **A**: Accessible
- **I**: Interoperable
- **R**: Reusable

(FAIR data is not always open data)

**Tier-0**: On-site computing (near real time processing)

**Tier-1**: On site and/or federated (analysis after experiment)

Graphic: Patrick Fuhrmann DESY
PETRA-IV will offer complete data life cycle services

Data management for the non expert user community

- Integration data capture
  - Electronic log books
  - SampleID database
  - Standard file formats
  - Integration to instrumentation
  - Integrated metadata harvesting

What does FAIR provide?
- Findable
- Accessible
- Interoperable
- Reusable

(FAIR data is not always open data)

Save
- Curate, Store and Archive Metadata & Data

Publish
- Create Papers

Evaluate
- Tiered central computing model
  - Tier-0: On-site computing (near real time processing)
  - Tier-1: On site and/or federated (analysis after experiment)

Graphic: Patrick Fuhrmann DESY
PETRA-IV will offer complete data life cycle services
Data management for the non expert user community

**Plan**
- Data formats
- Storage Sources
- Metadata

**Process**
- Create Experiment
- Collect Metadata
- Measure
- Process Store Data
- Validate Data
- Visualize Data
- Analysis
- Integrate Data
- Create Output
- Publish Results

**Integrate data capture**
- Electronic log books
- SampleID database
- Standard file formats
- Integration to instrumentation
- Integrated metadata harvesting

**Evaluate**
- Tiered central computing model

**Infrastructure for data evaluation**
- Tier-0: On-site computing (near real time processing)
- Tier-1: On site and/or federated (analysis after experiment)

**Open repositories**
- Searchable
- Interlinked
- Federated
- Reused

**Open data**
- Impact Research
- Reviews
- Teaching

**Reuse**
- Curate, Store and Archive Metadata & Data

**Access**
- Share Data
- Open Access
- Access rules and control

**Curate or destroy**

**What does FAIR provide?**
- Findable
- Accessible
- Interoperable
- Reusable

(FAIR data is not always open data)

**Save**
- Central HPC resources
- Sustainable and reusable software ecosystem
- Power user software deployed for all users
- Remote data evaluation
- Containerisation

**Graphic: Patrick Fuhrmann DESY**
PETRA-IV will offer complete data life cycle services

Data management for the non expert user community

**Plan**
- Data formats
- Storage Sources
- Metadata

**Create**
- Experiment
- Measurements

**Collect**
- Metadata

**Process**
- Store Data
- Validate Data

**Visualize**
- Data

**Integrate**
- Analysis
- Create Output

**Publish**
- Results

**Reuse**
- Impact Research
- Reviews
- Teaching

**Access**
- Share Data
- Open Access
- Access rules and control

**Save**
- Curate, Store and Archive Metadata & Data

**Evaluate**
- Tiered central computing model

**Tier-0**: On-site computing (near real time processing)
- Central HPC resources
- Sustainable and reusable software ecosystem
- Power user software deployed for all users
- Remote data evaluation
- Containerisation

**Tier-1**: On site and/or federated (analysis after experiment)

**(Open) data repositories and catalogues**
- Raw data can be made open
- Searchable federated catalogues (with access control)
- Common user IDs (AAI)
- DOI minting
- Place to put open results with processed data

**What does FAIR provide?**
- Findable
- Accessible
- Interoperable
- Reusable

**Graphic**: Patrick Fuhrmann DESY
PETRA-IV will offer complete data life cycle services

Data management for the non expert user community

**Integrated data capture**
- Electronic log books
- SampleID database
- Standard file formats
- Integration to instrumentation
- Integrated metadata harvesting

**Evaluate**
Tiered central computing model

**Infrastructure for data evaluation**
- Central HPC resources
- Sustainable and reusable software ecosystem
- Power user software deployed for all users
- Remote data evaluation
- Containerisation

**Tier-0**: On-site computing (near real time processing)

**Tier-1**: On site and/or federated (analysis after experiment)

**Open repositories and catalogues**
- Raw data can be made open
- Searchable federated catalogues (with access control)
- Common user IDs (AAI)
- DOI minting
- Place to put open results with processed data

What does FAIR provide?
- Findable
- Accessible
- Interoperable
- Reusable

**Plan**
- Proposal
- Data formats
- Storage
- Sources
- Metadata

**Analysis**
Integrate Data

**Save**
- Open data
- Curate
- Store and Archive

**Diagram**
Graphic: Patrick Fuhrmann DESY

**Open repository**
- Searchable
- Interlinked
- Federated
- Reused

**User portal**
PETRA-IV will offer complete data life cycle services

Data management for the non expert user community

**Integrated data capture**
- Electronic log books
- SampleID database
- Standard file formats
- Integration to instrumentation
- Integrated metadata harvesting

**Evaluate**
Tiered central computing model

**Infrastructure for data evaluation**
- Central HPC resources
- Sustainable and reusable software ecosystem
- Power user software deployed for all users
- Remote data evaluation
- Containerisation

**Tier-0**: On-site computing (near real time processing)

**Tier-1**: On site and/or federated (analysis after experiment)

**(Open) data repositories and catalogues**
- Raw data can be made open
- Searchable federated catalogues (with access control)
- Common user IDs (AAI)
- DOI minting
- Place to put open results with processed data

Graphic: Patrick Fuhrmann DESY
PETRA-IV will offer complete data life cycle services

Data management for the non expert user community

**Plan**
- Data formats
- Storage sources
- Metadata

**Create**
- Experiment measurements

**Collect**
- Metadata

**Process**
- Store data
- Validate data

**Visualize**
- Data

**Analysis**
- Integrate data
- Create output
- Publish results

**Reuse**
- Impact research
- Reviews
- Teaching

**Access**
- Share data
- Open access
- Access rules and control

**Save**
- Curate, store, and archive metadata & data

**Evaluate**
- Tiered central computing model

**Tier-0:** On-site computing (near real time processing)

**Tier-1:** On site and/or federated (analysis after experiment)

**Infrastructure for data evaluation**
- Central HPC resources
- Sustainable and reusable software ecosystem
- Power user software deployed for all users
- Remote data evaluation
- Containerisation

**Open repositories and catalogues**
- Raw data can be made open
- Searchable federated catalogues (with access control)
- Common user IDs (AAI)
- DOI minting
- Place to put open results with processed data

**Integrated data capture**
- Electronic log books
- SampleID database
- Standard file formats
- Integration to instrumentation
- Integrated metadata harvesting

**What does FAIR provide?**
- Findable
- Accessible
- Interoperable
- Reusable

**Graphic:** Patrick Fuhrmann DESY
SciCat as a catalogue foundation

We are in the process of deploying and developing SciCat as our data catalogue.

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
  - research group data

Initial development by

DESY
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* 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.
Acknowledgments

Special thanks for contributions, ideas and inspiration from

**FS-SC:** Anton Barty, Tom White, Christoph Rosemann, Alexandra Tolstikova, Tim Schoof, Vijay Kartik, Mads Jakobsen, Sam Flewett, Gudrun Lotse, Diana Rueda, Marc-Olivier Andrzej, Michael Größler, Lisa Amelung, Nicola Baark, Igor Khokhriakov, Olga Merkulova, Mikhail Karnevinsky, Abdullah Malik, Silvan Schön

**Daphne4NFDI:** Anton Barty, Bridget Murphy, Lisa Amelung, Christian Gutt, Astrid Schneidewind, Wiebke Lohstroh, Sebastien Busch, Frank Schreiber, Tobias Unruh, Jan-Dierk Grunwaldt and at least 50 others

**Other DESY:** Volker Gülzow, Martin Gasthuber, Patrick Fuhrmann, Paul Millar, Sophie Servan, Mikhail Karnevinsky, Kars Ohrenberg (Central IT), Thorsten Kracht, Linus Pithan (FS-EC), Harald Reichert, Kai Bagschik, Stephan Klumpp (PETRA-IV), and many others

**Others:** Valerio Mariani (SLAC)
Final thoughts
Final thoughts

- Keeping all detector output is feasible but can get very expensive
  - Who pays?
  - Who are we keeping it for?
  - Is it worth the cost?
Final thoughts

• Keeping all detector output is feasible but can get very expensive
  • Who pays?
  • Who are we keeping it for?
  • Is it worth the cost?
Final thoughts

- Keeping all detector output is feasible but can get very expensive
  - Who pays?
  - Who are we keeping it for?
  - Is it worth the cost?

- What is the ‘raw data’ we aim to keep?
  - Photons not ADU, 1D powder …
  - For what purpose is the data being kept?
Final thoughts

• Keeping all detector output is feasible but can get very expensive
  • Who pays?
  • Who are we keeping it for?
  • Is it worth the cost?

• What is the ‘raw data’ we aim to keep?
  • Photons not ADU, 1D powder …
  • For what purpose is the data being kept?

• Clarity on when to discard data is needed
Final thoughts

• Keeping all detector output is feasible but can get very expensive
  • Who pays?
  • Who are we keeping it for?
  • Is it worth the cost?

• What is the ‘raw data’ we aim to keep?
  • Photons not ADU, 1D powder …
  • For what purpose is the data being kept?

• Clarity on when to discard data is needed

• Temptation is to invest in new outcomes rather than old data
  • Money is limited and may come from the same (limited) budget
Final thoughts

• Keeping all detector output is feasible but can get very expensive
  • Who pays?
  • Who are we keeping it for?
  • Is it worth the cost?

• What is the ‘raw data’ we aim to keep?
  • Photons not ADU, 1D powder …
  • For what purpose is the data being kept?

• Clarity on when to discard data is needed

• Temptation is to invest in new outcomes rather than old data
  • Money is limited and may come from the same (limited) budget

• Persistent availability of data requires persistent funding
  • What happens at the end of a 5 year project?
End