# Welcome
## to the Round Table on Large Volume Data Management!

ESRF

SRI2012

SOLEIL SYNCHROTRON

# Panel Members

**Dr. Oliver Bunk**

Swiss Light Source (SLS) at PAUL SCHERRER INSTITUT PSI

Oliver Bunk is heading the laboratory for macromolecules and bioimaging (LSB) at PSI since mid 2011. Before that time he led the coherent X-ray scattering group that operates the cSAXS beamline at the SLS. The LSB laboratory comprises several sources of high data rates, i.e. the detector, MX, X-ray tomography and coherent X-ray scattering groups.

**Dr. Eric Dooryhee**

National Synchrotron Light Source II (NSLS-II) at BROOKHAVEN NATIONAL LABORATORY

Eric Dooryhee is leading the Powder Diffraction Beamline group at NSLS-II. His science focus areas range from hybrid organic-inorganic materials, expitaxial perovskite films and multi layers, phase transitions, microstructures to cultural heritage materials. Before his assignment at Brookhaven he has worked at Neel Institute and as beamline scientist at ESRF.

# Panel Members

**Dr. Lukas Helfen**

Karlsruhe Institute of Technology (KIT)

Lukas works for the Karlsruhe Institute of Technology at the Imaging Beamline ID19 of the ESRF in order to develop and apply advanced x-ray imaging methods. Before that he worked for the Fraunhofer Institute for Non-Destructive Testing (Dresden, Germany) and from 2004 onwards for the synchrotron light source ANKA on the development of synchrotron laminography.

**Dr. Thomas Ursby**

The MAX IV Laboratory

Tomas is project manager of the future BIOMAX beamline at MAX IV. His interests cover hard X-ray optics, crystallographic methods and structural biology and instrumentation for MX.

# Panel Members

**Dr. Heinz-Josef Weyer**

PAUL SCHERRER INSTITUT

Swiss Light Source (SLS) and now SwissFEL at PSI

Heinz-Josef was for many years scientific coordinator for the SLS taking care of the user office and the development of the Web-based User Office. Since 2008 he is involved in several EU FP7 projects and driving the progress for a pan-European Authentication and Authorization Infrastructure (AAI) within EuroFEL, PaN-data, and CRISP.

# Panel Members

**Animators:**

**Dr. Cameron Kewish**
Synchrotron SOLEIL
Beamline scientist at the Nanoscopium beamline of SOLEIL

**Rudolf Dimper**
Head of the Technical Infrastructure Division at ESRF
Involved in the EU FP7 projects PaN-data, CRISP, LinkSCEEM-2

# On the menu today

- **Setting the scene**
- **Data acquisition**
- **Data storage and transport**
- **Data Policy**
- **Wrap up**

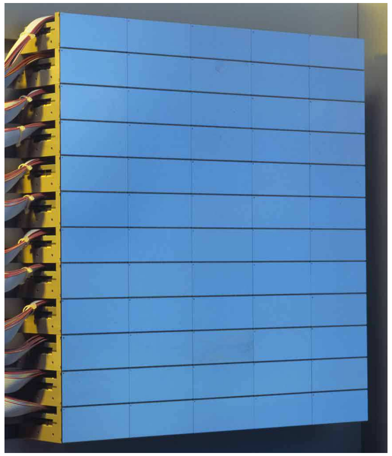
# Setting the scene




"Large Volume Data Management"

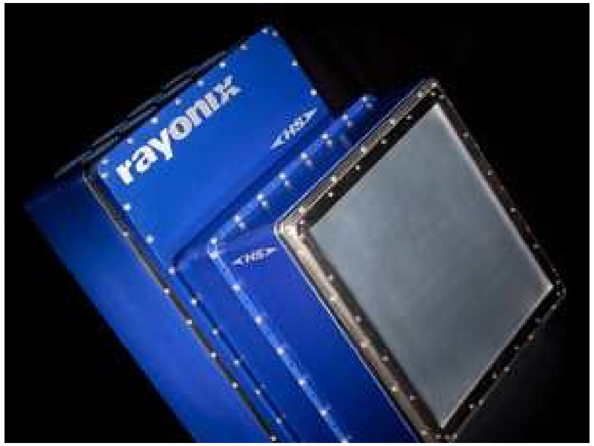
**What is large?**

- **Detectors evolve quickly**
  - Higher resolution
  - Faster readout, less dead-time
  - New experimental methods become possible
  - Single experiments can now generated **TBs of data, 100 000's of files**



Pilatus 6M


PCO dimax




Rayonix MX-340 HS

# Setting the scene

"Large Volume Data Management"

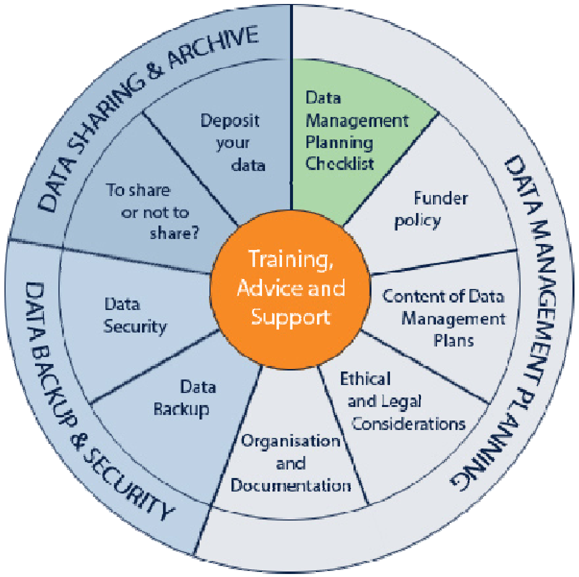
**Where is the problem?**


- **It is simply not the same to deal with 100's or 100 000's of files**
  - Latency – the time it takes to write/read/analyze data
  - Tools – to deal efficiently with the data deluge
- **Data management, i.e. a structured/organized approach to handle data is required:**
  - IT infrastructure → fast networks, data storage, backup, data analysis
  - Software → metadata capture, data catalogues, authentication, authorization, data preservation, data visualization, data analysis
  - Data policy
- **The facilities are at center stage to**
  - provide IT and data management services
  - implement a data management plan

# Setting the scene

**Data Management: data policy → data sharing → data preservation**

- ✓ Data Management is currently a hot topic
- ✓ Facilities struggle to agree and implement a data policy
- ✓ Facilities work together in PaN-data and CRISP to develop tools for data management:
  - Harmonize authentication and authorization
  - Standardize data formats and annotation of data
  - Allow transparent and secure remote access to data
  - Establish sustainable and compatible **distributed** data catalogues
  - Link data permanently to publications
  - Allow long term preservation of data
  - Provide tools/interfaces for curating data
  - Provide compatible open source data analysis software




**Source: University of Oxford**

- ✓ The IUCr has taken up the issue via its Diffraction Data Deposition Working Group (dddwg) – meeting in Bergen on 6 August

# Setting the scene



**Open Access to Data**

A remarkable report has been published by the Royal Society: "Science as an open enterprise"

Chapter 1: The purpose and practice of science

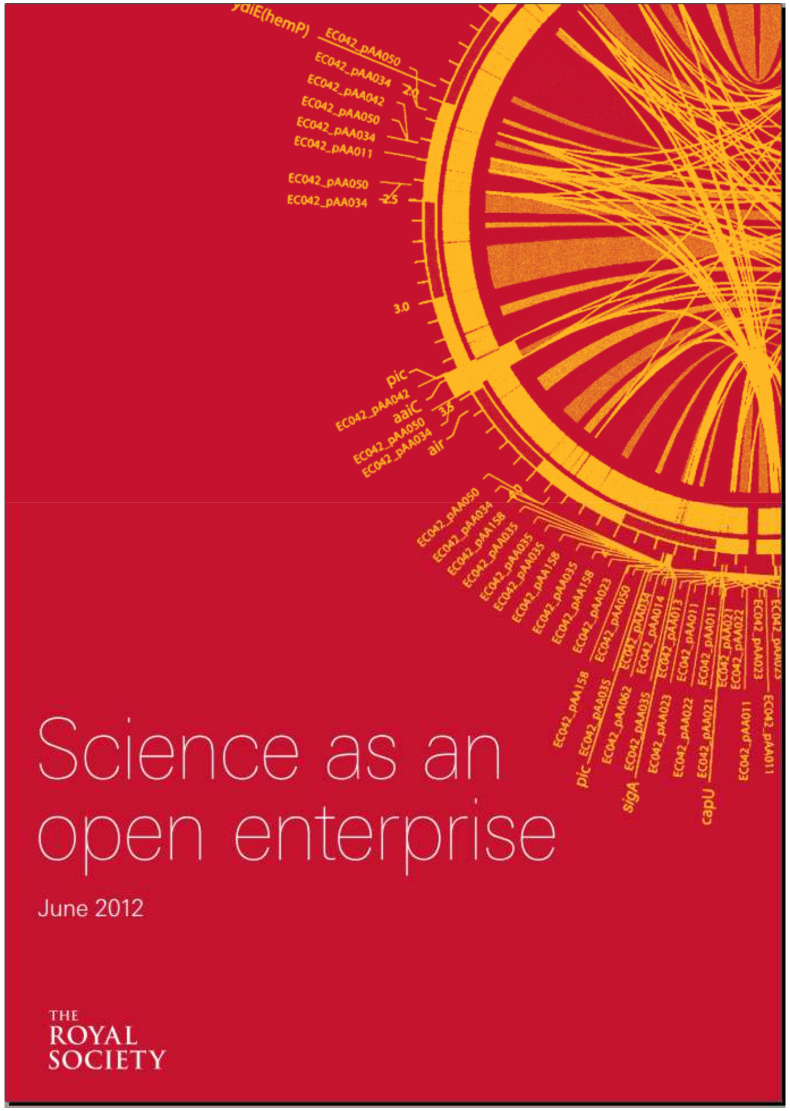
Chapter 2: Why change is needed: challenges and opportunities

Chapter 3: The boundaries of openness

Chapter 4: Realising an open data culture: management, responsibilities, tools and costs

Chapter 5 Conclusions and recommendations

10 Recommendations



# Data acquisition

The main issue at the ESRF is make the IT infrastructure evolve to get the data out of the detector (guaranteed bandwidth)

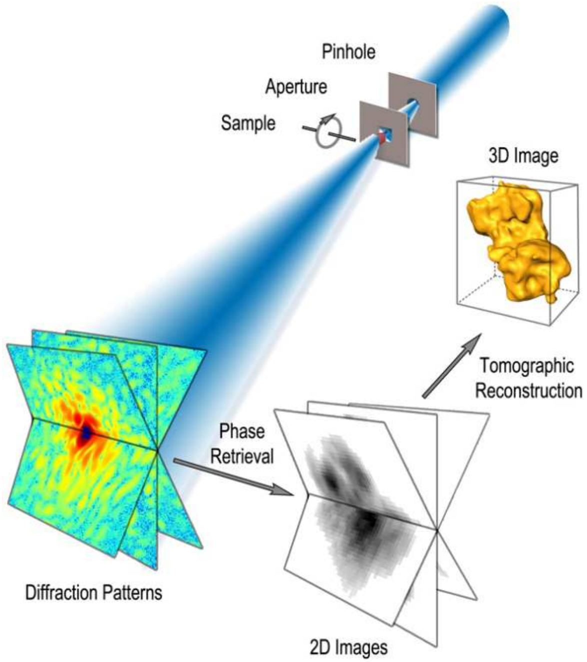
→ The Pilatus 6M detector was difficult to integrate into the ESRF IT infrastructure

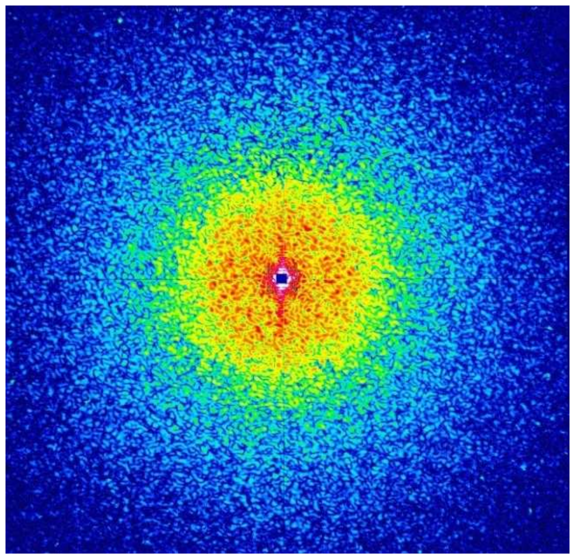
Similarly it is difficult to guarantee bandwidth for the detector readout while reading the data to perform on-line data analysis.

It will be difficult over the next years to have the funds to make the IT infrastructure evolve as fast as the detectors

# Ptychographic X-ray computed tomography at the nanoscale

- Coherent X-ray Diffraction Imaging together with ptychography at HXN or CHX has the potential to extend structural science for both crystalline & noncrystalline materials
- Optimized experiment on a 2 μm object at ~ 10 nm resolution will require a 2D area detector array with 6M pixel per frame of diffraction pattern
- Results in .1 Gb/frame and .1Tb/sec peak data rate at 1 kHz frame rate
- 3D dataset requires 100x1000 frames, leading to ~1.2 TB per dataset
- Such a dataset may be collected in 1-2 hours at NSLS-II
- Data analysis includes FFT and inverse FFT with many thousands of iterations, requiring 4x as much data during analysis



Coherent diffraction pattern from a nanoporous Au microparticle

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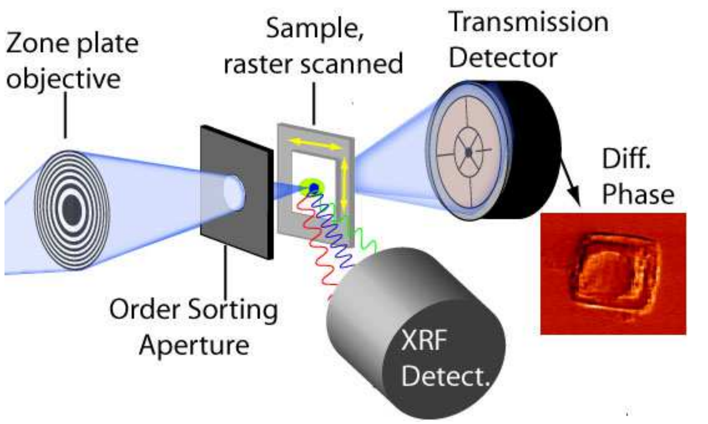
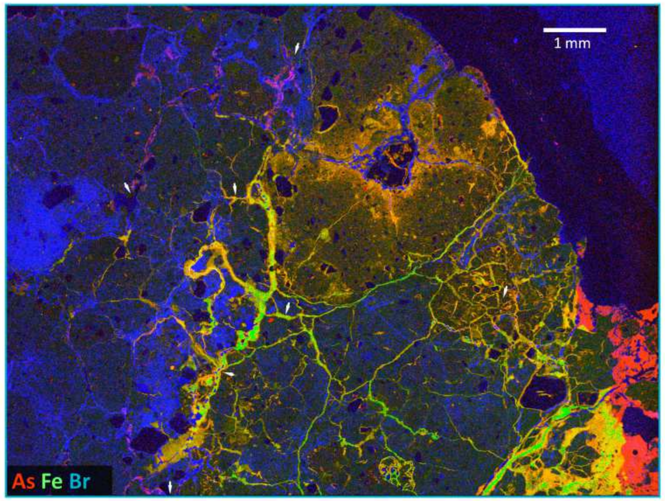
# Scanning XRF Microscopy & Tomography

- X-ray fluorescence microscopy at SRX or HXN will offer high elemental sensitivity, easy quantification, chemical state mapping, & 3D tomographic imaging
- Optimized experiment on a 10 μm biological multi-cell complex at 10 nm resolution may make use of a 400 element fluorescence detector array that covers 30% of 4π solid-angle
- Each detector element gives an energy spectrum which is digitized to 1024 channels at 12 bit dynamic range, with 0.1 ms dwell time
- This leads to a peak data rate of 400x1024x12x10000 = 50 Gb/sec
- Complete 3D dataset on the 10 μm cell complex at 10 nm resolution will consist of 1000x1000 x1000 pixels, leading to 4 TB per 3D dataset
- Such a 3D dataset may be collected in ~ 1.2 days



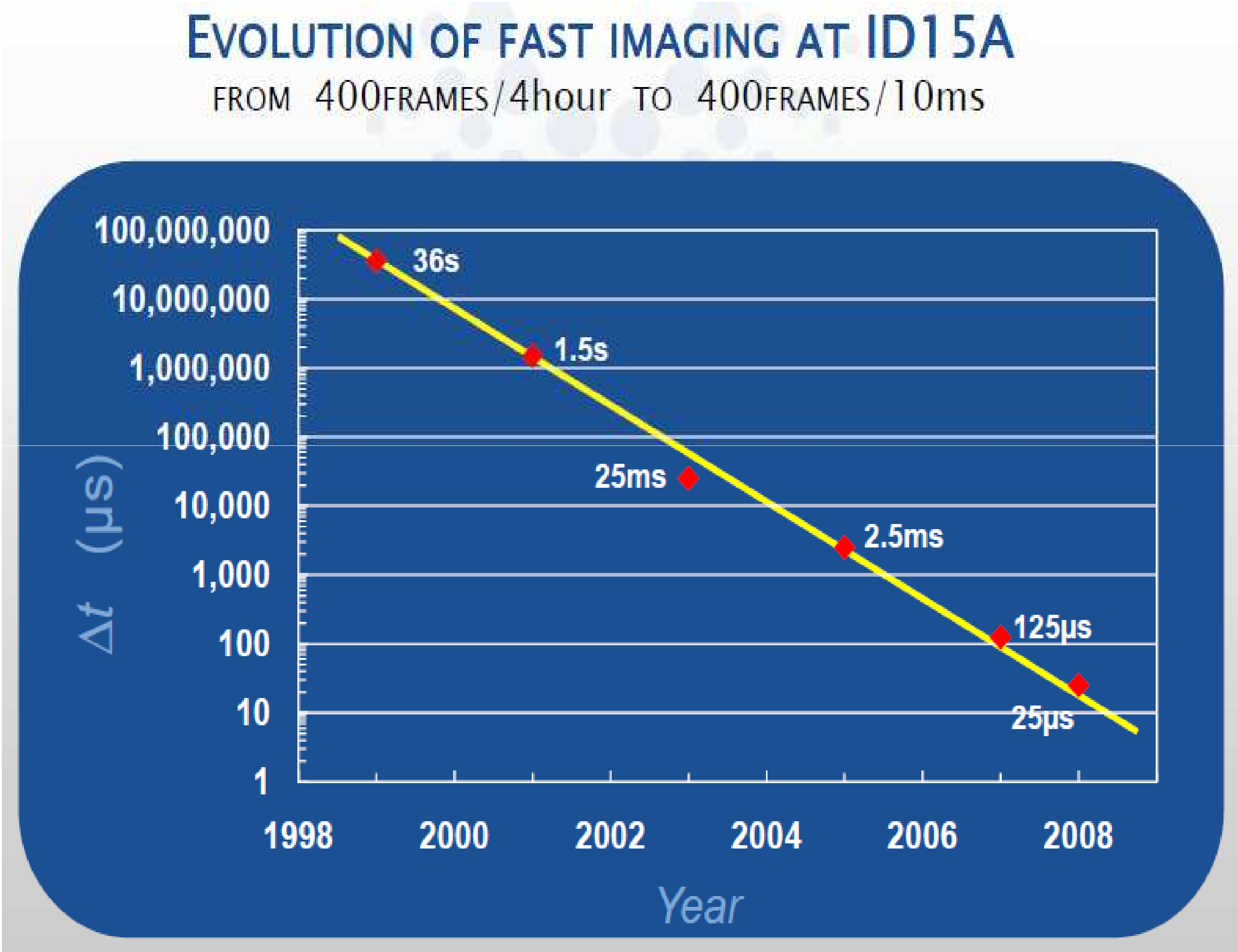
# Drivers in future Data Management

- Ultra-high brightness, flux and nanometer scale beams
  - enable new types of data intensive measurements
  - drive substantial increases in data throughput for many experiments


- Tomography
- Diffraction microscopy
- Coherent Diffractive Imaging
- Ptychography
- Fluorescence microscopy
- X-ray Photon Correlation Spectroscopy
- Macro-molecular Crystallography

- A new generation of detectors will drive higher data rates:
  - Dectris PILATUS 100k 100kpix frames @ 300Hz yields 600Mbps
  - PILATUS 6M mounts multiple 100k modules to generate up to 1500Mbps
  - Medipix2/3 (in development) 256x256 photon counting matrix – 1Gbps
  - Fast CCD cameras running up to 6000 fps @ 800x600pix
  - EIGER (prototype) 4Mpix @ up to 20kHz

# Courtesy: V. Honkimaki (ESRF)

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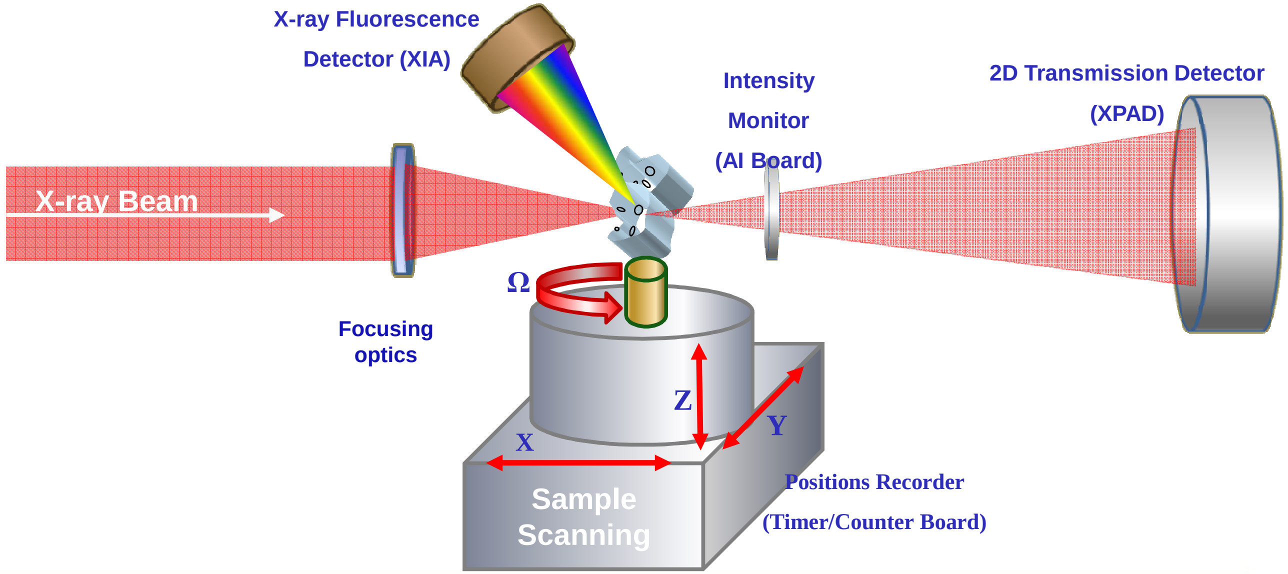
BROOKHAVEN SCIENCE ASSOCIATES

# Data management at Soleil

# Acquisition: FLYSCAN

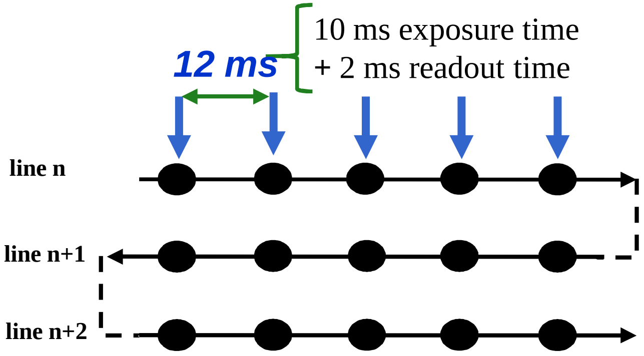
- Objective: Develop and implement a global and modular solution for experiments requiring simultaneous and correlated measurements:
  - taking data while beamline components are in motion…
    - to save time during measurements
    - to make best use of the high flux of photons
  - from several detectors in parallel (including encoders) …
    - to profit from complementary techniques (imaging, fluorescence, …)
    - to ensure temporal and spatial consistency of data between techniques



# Acquisition: FLYSCAN

- **Projected performance in megapixel differential phase contrast imaging:**

  Continuous motion along X-axis at ~0.1 mm $s^{-1}$, zig-zag scan pattern




12 sec acquisition

+ 3 s dead time (*transfer and storage of 1000 detector images*)

+ 0.5 s = time for moving between lines

➡ **Total time for 1×1 mm²**
**~ 4.3 hr**

➡ **1 map = 1 megapixel**

➡ **= $10^6$ frames**

➡ **= 150 GB**

(150 KB = detector frame + intensity monitor data + motor encoder positions)

- **Challenges:**
  - Volume of data: **~1 TB /day /beamline**

    *(Compared to current average of ~1TB /week for all Soleil beamlines combined.)*

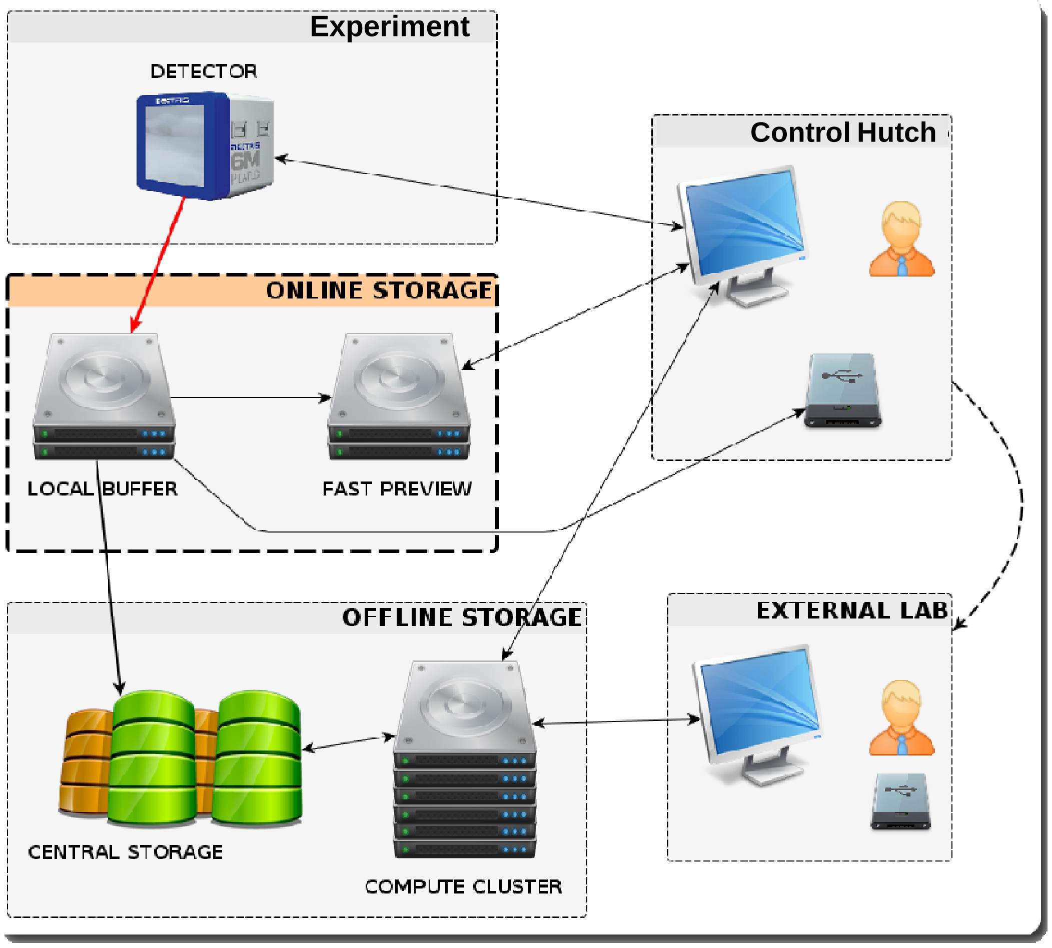
    ➡ Using a larger pixel array detector (e.g. 1Mpixel, without binning): 1 TB per map

    ➡ 5 maps /day = 1000 maps /year = **~1 PB /yr /beamline**
  - Necessity to adapt: network infrastructure, storage, online data inspection & reduction, calculation methods (e.g., GPU cluster, …)
  - How to provide access to data? Will be difficult for users to transfer/handle such volumes…
  - How long to retain data on-site? What methods of treatment…

# Data acquisition

**Requirements for fast buffer storage:**

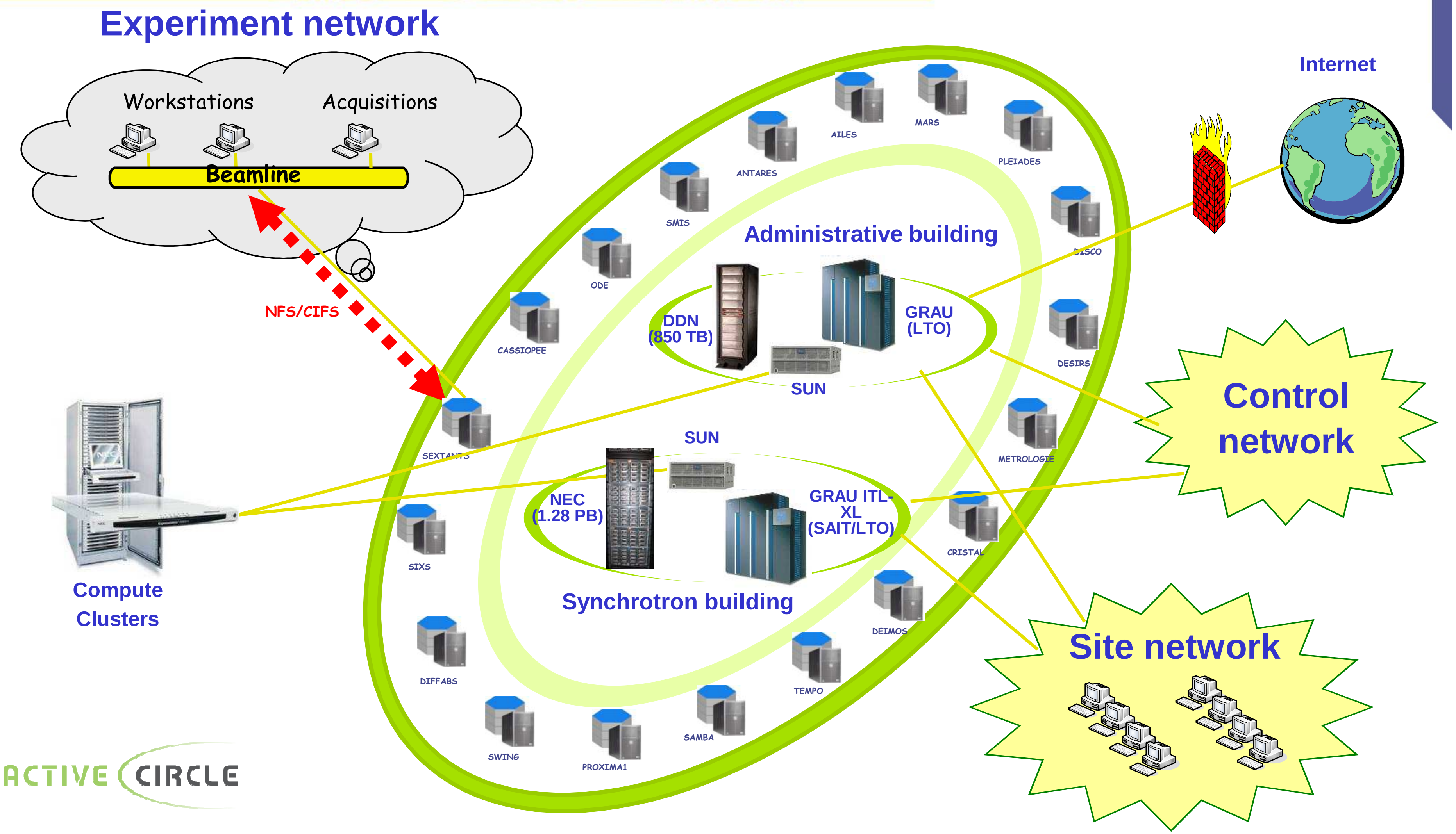
- ✓ fast preview
- ✓ 2 days capacity
- ✓ raw export
- ✓ central storage push
- ✓ multiple 10 Gbps
- ✓ NFS (V4+V3) and CIFS
- ✓ list 10 000 files < 3s
- ✓ today: write > 200 MB/s
- ✓ tomorrow: write > 1GB/s
- ✓ read ≥ write speed
- ✓ sustained performances much lower



# Data acquisition

1. What data volume or data rates are expected to be generated in the next 5 years?
2. Do we have the means (money/manpower) to keep up with the data avalanche?
3. Should facilities provide data analysis services?
4. Can we develop on-the-fly data reduction or vetoing, so that only good data are stored?
5. Would it make sense to build an EU data analysis centre for SR data?

# Soleil's storage architecture



# Soleil's storage architecture

Active Circle is used to store, protect and manage large and rapidly growing volumes of data. It aggregates heterogeneous devices into a single storage pool.

Main features:

- Hardware-independent software running on standard x86 servers
- Optimization through the use of hierarchical storage and data lifecycle management, data storage on disk or tape libraries
- Data protection and high availability provided by versioning, replication, and clustering

# Data storage and transport

- ESRF has 1.2 PB of disk storage for temporary storage of beamline data
- Users are supposed to transfer or carry away the data after their experiment
  - This becomes problematic for large data volumes:
    - Internet speed insufficient – ESRF has a 10Gbps Internet connection, but generally this is not the case of the other end
    - Copying data to USB disks may take longer than the experiment itself
    - USB-3 helps…but not for long
    - Users may be forced to leave the raw data at ESRF and do the analysis on the spot or remotely
- Users doing experiments in several facilities or coming back several times may require to keep the data on-line
- In case experiments are done in several facilities, the data format may become an issue
- Users may experience problems off-loading the data in the home lab…the same for the data analysis
- Users are not requested to think about a data management plan when submitting a proposal

# Data storage and transport

1. Where to store data (beamline, central: data centre, cloud (legal problem), grid)?
2. How to transport data from the beamlines to the users institution?
3. Is the Internet up to the task?
4. Would it make sense to contact the NRENs?
5. What is the life-cycle to consider (how long can the data be stored at the beamline)?
6. How to access data from home institution?
7. What is a reasonable response time for a request to access data?

# Soleil's current data policy

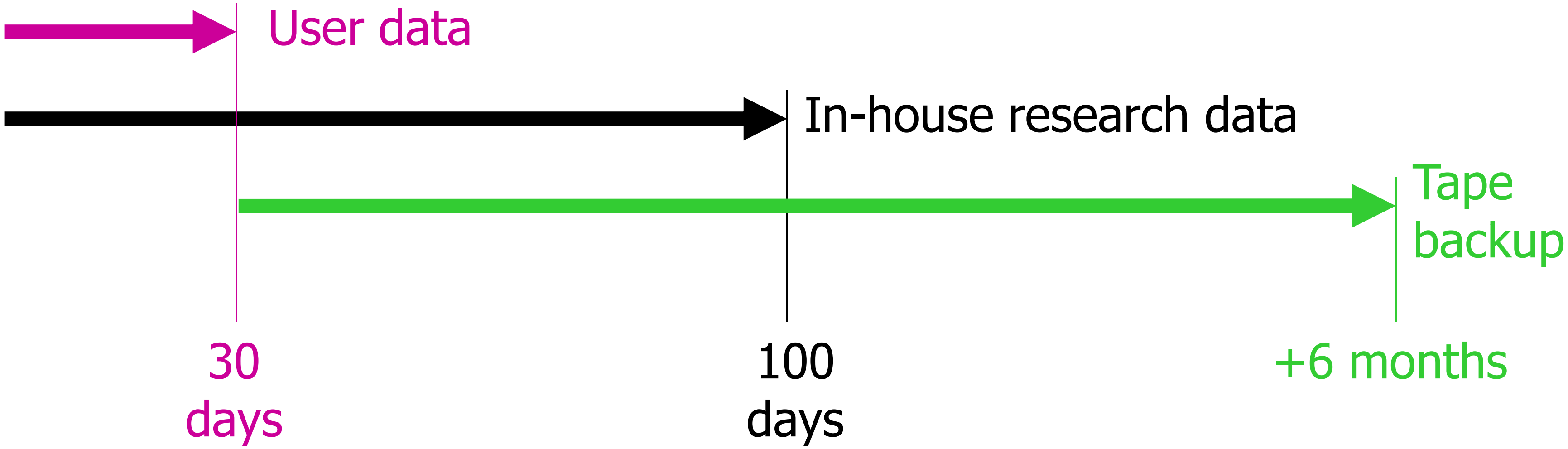
- Data is deposited on the beamlines storage point (or HPC facility)
- 4 Copies are immediately made in 2 separate server rooms on site:
  - 2 on disk arrays, and 2 on tape libraries
- Data is kept (if possible) at least 4 days locally, and until space is required
- After 100 days, the 2 disk copies expire; the 2 tape copies are kept
- The 2 tape copies expire after further weeks, months or years depending on the beamline and the file system (as contracted).
- At any time, users can request for their data to be archived
- Following each technological disruption, the beamline leader and IT department analyze which data are to be restored from backup

# Soleil's current data policy

- Data belongs to the owner of the sample
- Data access is restricted to the experiment account/proposers
- Other access modes are the subject of internal discussion…

- For the future: we are discussing
  - How long can the facility preserve data under heavy load?
  - Whose responsibility is it to process the data, or provide tools?
  - What happens in special cases, extra-long term proposals, proprietary beam use?

## ESRF's current policy for storing scientific data

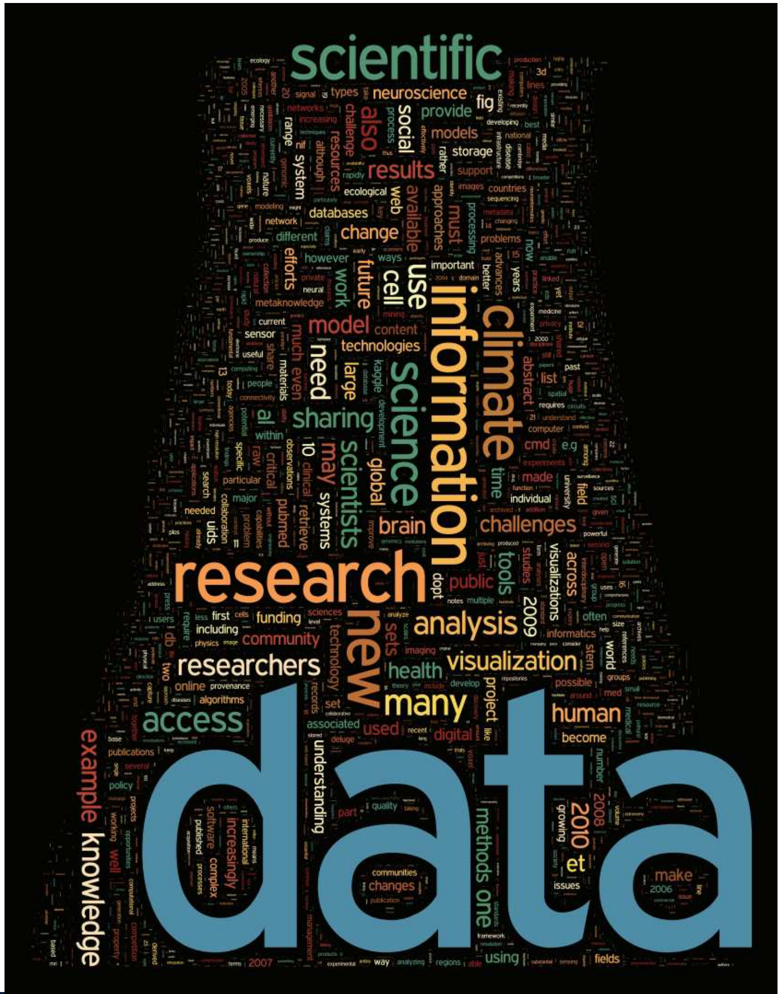



- **After 6 months all data has disappeared from our central storage!**
- **Archiving of the data is currently left to the users!**

# Data policy

- scientific data is often (almost always) considered private property
- open access to scientific data is almost impossible
- scientific data is not managed professionally
- Consequence:
  - invaluable data sets are lost or inaccessible
  - Re-analysis is impossible
  - Publications and data are not linked
- barriers to interact with data must be lowered

- Data must be made accessible and useable



# Data policy

- The ESRF struggles to adopt the PaN-data data policy
- Internal discussion continue about the:
    - Embargo period
    - Effort required to enter metadata information
    - Cost of building a publicly accessible data repository
    - Legal issues, e.g. liability

# Data policy

1. Who owns the data?
2. Should data be professionally preserved and why? For how long?
3. Should all data be preserved?
4. If not, who will decide which data to preserve?
5. Should data become open access after an embargo period?
6. Does this apply to ALL data, and if not, who decides?
7. How long should an embargo be to allow sufficient time for analysis/publication, yet open the data while still scientifically relevant?
8. Is it problematic to combine data generated at different facilities for analysis?

# Outlook/Summary

NSLS II will immediately have to deal with large data volumes (100k files)

1.2 TB/dataset x 4 for just one experiment

50TB/day → 10-11PB data storage facility

Soleil: Nanoscopium beamline → 1TB/day/beamline, larger detectors will generate even more

Panel Discussion:

- ✓ We should implement data management plans prior to the experiment. Also, reduction of data volume prior to storage via filtering, for example as is done in particle physics.
- ✓ Data preservation could be pragmatically limited to the life-time of the storage technology
- ✓ Data storage for ever could be interesting so that other groups can re-process published data. The policy could vary between small and large data beamlines.
- ✓ Good discussion on metadata: will it be possible to store enough meta data to reuse data sets? Must be automated, is difficult, very dependent on the experiments. Metadata should also include processing steps.
- ✓ EU wide central storage? It would be simpler to make public files available worldwide but stored at home.
- ✓ Embargo period could be minimum the duration of a PhD thesis, to allow time for the processing prior to opening the data. The cost of storage could be prohibitive.

# Thank you
# for your participation!

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