TALK OUTLINE

Who we are

User community

Example experiments

What our users need

Data analysis as a Service

How to get there with e-infrastructures

Conclusion
PHOTON AND NEUTRON SOURCES + COMMUNITY

- 10 photon sources
- 7 neutron sources
- Represents ~40,000 users/year
- PaN is not CERN
PHOTON AND NEUTRON SOURCES
HOW DOES A SYNCHROTRON WORK
PAN USER COMMUNITY

• Counted users between 2012 + 2014: see http://pan-data.eu/Users2012e-Results for details

• Total of 38338 users of which 14347 new each year
PAN USER COMMUNITY

- Counted users between 2012 + 2014: see http://pan-data.eu/Users2012e-Results for details
- Total of 38338 users of which 14347 new each year
PAN USERS COUNTRY DISTRIBUTION

France
Germany
United Kingdom

Other countries include:
- United States
- Italy
- United Kingdom
- France
- Germany

Countries with smaller percentages include:
- Slovakia
- Turkey
- Ukraine
- Greece
- Estonia
- South Africa

Countries with very small percentages include:
- Afghanistan
- French Guiana
- Guam
- Macau
Two quite different types of data analysis tasks:

- **Analysis of experimental data (~3/4)**
  - processing time / dataset typically short (seconds)
  - but large amounts of data (10 TB / day)
  - difficult to move data off site e.g. cloud (so far)

- **Theoretical calculations and modeling (~1/4)**
  - small amounts of input+output data (a few GB max)
  - but long processing times (80 cores for 5 days not uncommon)
  - not difficult to move to cloud

→ theoretical calculations and modeling are candidates for cloud
• 499 experiments produced:

4 PetaBytes in 2016

• Data volume is growing each year

• Next generation experiments can produce 10 PB in 1 week
EXAMPLE – DIAMOND DATA SINCE 2007

Total Data Archived at Diamond Light Source

- Data in GB
- Dates from Jan 07 to Jan 15
- Total data archived by Jan 16: 5,779,087 GB
1. Data management and policy
2. Medium to Huge and increasing data volumes
3. Helping (new) users to analyse their data
4. Developing Data Analysis as a Service
5. Software development resources
6. Integrating private and public clouds
7. PAN community not well known
8. How the e-infrastructures can help

Conclusion
MULTIPLE DATA BOTTLENECKS

1. Acquiring data from detectors to storage (Gigabytes/s)
2. Reducing data online fast enough (Gigabytes/min)
3. Analysing data fast enough (Terabytes/day)
4. Getting results to users efficiently (Giga to Terabytes)
5. Scientific + infrastructure software bottleneck ...

REDUCING THE BOTTLENECK EFFECT:
"What we're trying to do here is expedite the time to discovery. Scientists should be able to focus on their science without having to become experts in data management."

—Shawn McKee
research scientist in physics

credit: http://arc.umich.edu/
PARALLEL ALGORITHMS + DEVELOPERS NEEDED

- PyFAI – radial integration
- PyMCA – multi-variate analysis
- PyNX – ptychography
- PyHST – tomography
- XPCS – coherent diffraction correlation
- List keeps on growing …
- Parallel programming on GPUs / CPUs with MPI / OpenCL / OpenMP requires specialised skills
PyFAI – radial integration code (pyfai.readthedocs.org)

Hosted on GitHub: https://github.com/pyFAI/pyFAI
- 23000 lines of Python (plus 5000 for the test)
- 8000 lines of Cython which are converted into ... C (about half a million lines)
- 5000 lines of OpenCL kernels

4 years of almost constant development – speedup, new detectors, ...
Probing the structure of heterogeneous diluted materials by diffraction tomography
Pierre Bleuet, Eléonore Welcombe, Eric Dooryhée, Jean Susini, Jean-Louis Hodeau & Philippe Walter
Data rate = 250 Hz
Experiment = 1 week
Sample volume = $1000^3$
Data volume = 10 PB
Have to reduce data online to < 10 TB
Use PyFAI accelerated on GPU to reduce data in realtime a factor of 1000
Main issues are
- How to develop maintainable software
- How to avoid scientific software developers wasting time developing non-scientific software e.g. gui code, input/output, standard algorithms
- How to get developers to adopt best practices

ESRF approach
- Develop a common library which implements common low-level functionality
- Use best practices (unit tests, continuous integration, documentation, …)
- Python-based, C++ for speed, Open Source, simple licence (MIT), Github
- Hire software engineers to develop the library
- Build scientific applications on top
- Encourage collaborations

Sustainability
- The library saves development time + improves maintenance of scientific applications
TOOLKIT APPROACH
Open Source development model works!
Conclusion: need a similar effort for web applications
USE CASE – RECIPROCAL SPACE STRAIN SCANNING

- **Kmap** – strain scanning
- **Experiment** = 10 minutes
- **Sample size** = 100x100 um
- **Resolution** = 100 nm
- **Data reduction** = 10 hrs
- **Data analysis** = bottleneck for users i.e. needs specialist

**Solution** : hire data scientist for 18 months to rewrite scientists application

*Figure 8*
(a) Two-dimensional map distribution of the tilt magnitude (°) and (b) directional representation (arrows) of tilted [001] atomic planes with respect to the sample surface normal.
USE CASE – RECIPROCAL SPACE STRAIN SCANNING

- Financing = IRT-Nanoelec
- File format = HDF5
- Optimise = legacy code
- Execution = 2 minutes
- Speedup = 300 times!
- Next step = make available remotely as a service
- Long term = new program is based on SILX and therefore easier to maintain

Scientist: « Amazing - I have never seen my data like this! »

Conclusion: hire more data scientists to rewrite scientific application + do similar effort for web applications
MANY DIFFERENT USE CASES

- **Life sciences** – single crystal diffraction, and (soon) cryo electron microscope
- **Spectroscopy** – small to medium sized data sets, lots of modelling (DFT calculations)
- **Small Angle Scattering** – medium data sets but lots of modelling (Molecular Dynamics)
- **Coherent diffraction** – large data sets + iterative processing
- **Tomography** – currently the main data producer (<80%) has the highest needs in terms of data processing
- **Cultural heritage**: archeology, paleontology
Fast synchrotron tomography at KIT

- Fast high-throughput synchrotron-based X-ray tomography for material science, biology & paleontology

- ASTOR virtual infrastructure (astor.kit.edu)
  - Virtual analysis infrastructure based on cloud technology
  - Remote access for external users
  - Automated segmentation tools

- Example: Digitalization of 30 million-year-old phosphatized insects
  - Collections from the Natural History Museums Basel & Stockholm
  - Datasets scanned in one week: 1408
  - Data created: ~ 79.2 TB (without post-processing!)
    - raw data: ~36.3 TB
    - reconstructed tomograms: ~ 42.9 TB

DATA POLICY

- What about Data Policy and PaNs?

- PAN RIs had no open data policy prior to 2011

- PANDATA-EUROPE (FP7) deliverable produced a generic open data policy
  (http://wiki.pan-data.eu/imagesGHD/0/08/PaN-data-D2-1.pdf)
• PaN-Data Open Data Policy now accepted

• First adopted by neutron sources:
  – ISIS and ILL

• Then adopted by photon sources:
  – ELETTRA, ESRF, HZB, PSI

• Other sources following:
  – ALBA, DESY, XFEL, …

• Just in time for Springer + Nature journals
• ESRF is custodian of data and metadata
• ESRF to collect high quality metadata to facilitate reuse of data
• ESRF will keep metadata forever
• ESRF will keep raw (or reduced) data for 10 years
• Data will be registered in a data catalogue (ICAT)
• Data will be published with a Digital Object Identifier (DOI)
• The experimental team has exclusive access to data during the embargo period (3 years which can be extended on request)
• Data will be made public after the embargo period under licence CC-BY 4.0
• Data Policy will be implemented on all beamlines by 2020
• **Volume**
  - 100s of Petabytes for each RI over 10 years

• **Cost**
  - Hundreds of thousands euros per year

• **Metadata**
  - Big effort to define metadata (years) but can be shared

• **Open access**
  - Scientists are encouraged by Journals + H2020

• **Reusability** – depends on metadata
Many data sets are medium to small
How to go from Infrastructure to Platform to Software to Data Analysis as a Service?

IAAS → PAAS → SAAS → DAAS

e-infrastructures / commercial clouds

RI(s)
SETTING UP PRIVATE CLOUD MODEL

MAIN BOTTLENECK IS SOFTWARE !!!
Photon and Neutron Data Analysis as a Service is a common proposal between all synchrotrons + neutron sources in EU (not funded).
The need for Data Analysis as a Service has not gone away – instead it has got stronger

Photon and Neutron sources are working on it with own resources

ESRF continues to play the rôle of coordinator for PANDAAS

Organised followup meetings:
- July 2016 @ ESRF
- December 2016 @ ESRF
- ESRF to present PANDAAS @ e-IRG meeting next week
- Activities reported here: http://pan-data.eu/node/103

Currently active tasks:
- Packaging scientific software with Docker containers
- Setting up and giving users access to private clouds
- Testing commercial cloud services (AWS, HNSciCloud, …)
• Amazon provides HPC resources → why not use them?

• Check out https://aws.amazon.com/hpc/

• AWS `cfncluster` script allows us to create an HPC cluster in 10 minutes with pre-installed MPI, fast interconnect, batch scheduler, ...
## Results of tests:

<table>
<thead>
<tr>
<th>Software</th>
<th>Intel Cpu ESRF clock, #cores</th>
<th>Intel Cpu AWS clock, #cores</th>
<th>elapsed time ESRF</th>
<th>elapsed time AWS</th>
<th>time ratio ESRF / AWS</th>
<th>theory speed AWS / ESRF</th>
<th>cost AWS</th>
</tr>
</thead>
<tbody>
<tr>
<td>FDMNES</td>
<td>E5-2680 2.7 GHz, 16</td>
<td>E5-2666 v3 2.9 GHz, 8</td>
<td>17 h 14 min (1034 min)</td>
<td>24 h 57 min (1497 min)</td>
<td>0.69</td>
<td>0.70 (0.5 * 1.07 * 1.3)</td>
<td>26.73 $ (25.0 * 1.069)</td>
</tr>
<tr>
<td>FDMNES</td>
<td>as above</td>
<td>E5-2666 v3 2.9 GHz, 10</td>
<td>as above</td>
<td>20 h 17 min (1217 min)</td>
<td>0.85</td>
<td>0.87 (0.625 * 1.07 * 1.3)</td>
<td>43.40 $ (40.6 * 1.069)</td>
</tr>
<tr>
<td>Geant4</td>
<td>E5-2680 2.7 GHz, 16</td>
<td>E6-2670 v2 2.5 GHz, 8</td>
<td>2 h 05 min (125 min)</td>
<td>3 h 42 min (222 min)</td>
<td>0.56</td>
<td>0.60 (0.5 * 0.93 * 1.3)</td>
<td>5.92 $ (3.7 * 1.60)</td>
</tr>
<tr>
<td>Geant4</td>
<td>as above</td>
<td>E6-2670 v2 2.5 GHz, 16</td>
<td>as above</td>
<td>1 h 54 min (114 min)</td>
<td>1.10</td>
<td>1.21 (1.0 * 0.93 * 1.3)</td>
<td>6.08 $ (1.9 * 3.201)</td>
</tr>
<tr>
<td>Quanty</td>
<td>E5-2680 2.7 GHz, 4</td>
<td>E5-2666 v3 2.9 GHz, 2</td>
<td>5 h 40 min (340 min)</td>
<td>7 h 38 min (458 min)</td>
<td>0.74</td>
<td>0.70 (0.5 * 1.07 * 1.3)</td>
<td>2.03 $ (7.6 * 0.267)</td>
</tr>
<tr>
<td>Quanty</td>
<td>E5-2680 2.7 GHz, 8</td>
<td>E5-2666 v3 2.9 GHz, 4</td>
<td>4 h 33 min (273 min)</td>
<td>5 h 32 min (332 min)</td>
<td>0.82</td>
<td>0.70 (as above)</td>
<td>2.94 $ (5.5 * 0.534)</td>
</tr>
<tr>
<td>Quanty</td>
<td>E5-2680 2.7 GHz, 16</td>
<td>E5-2666 v3 2.9 GHz, 8</td>
<td>5 h 09 min (309 min)</td>
<td>5 h 33 min (333 min)</td>
<td>0.93</td>
<td>0.70 (as above)</td>
<td>5.99 $ (5.6 * 1.069)</td>
</tr>
<tr>
<td>Quanty</td>
<td>as above</td>
<td>E5-2666 v3 2.9 GHz, 18</td>
<td>as above</td>
<td>6 h 26 min (386 min)</td>
<td>0.80</td>
<td>1.60 (1.125 * 1.07 * 1.3)</td>
<td>13.68 $ (6.4 * 2.138)</td>
</tr>
</tbody>
</table>

### Remarks:
1) the ESRF computer have 1 thread / core, the AWS comuters have 2 threads / core (i.e. hyperthreading)
2) theory speed: cores(AWS / ESRF) * clockrate(AWS / ESRF) * (estimated speedup hyperthreading)
3) the second FDMNES run on AWS used 10 cores of 2 nodes with 8 cores each
4) the nodes used in all Quanty runs at the ESRF have 16 cores, but only part of them were used
5) AWS prices are "on demand prices" for the region "EU Frankfurt", excluding taxes
• **Conclusions from AWS cloud tests**
  - Cloud is adapted for HPC applications
  - AWS HPC offer is easy to use and adapted to our needs
  - Could be used to absorb peak demand for HPC @ ESRF

• **Issues still to solve**
  - How to optimise best price
  - How to manage access + budget / user
  - How to transfer large volumes of data to cloud
  - How to make it even easier for our non-cloud savvy users e.g. portal

• **Hype about cloud is not just hype …**
  - See Viewpoint in Cern Courier « *End of steam age of computing* »
    by *Eckhard Elsen* CERN director for research and computing
Web notebooks provide easy access to data + algorithms for users familiar with scripting e.g. Python

« UGA 2.0 la science augmentée » project submitted to IDEX
• Organise yourselves!
  - PaN-Data collaboration ([http://pan-data.eu](http://pan-data.eu))

• Elaborate on and drive their e-infrastructure needs
  - PaN-DaaS project (but lack of funds)

• Participate in the innovation of e-Infrastructure services
  - Participate in HNSciCloud, AWS, e-IRG ...

• Contribute to standards and take care of their data
  - Adopting Open Data Policies, Nexus/HDF5
EOSC AND PAN-DATA

- EOSC is proposed to be a federation of services, but not clear what services will be useful for Photon and Neutron source users.

- PaN-Data trends:
  - Large data volumes + Open data policy will mean data stays at the sources in the future.
  - Compute power to be at sources i.e. most PaN RI’s will set up private clouds.
  - Assist users to move data+software to commercial/public cloud where possible.
  - Need domain specialists to (sup)port software.
PAN-DATA COMMONS IS HAPPENING

- Common users
- Common technology
- Common techniques
- Common software
- Common (meta)data
- Common catalogues
- Common data policy
- Common data analysis service
- Common e-infrastructure needs
E-INFRASTRUCTURES AND PAN-DATA

• E-IRG Roadmap
  − Good proposals but very high level

• e-infrastructures
  − No interaction so far (except GEANT indirectly),
  − Not sure how scalable e-infrastructures are to cater for PaN-Data community and all the others
  − Easier to get IaaS from commercial companies
  − What could e-infrastructures provide that commercial companies don’t and which Ris need? Expert advice + help with software development

No mention of PaN-Data community in roadmaps / white papers
CONCLUSION

• PaN-Data community is adopting best practices in data management to create a Data Commons and enable Open Science

• Data analysis of synchrotron and neutron data is a major bottleneck for users (TBs to PBs)

• Providing Data Analysis as a Service (PaNDaaS) is still a strategical issue, work continues very slowly but PaN community needs funds for developing DaaS

• e-infrastructures are not seen as service providers but could be advisors on how to setup e-infrastructures, hybrid clouds and develop SaaS/DaaS