



# *The ESS Data Management and Software Centre*

*Getting the most out of data*

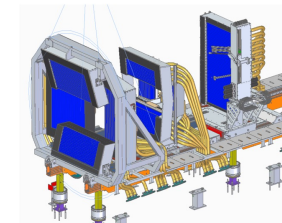
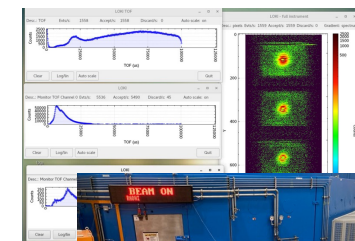
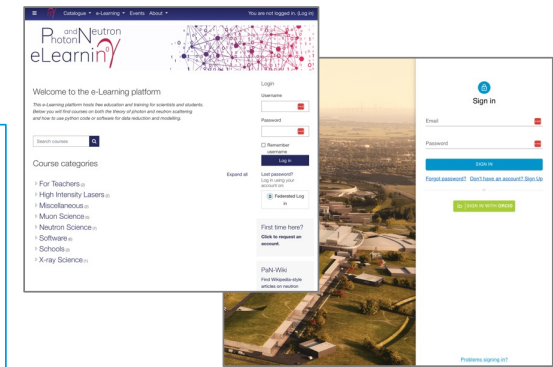
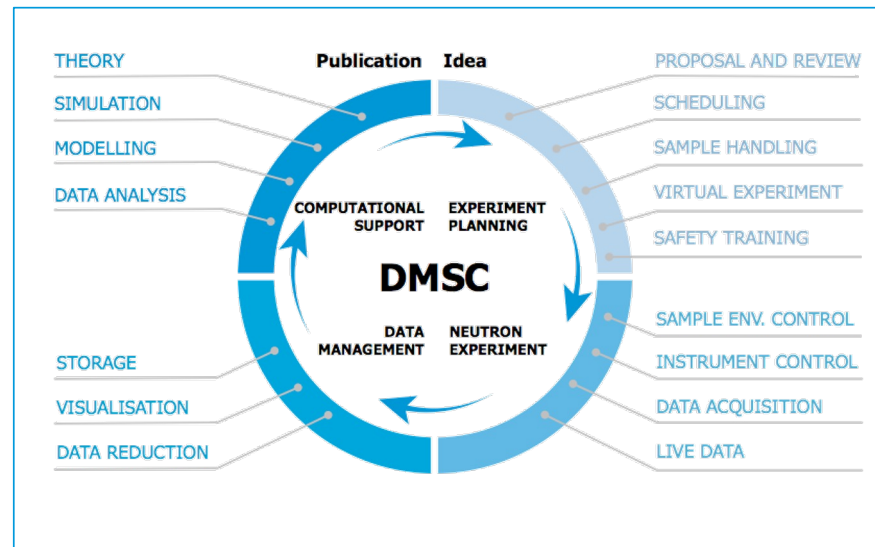
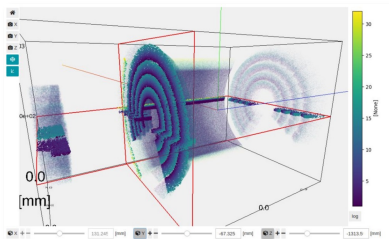
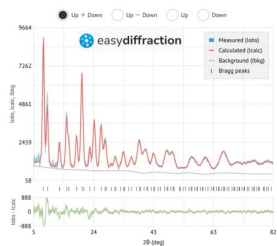
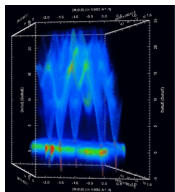
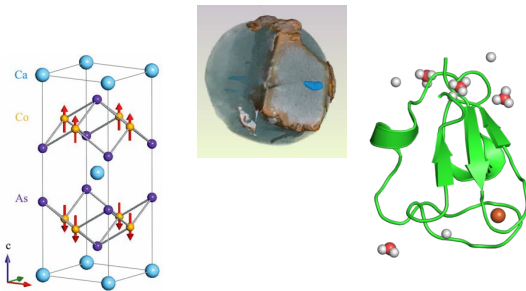
THOMAS HOLM ROD, HEAD OF THE DMSC DIVISION

# Technical Design Report (2013)

Importance of computing was emphasized already in design phase



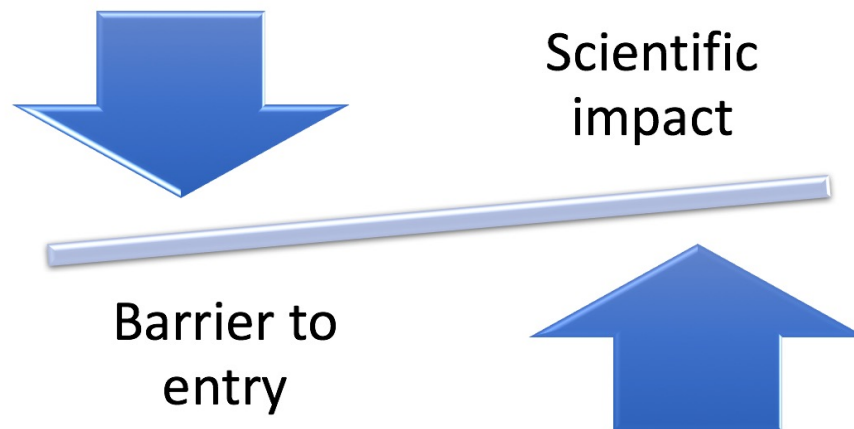
Support user from idea to publication with scientific computing tools & services



# DMSC objective



Minimise the time it takes to analyze and interpret experimental data



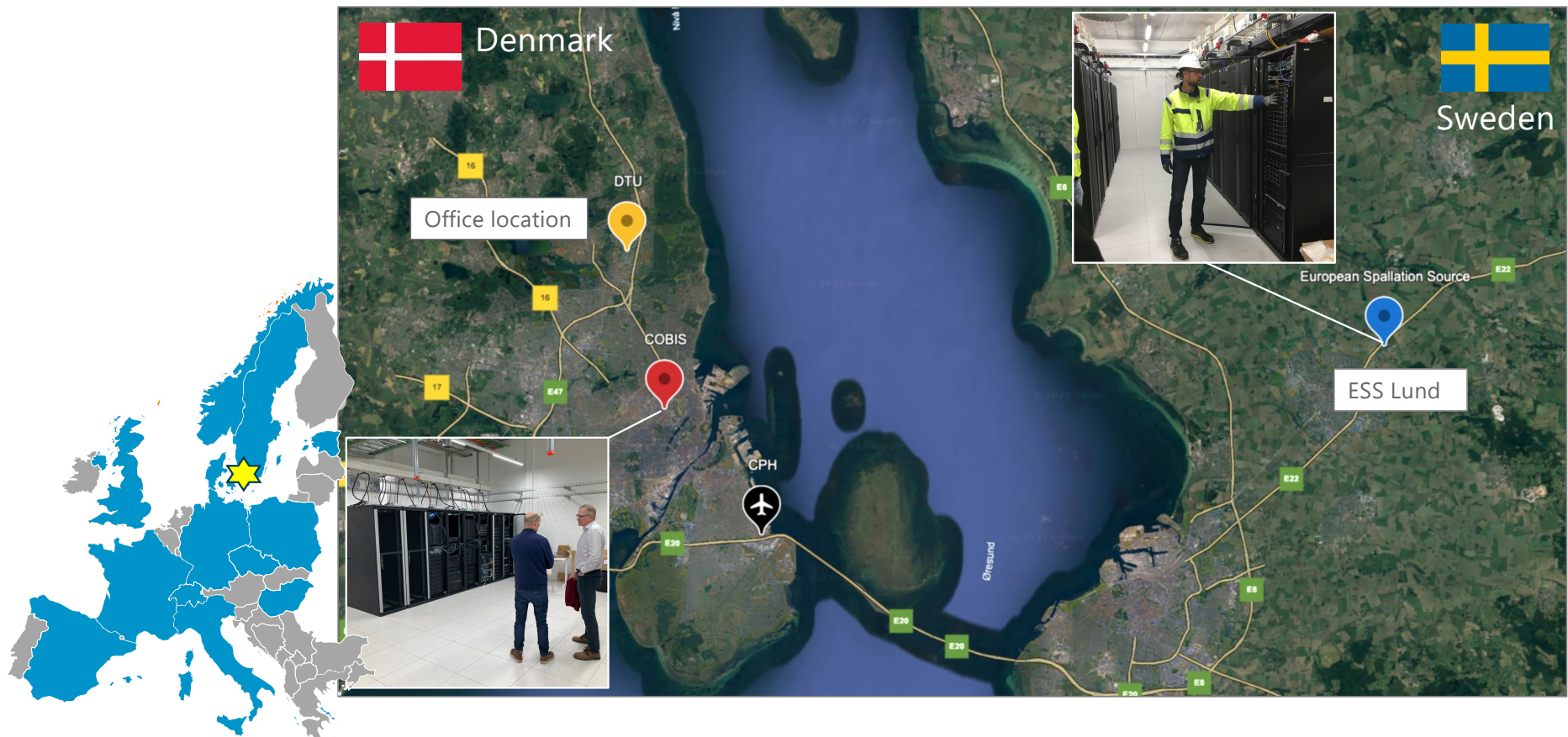
This is particular important for neutron sources due to the cost of producing neutrons

Maximise the scientific impact and success of ESS by serving the needs of both non-expert and advanced users



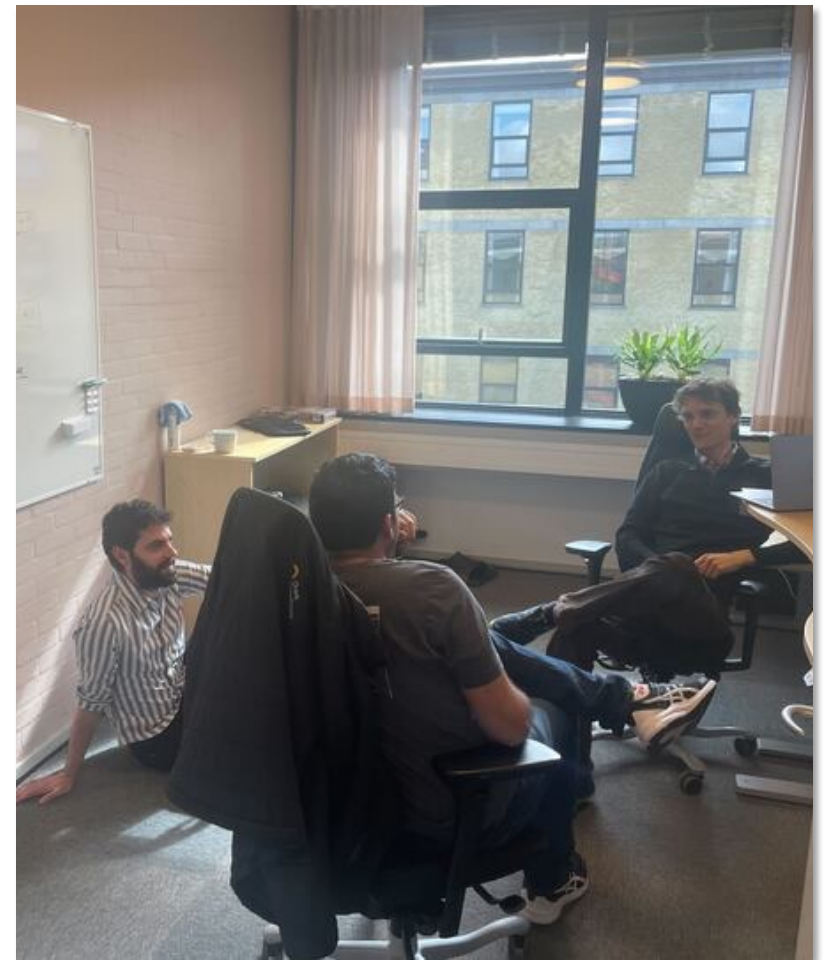
# ESS has two host nations

DMSC is located in Denmark



# New DMSC offices

In the campus of Technical University of Denmark





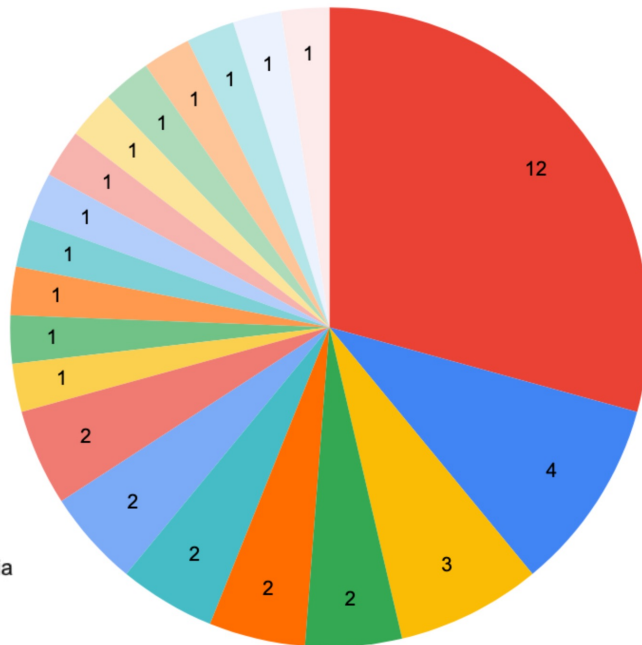
# Who are we at DMSC?

DMSC has attracted highly skilled staff internationally

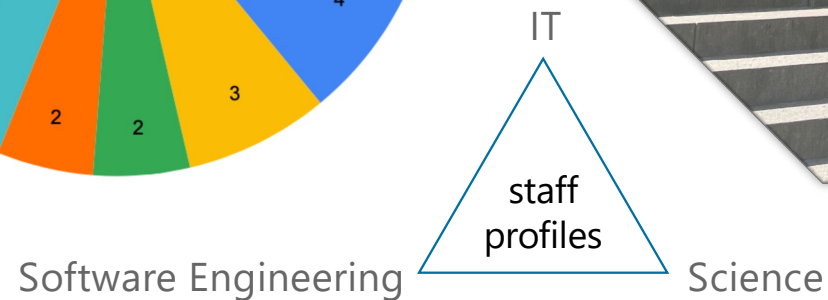
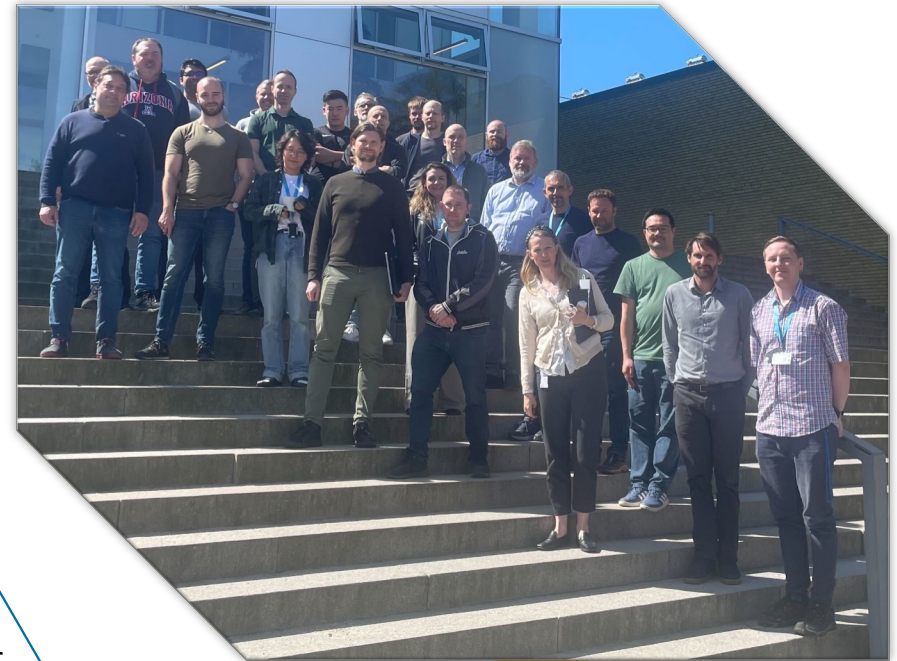


## Nationalities

- Denmark
- Sweden
- Germany
- France
- Hungary
- India
- UK
- USA
- Australia
- Belarus
- Brazil
- Bulgaria
- China
- Iceland
- Italy
- North Macedonia
- Poland
- Romania
- South Korea



41 staff members (incl. ECDC-DK, consultants and student workers)

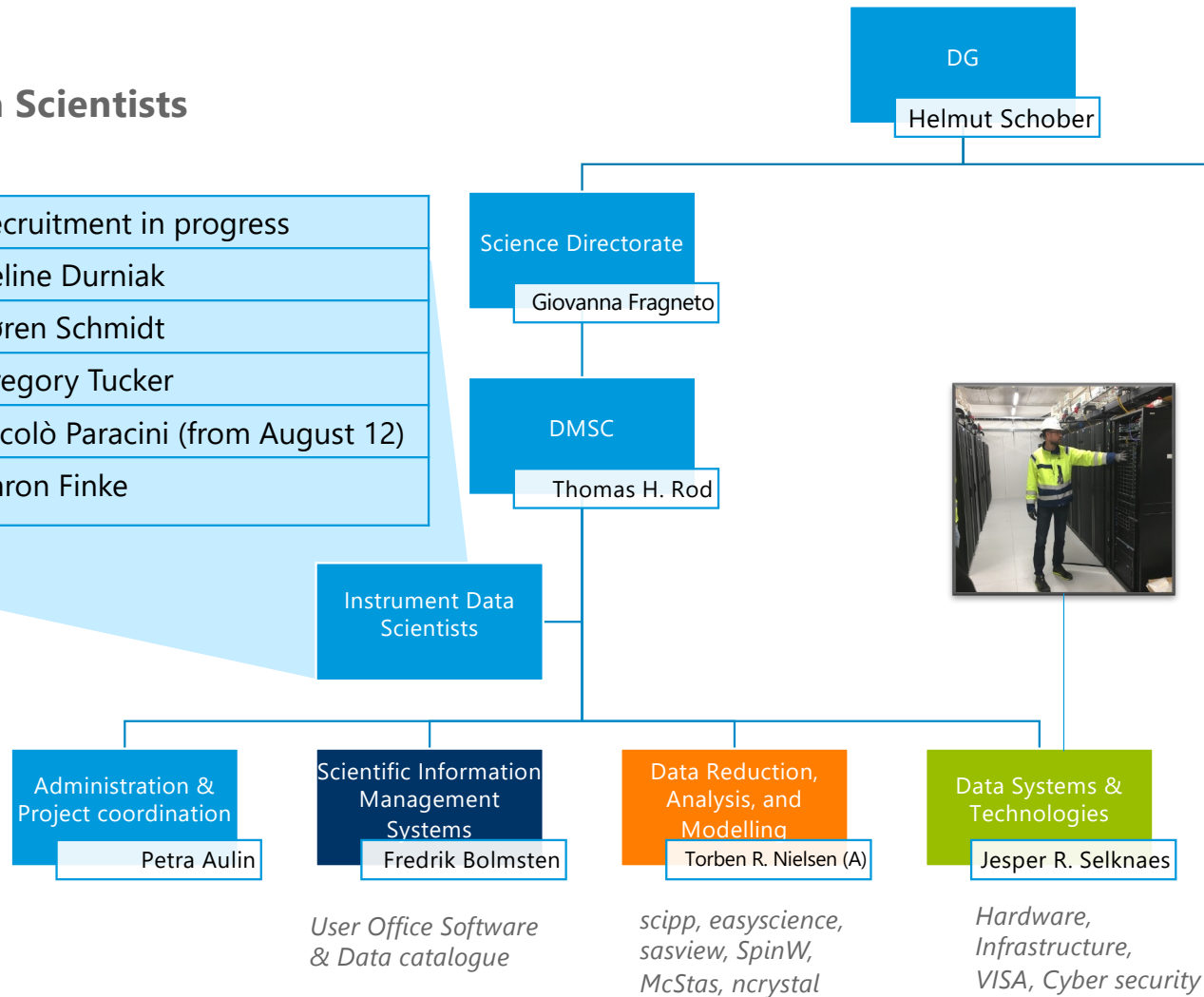


# DMSC organisation



## Instrument Data Scientists

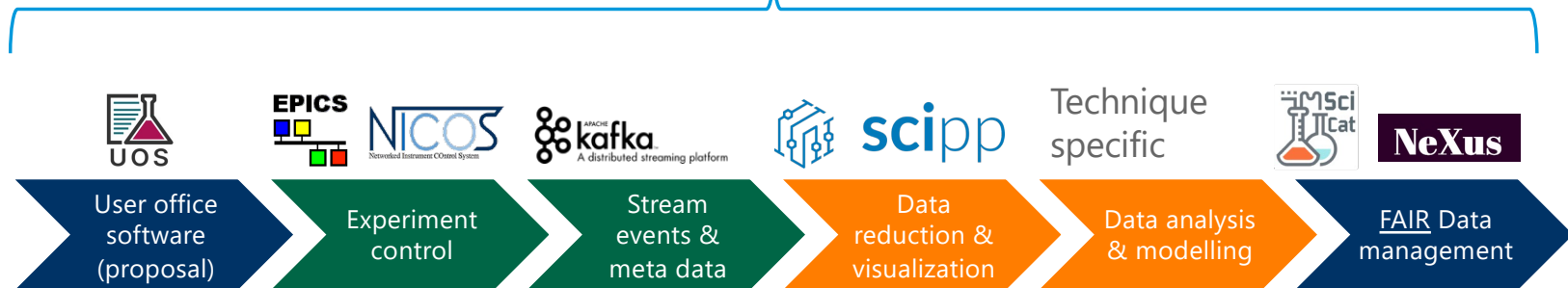
<b>LOKI</b> (& SKADI)	Recruitment in progress
<b>DREAM</b> (& MAGIC)	Céline Durniak
<b>ODIN</b> (& BEER)	Søren Schmidt
<b>BIFROST</b> (& CSPEC)	Gregory Tucker
<b>ESTIA</b> (& FREIA)	Nicolò Paracini (from August 12)
<b>NMX</b>	Aaron Finke



# Integrated data pipeline for each instrument

## Instrument Data Scientists:

- Interface to instrument teams
- Customization to instruments
- User support



## Data Systems & Technologies:



# Integrated data pipeline for each instrument

## Instrument Data Scientists:

- Interface to instrument teams
- Customization to instruments
- User support



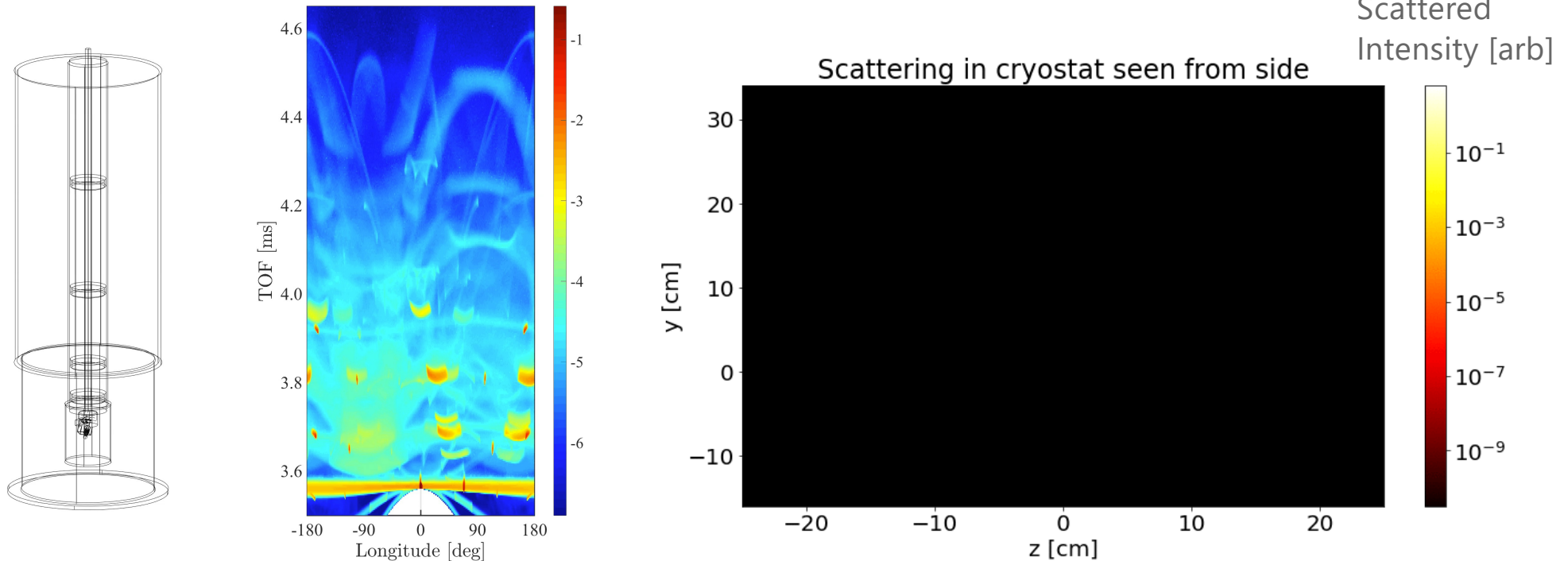
## Data Systems & Technologies:



Remote Access



# Simulating experimental artefacts



Library of instrument models and sample environments  
... that enables the plugin of theoretical sample models

*Credit: Mads Bertelsen, ESS*



# Analysis with the EasyScience family of analysis software

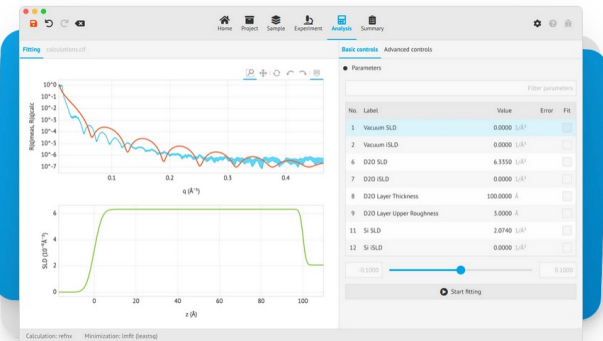


## easydiffraction

Simulation of diffraction patterns based on structural models and refinement against experimental data.

Integrates such crystallographic data analysis libraries as [CrysPy](#) and [CrysFML](#).

[Visit easydiffraction.org](http://easydiffraction.org) →



## easyreflectometry

Simulation of reflectometry profiles based on layered structures and refinement against experimental data.

Integrates such reflectometry data analysis libraries such as [refnx](#) and [refl1d](#).

[Visit easyreflectometry.org](http://easyreflectometry.org) →

## UNIFIED USER INTERFACE?

Same look and feel for different techniques

✓ EasyDiffraction analysis

✓ EasyReflectometry analysis

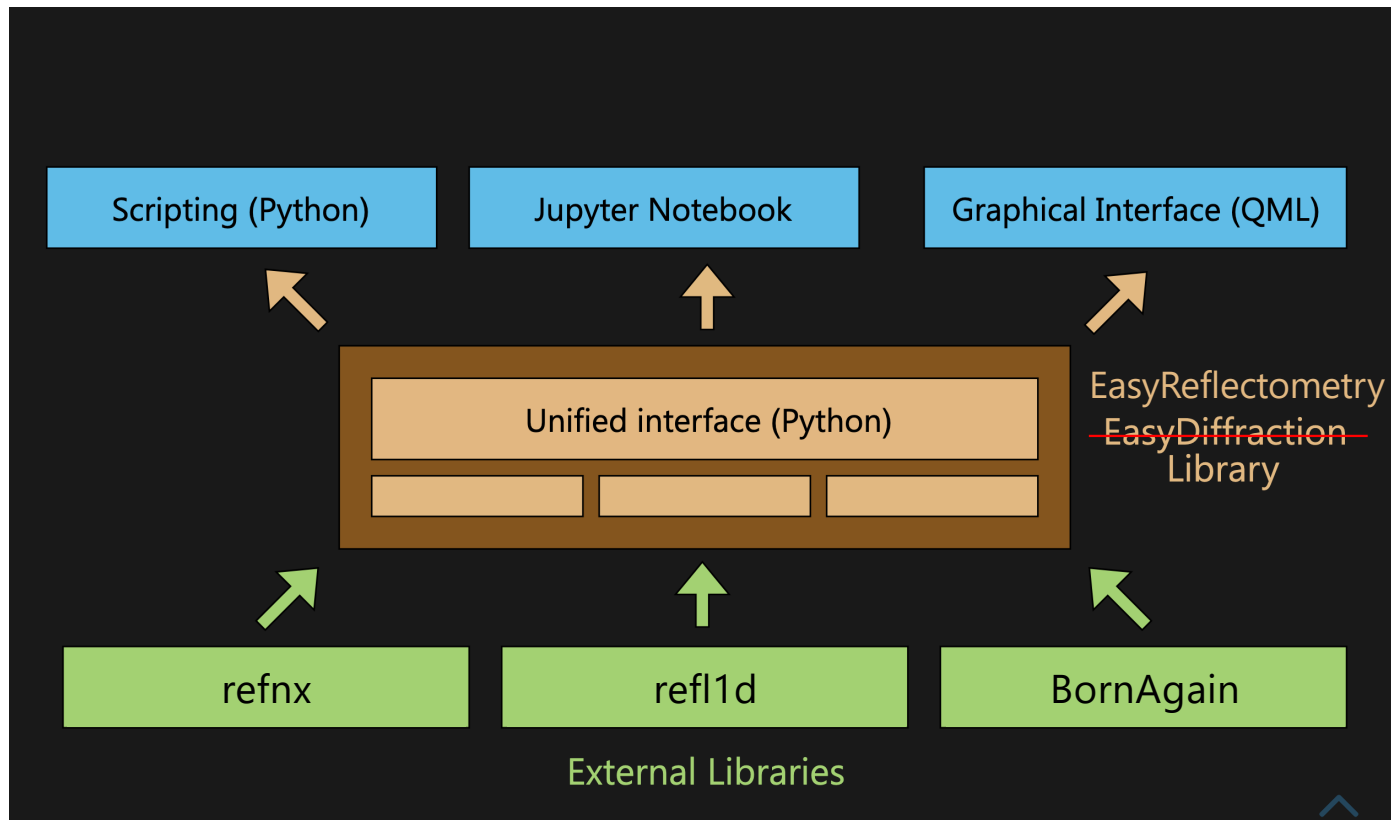
? EasyQens analysis

? EasyBragg analysis

✓ ? EasyTexture reduction

# Architecture

<https://easyscience.software>  
<https://easydiffraction.org>  
<https://easyreflectometry.org>



Courtesy: Andrew Sazonov

# European Open Science Cloud & FAIR data

How does the simulation community position itself?




Implementation of FAIR data and open science across Europe  
(+1 billion €)



Implementation of FAIR data for photon and neutron sources

# FAIR data management

SciCat is used as data catalogue by several facilities



Items per page: 25 1 - 25 of 2894

Search							
Clear							
PID	Name	Run No.	Size	Start Time	Type	Image	Proposal ID
20.500.12269/4f8c991e-a879-4e00-9095-5bb13	LDP data		212 MB	2020-02-21 Fri 10:01	derived		
20.500.12269/7d457282-ab2d-bdc9f440cb30	Fe3O4		14 KB	2020-02-20 Thu 10:30	raw		
20.500.12269/2d5af6ef-V20	sample data		0 B	2020-02-06 Thu 13:02	derived		
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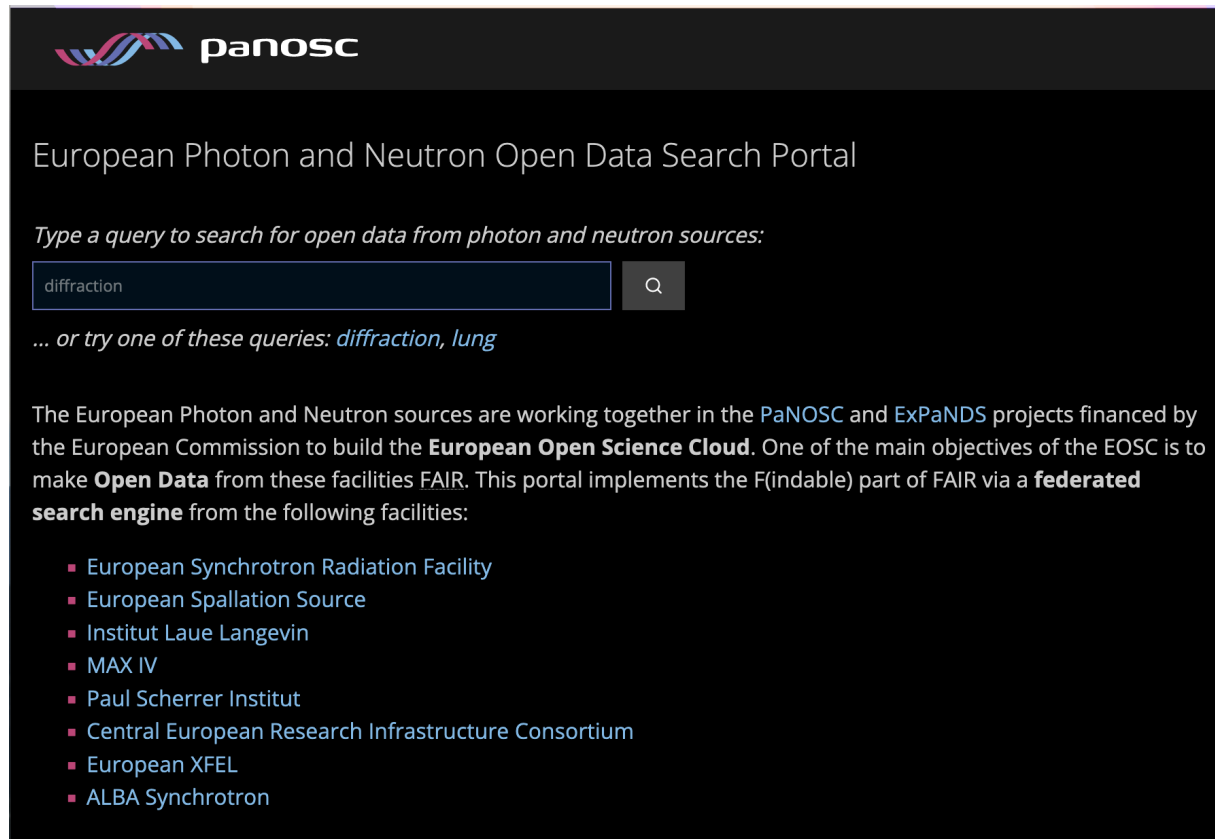
Data will be made public after 3 years



# Federated data portal

You can find and access data from multiple photon and neutron sources from one place

<https://data.panosc.eu>



https://pan-training.eu

The screenshot shows the homepage of the pan-training.eu website. The header includes a navigation bar with 'Catalogue', 'E-learning', 'Events', and 'About' links, along with a 'Log in the catalogue to register content' link. The main section features the 'Photon and Neutron Training' logo and a search bar. Below the search bar, there are four icons representing 'Materials', 'Events', 'Workflows', and 'Providers', each with a brief description. A 'We have:' section lists statistics: 190 materials (48 PaN E-learning courses and 142 other materials), 335 events, and 11 workflows. A 'Register new content' button is also present. The 'E-Learning Courses' section highlights online interactive courses on PaN science theory and experimental data reduction and analysis, with links to 'Practice data reduction and analysis' and 'Run Jupyter notebooks remotely'. The footer displays the date '2024-06-13' and the text 'PRESENTATION TITLE/FOOTER'.

Log in the catalogue to register content

Catalogue ▾ E-learning Events About ▾

Photon and Neutron Training

Search PaN training...

Training for photon & neutron science.  
Find educational material from institutes around Europe.

We have:

- 190 materials:
  - 48 PaN E-learning courses and
  - 142 other materials
- 335 events and
- 11 workflows

Register new content

Materials  
Find documents, videos and git repos

Events  
Browse events provided by our community

Workflows  
Guided processes for specific scientific management

Providers  
Browse by the institute providing content

Access Courses

PaN-wiki

Log on

E-Learning Courses

Online interactive courses on the theory of PaN science along with experimental data reduction and analysis.

- Practice data reduction and analysis.
- Run Jupyter notebooks remotely.

Latest Content in our training portal for the photon & neutron community

12-17 November 2023, International Conference on Molecular Energy Transfer in Complex Systems (ICOMET), Jaipur, India

2024-06-13 PRESENTATION TITLE/FOOTER





# Using simulations for training

## Combining Moodle & Jupyter

<https://pan-learning.org>

PaN-Training Catalogue ▾ E-Learning ▾ Events About ▾

Welcome to the Photon and Neutron E-learning platform that hosts free education and training for scientists and students.  
Below you will find courses on both the theory of pl

 + 

- ✓ Classes
- ✓ Assignments
- ✓ Quizzes
- ✓ Videos
- ✓ ...

- ✓ Instrument simulations
- ✓ Atomistic simulations
- ✓ Databases
- ✓ ...

### Available courses

Introduction to Neutron Reflectometry Fitting

Neutron Scattering Library

Introduction to Neutron Scattering

Advanced Topics in Neutron Scattering

Quasi-Elastic Neutron Scattering

swedness-online-2021

Introduction to Muon Spin Spectroscopy

Muons in Semiconductors

Muons in Magnetism

Muons in Superconductivity

Python Workshop (IKON21)

Python Workshop (IKON20)

SasView: Analysis of SAS Data

Including Jupyter Notebooks in your Course

Creating a Video Mini-Lecture

Collection of photon science slides

Quiz Taster

2024-0



PRESENTATION TITLE / FOOTER  
This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 823852



# More training



<https://workshops.ill.fr/event/425/>

**5-7 NOV**  
**GRENOBLE**  
**FRANCE**

**UNVEILING DYNAMICS**  
**MDANSE SCHOOL 2024**  
**MASTERING MATERIALS THROUGH DFT & MD**

Enter your search term

Application until 30th June 2024

**Piotr Rozyczko** 12:45 PM  
Applications are welcome (we actually need more applicants!) until June 30  
<https://workshops.ill.fr/event/425/>  
Only 200 €!  
Guesthouse, lunches, wine and cheese buffet and social dinner included!  
3 days of constant DFT and MD fun!

Contact

<https://indico.ess.eu/event/3514/>

**ESS Data Management and Software Centre**  
**Summer School**

**DMSC Summer School 2024**

Sep 2 – 6, 2024  
Copenhagen, Denmark

**Overview**  
Registration Information  
Important dates  
Programme  
Contact

**Organiser Email**  
✉ [symposia@ess.eu](mailto:symposia@ess.eu)

Welcome to ESS Data Management and Software Centre (DMSC) Summer School 2024!

The school will be held in Copenhagen from the **2nd to the 6th of September 2024**, with on-site registration and welcome reception on the afternoon of the 1st.

This summer school is being organised by the [European Spallation Source](#). We invite applications for participation to learn about the role of your data, from proposal to publication.

The role of data in neutron scattering is changing, with greater importance being placed on data reduction and analysis, as well as FAIR (findable, accessible, interoperable, and reusable) and open data. Therefore, neutron scattering scientists must be trained to understand fully the role that data has in their experiments and how to harness the tools that maximise the value of their data. This summer school will provide that training, covering the full ESS Data Pipeline.

The diagram illustrates the ESS Data Pipeline, a sequence of steps: User Office Software (UOS), Experimental Control, Stream Events & Metadata (Kafka), Data Reduction & Visualisation, Data Analysis (Technique Specific), and FAIR Data Management (MSci). Below this pipeline, logos for partner institutions are displayed: EPICS, NICOS, scipp, and NeXus.

# Summary



- The DMSC is responsible for supporting the science program with scientific computing solutions
- The DMSC will enable remote access so users can analyse data on ESS computers
- The DMSC will deliver an integrated data pipeline for each instrument
- The DMSC will support users from idea to publication with digital solutions and hands-on support
- DMSC staff encompasses both technical and scientific staff, who do science themselves and collaborates with universities
- DMSC is open for collaboration and already collaborates with many other facilities

# Questions?

