EUROPEAN
SPALLATION
SOURCE

Updates from the ESS-DMSC

PRESENTED BY THOMAS HOLM ROD

2023-09-19

Agenda

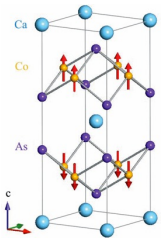
1 Introduction to DMSC

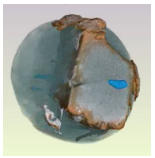
2 General updates from DMSC

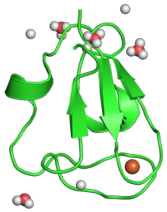
3 Specifically for reflectometry

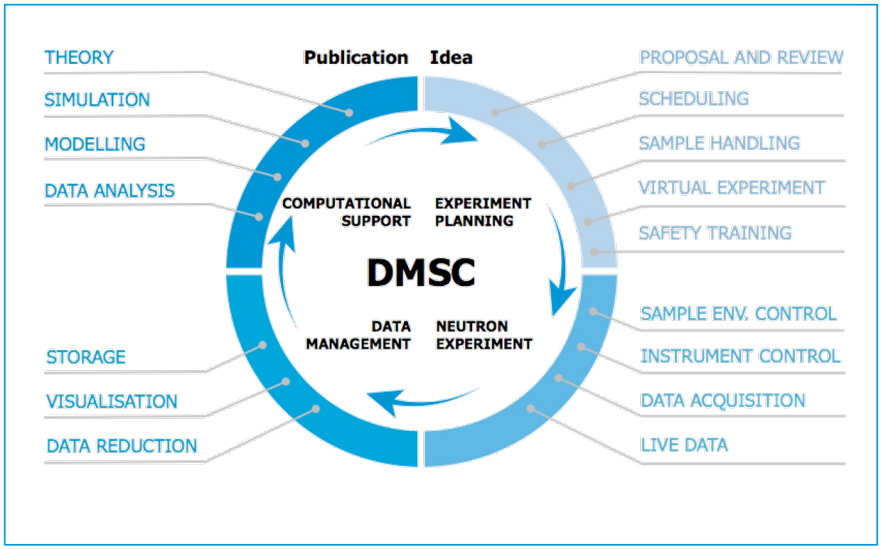
DMSC Scope

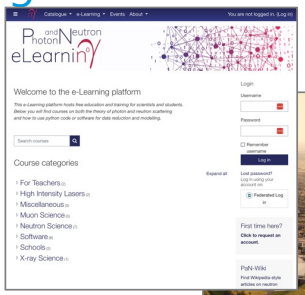
Support user from proposal to publication with scientific computing tools & services

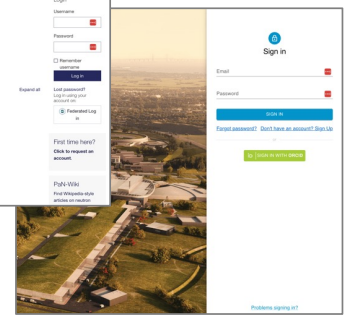


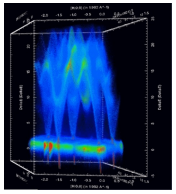


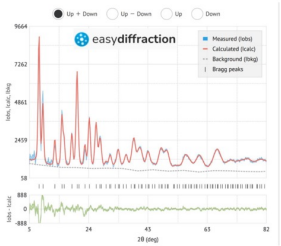


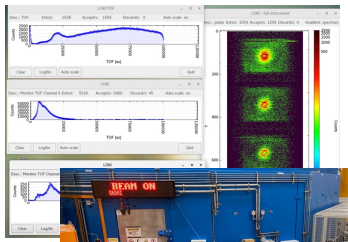


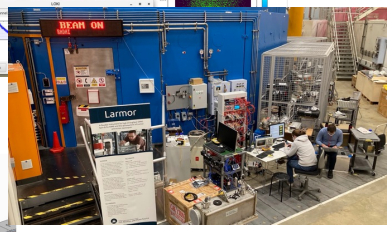


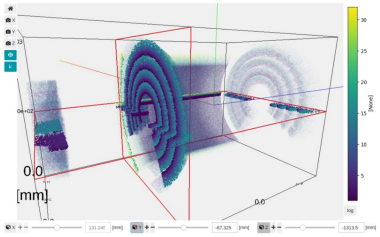


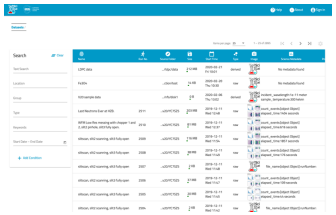


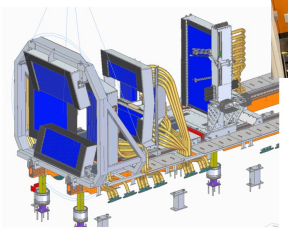




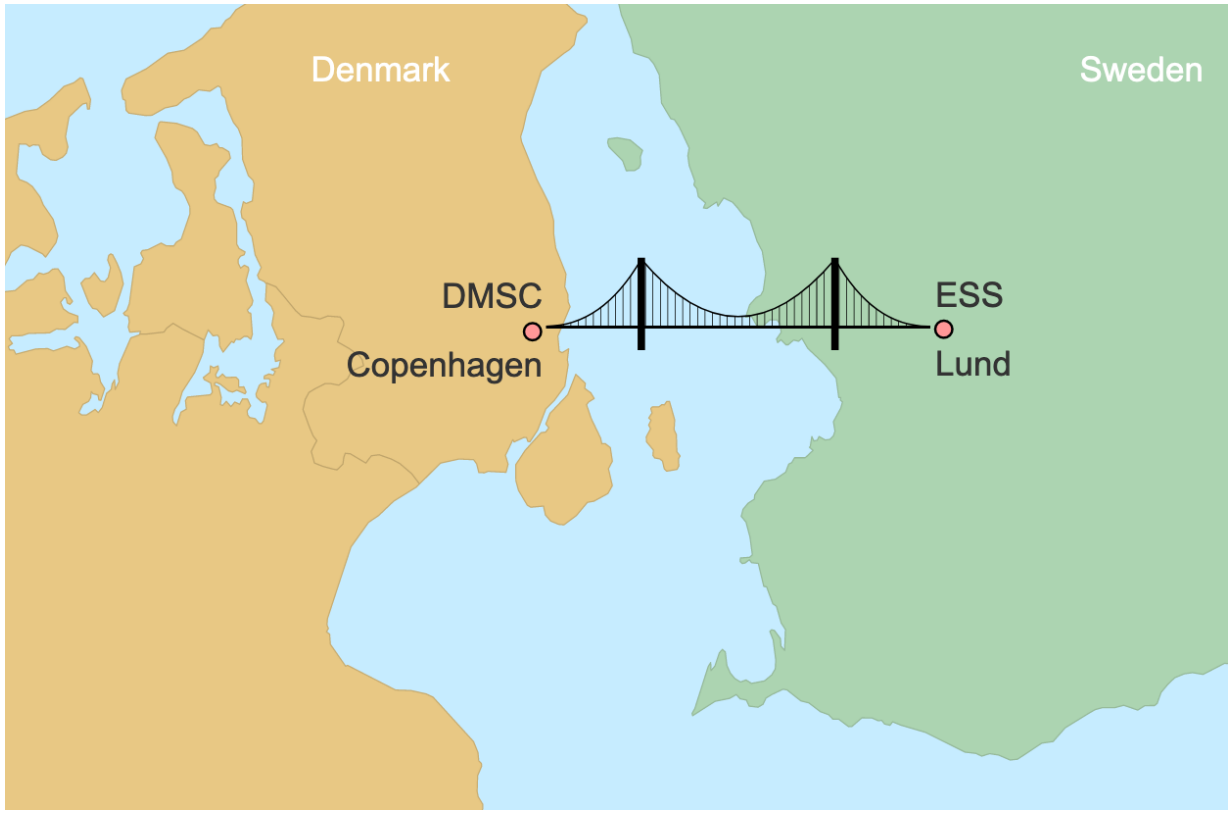








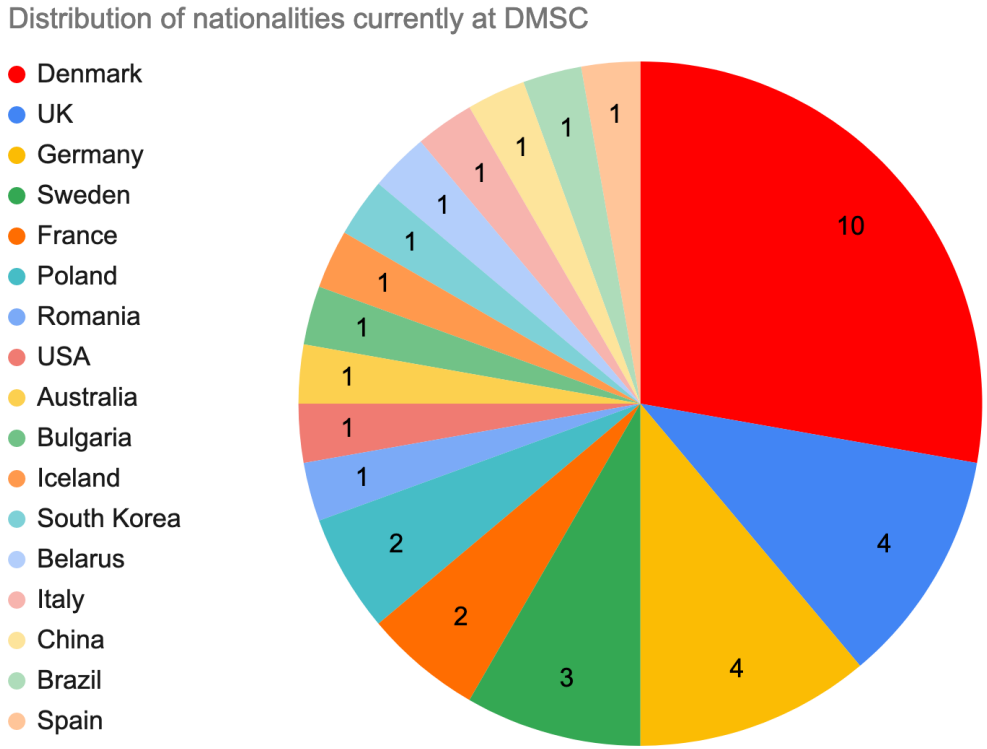
DMSC changes



- Most likely relocate to DTU north of Copenhagen (negotiations are ongoing)
- Interviews ongoing for Head of DMSC
- Instrument Data Scientist for reflectometry (Andrew McCluskey) resigned
    - Looking for replacement! (job ad out)

Staffing

DMSC DK staff April 2023

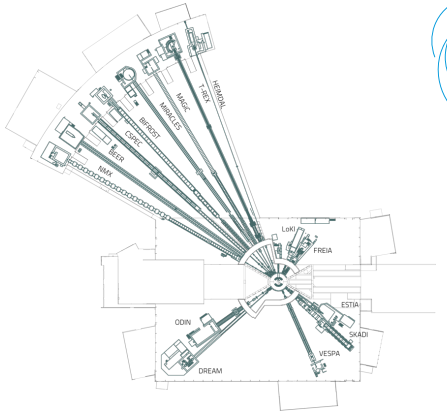


42 staff members in DK + 4 in SE

18 / 19 nationalities

66% has a PhD degree

Integrated data pipeline



EasyReflectometry
BornAgain
Refnx
Refl1d
rascal

User office software	Experiment control	Stream events & meta data	Data reduction & visualization	Data analysis	FAIR Data management
ISIS	TUM, PSI	ISIS	ISIS, MLZ, ORNL?	ORSO MLZ	PSI, MAX IV, …

Our Instrument Data Scientist resigned

but has handed over and has not abandoned us

Selene guide → Completed (for his part)

Data reduction → Jan-Lukas (scipp developer)

Scipp team has had challenges recruiting but we are getting there.

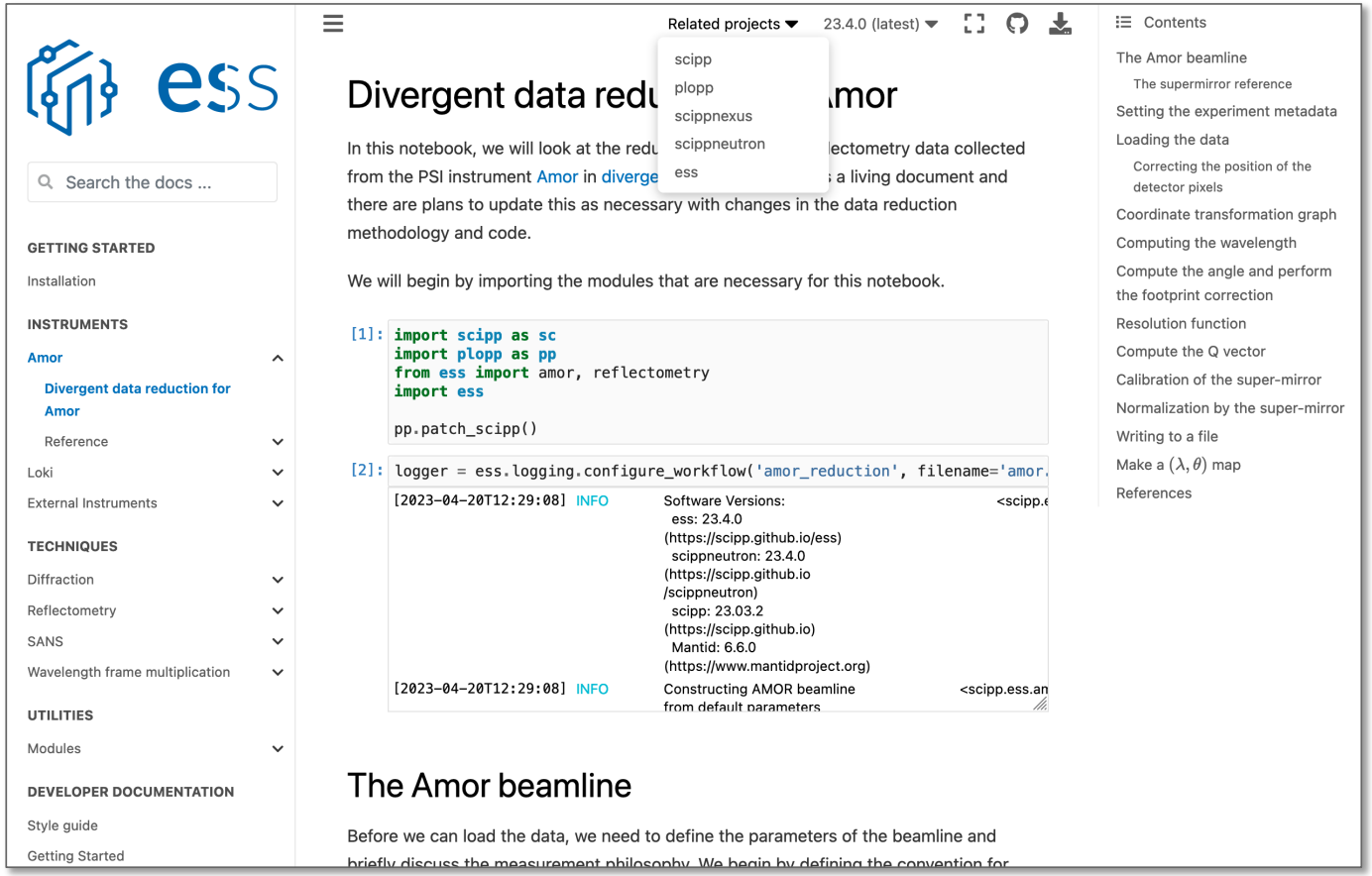
Data analysis → Piotr & Andrew S EasyScience developer

EasyScience team is at half capacity with 2 developers. Currently two open positions.

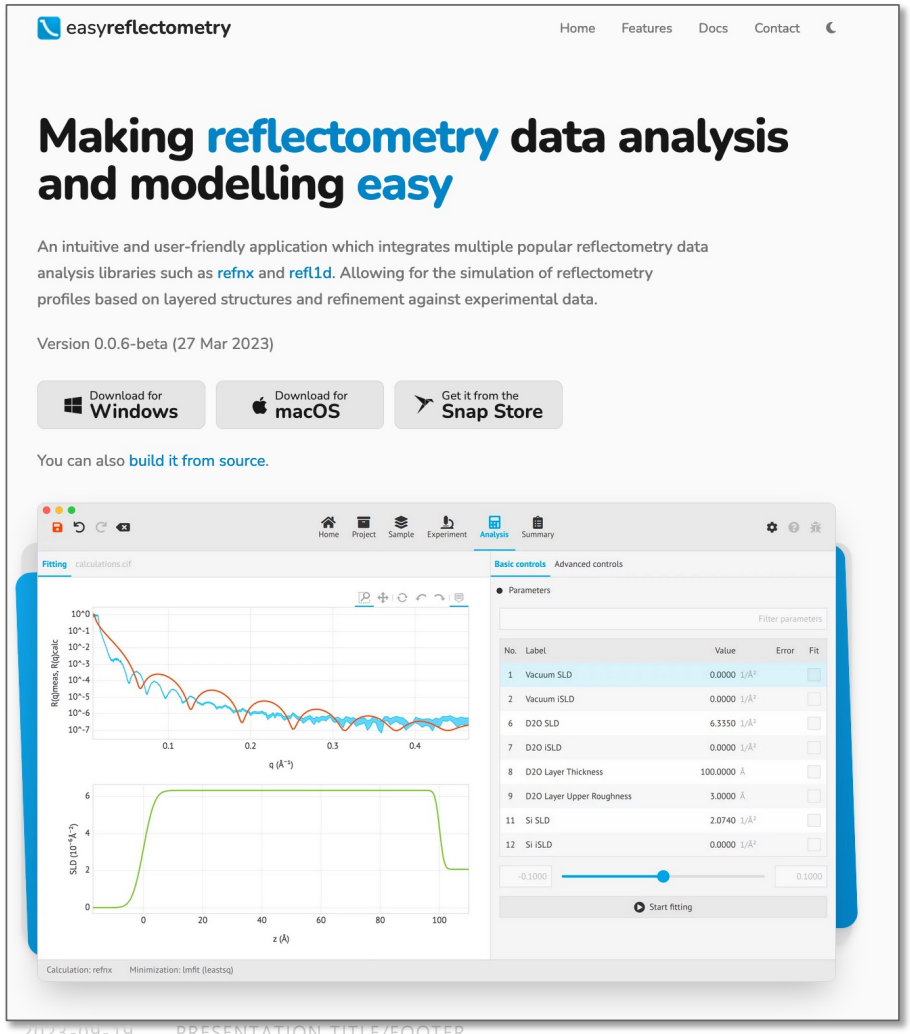
Jos (new Instrument Scientist)

Data reduction with scipp

https://scipp.github.io

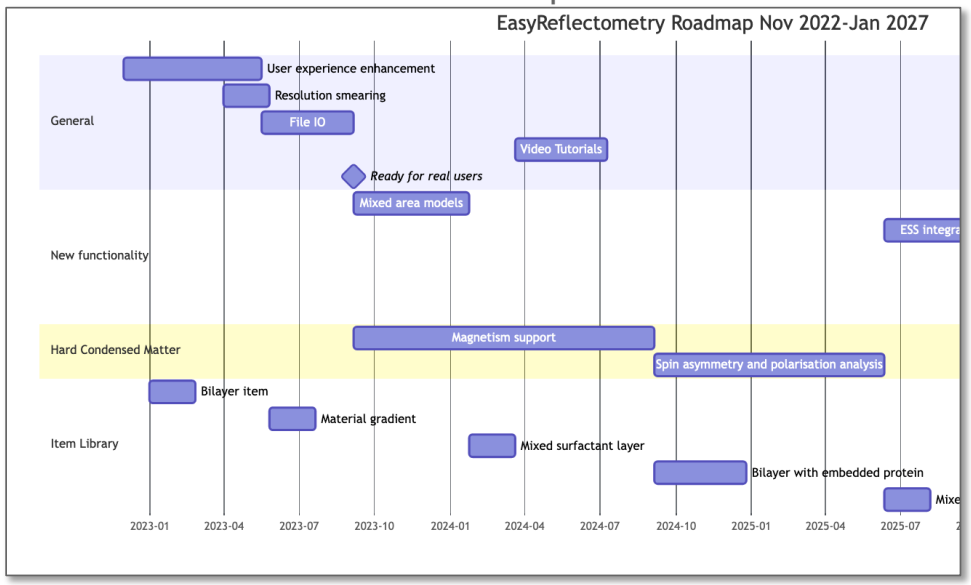


Data analysis with easyReflectometry



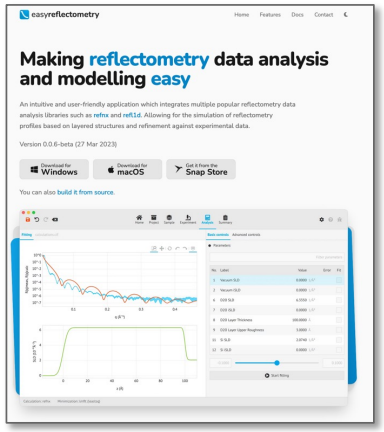
https://easyreflectometry.org

Roadmap



(needs to be updated)

Data analysis with easyReflectometry



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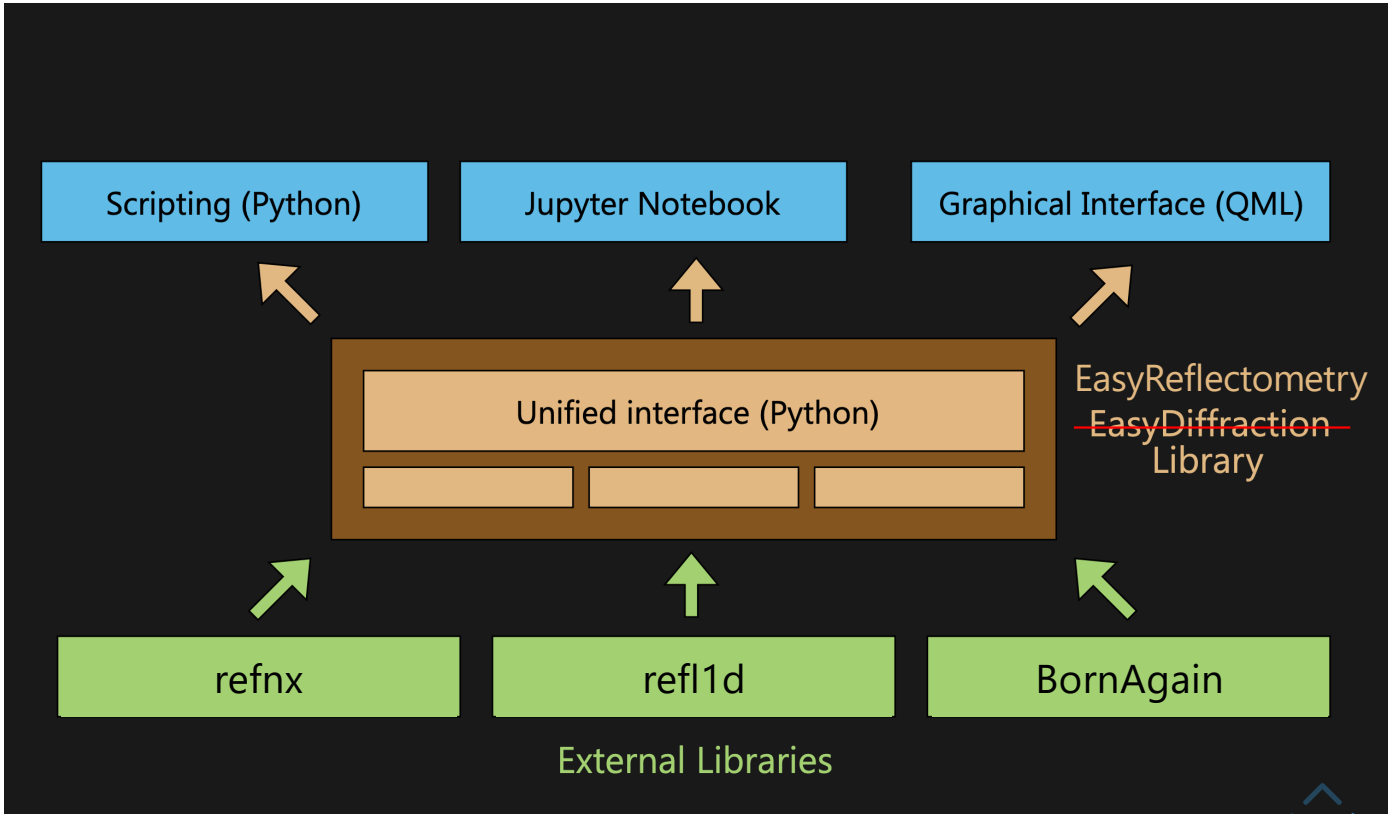
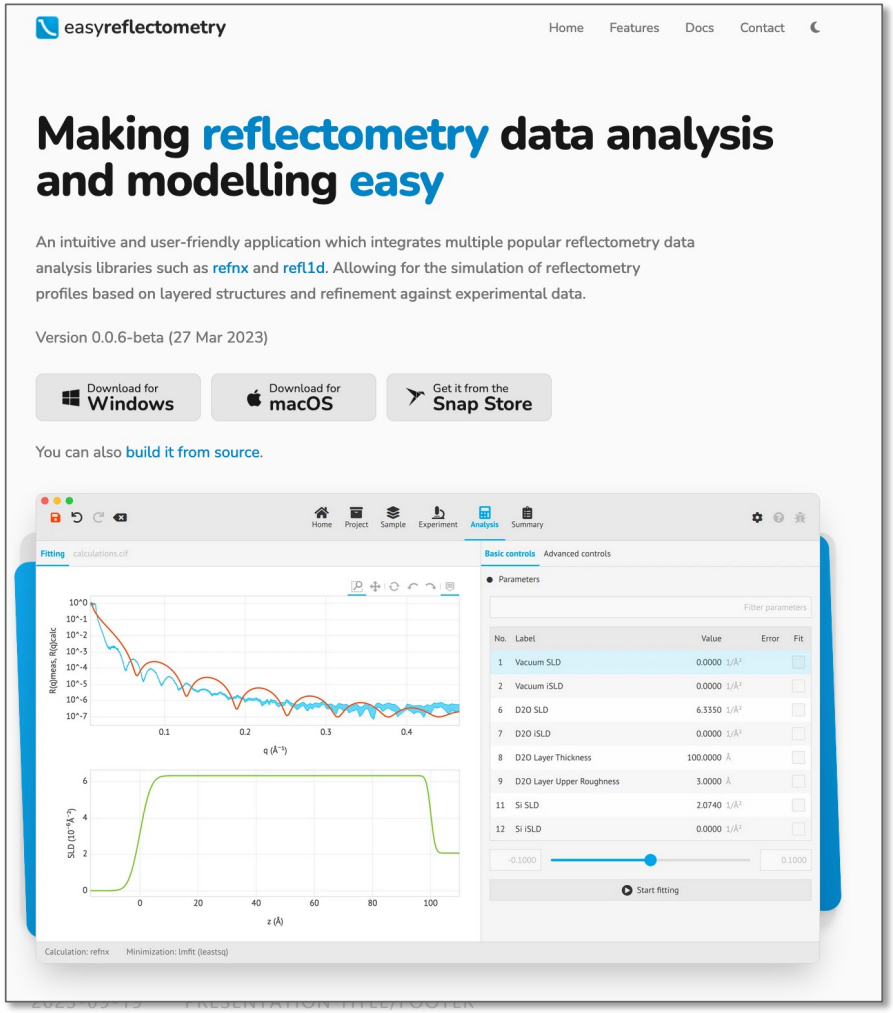


Courtesy: Andrew Sazonov

Data analysis with EasyReflectometry



EasyReflectometry is a member of the EasyScience family developed by DMSC

Popular without really being in use

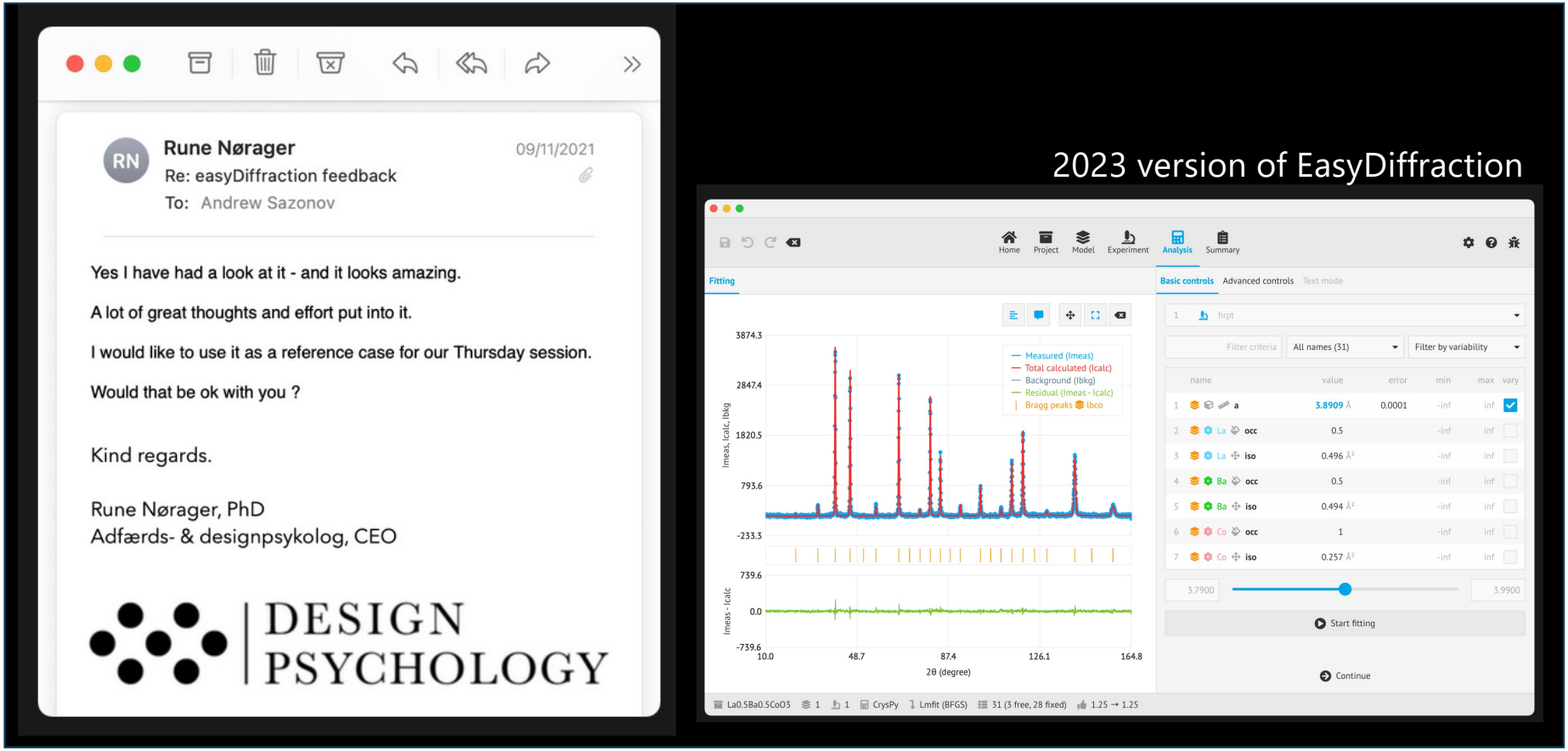
UNIFIED USER INTERFACE?

Same look and feel for different techniques

- EasyDiffraction — analysis
- EasyReflectometry — analysis
- EasyQens — analysis
- EasyBragg — analysis
- EasyTexture — reduction

Appealing GUI design:

Approval from expert



Job ad is out

Also on LinkedIn – please share

Instrument Data Scientist for reflectometry

ESD-36777

The European Spallation Source (ESS) is a "Big Science" project that aims to be the most powerful neutron source in the world when it is fully operational in 2027. It will enable scientists to study the structure and behavior of matter at the atomic level, opening new possibilities for research and innovation in material science.

ESS invites applications for an Instrument Data Scientist position at the Data Management and Software Centre (DMSC) in Copenhagen, Denmark. The DMSC is tasked with the mission of assisting users of ESS with all their scientific computing needs. This can range from data reduction to experiment control, and from data analysis to computing hardware.

About the role

As an instrument data scientist for neutron reflectometry at the ESS you will act as an interface between DMSC and the instrument team for reflectometry.

The role will focus on the following tasks:

- Project/product managing the deliverables from DMSC to the instrument team, allowing the maximum scientific impact to be generated from the instruments.
- Working with your colleagues and development teams at DMSC and the instrument team to provide the best user experience.
- Co-designing and co-developing data reduction, processing, and analysis software with your colleagues at DMSC using requirements from users and the instrument team.
- Providing direct support during experiments to users with analysis of their data, once the instruments have entered the ESS user program.
- Advancing neutron reflectometry with cutting edge data science and data analysis techniques.

The role will initially focus on ensuring that scientific user software is ready for operation of the instruments. The instrument data scientist will therefore play a central role during commissioning of the instruments, with duties in instrument control and data reduction. Part of this will require visits to the AMOR beamline at the Paul Scherrer Institute in Switzerland, where the software you develop can be tested before the ESS instruments are fully operational.

DMSC Summer school

Training in ESS software suite and FAIR data

(Andrew's McCluskey last task for ESS)

User office software → Experiment control → Stream events & meta data → Data reduction & visualization → Data analysis → FAIR Data management

- Following on from PaNOSC Summer school
- Focusing on ESS software suite and FAIR data
- 1st school in Sep 2023
- 14 participants (over-subscribed)

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Next steps for reflectometry

It all starts with recruitment

- Recruit new Instrument Data Scientist for reflectometry

  Resume activities for **data reduction**, data analysis, user journey, AMOR, etc.

- Expand development team for analysis with at least two persons
- Develop and release EasyDiffraction 1.0
- Resume development of EasyReflectometry
- Finding collaborators for EasyReflectometry

Finish presentation

Staffing for Analysis and Instrument Data Scientists

Instrument Data Scientists (½ IDS instrument)

Technique	Instruments	Who or When
Imag. & Eng.	ODIN & BEER	Søren
Reflectometry	ESTIA & FREIA	~~Andrew M~~
SANS	LoKI & SKADI	Wojtek
Diffraction	DREAM & MAGIC	Céline
Spectroscopy	BIFROST & CSPEC	Greg
Diffraction	NMX & HEIMDAL	Jan 2025
Spectroscopy	TREX & MIRACLES	Jul 2026

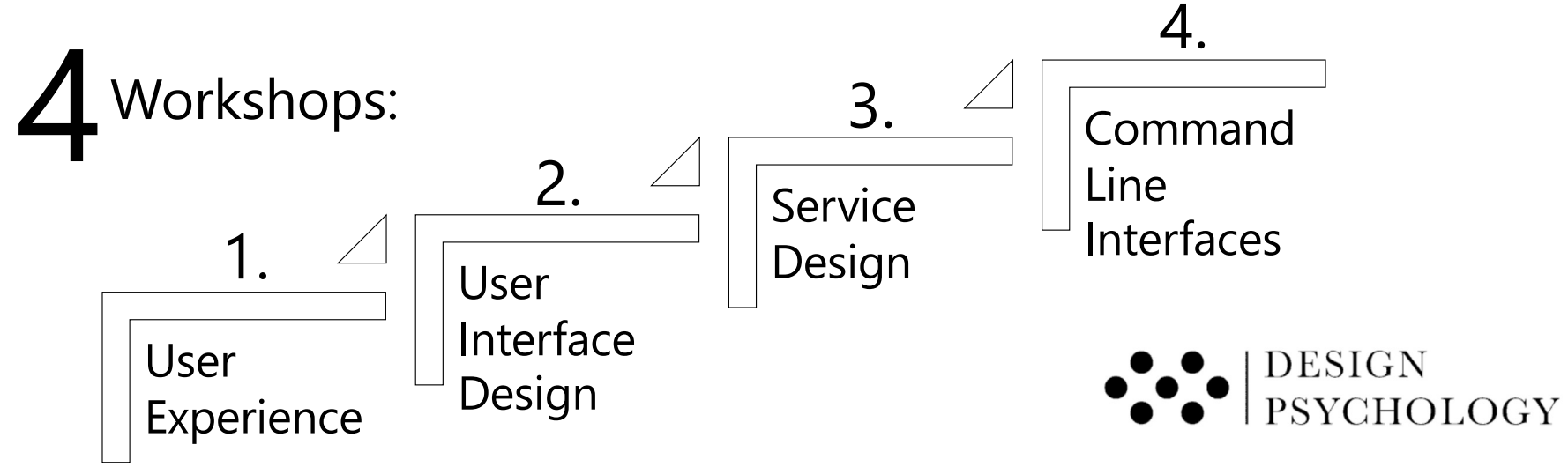
Data analysis core development

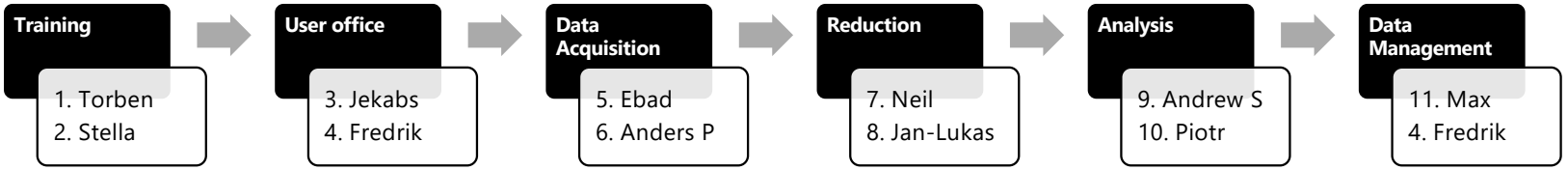
Technique	Who or When
Manager (Atomic sim)	Piotr
Diffraction	Andrew S
Spectroscopy	~~Simon W~~
Imaging (& Eng)	~~Nov 2023~~

- Ensure right expertise
- Able to collaborate on all techniques
- IDS for reflectometry and SANS contribute significantly to data analysis
- Data analysis developers to support IDSes during Hot Commissioning
- Conservative when using ESS budget
- More visionary / researchy when using external funding

User Experience Workshop

Competence development / Improvements of UX (e.g. GUIs) across DMSC





12. Céline
13. Søren
14. Greg
15. Andrew M
16. Wojtek

MODULAR STRUCTURE

https://easyscience.software