



**EUROPEAN
SPALLATION
SOURCE**



Updates from the ESS-DMSC

PRESENTED BY THOMAS HOLM ROD

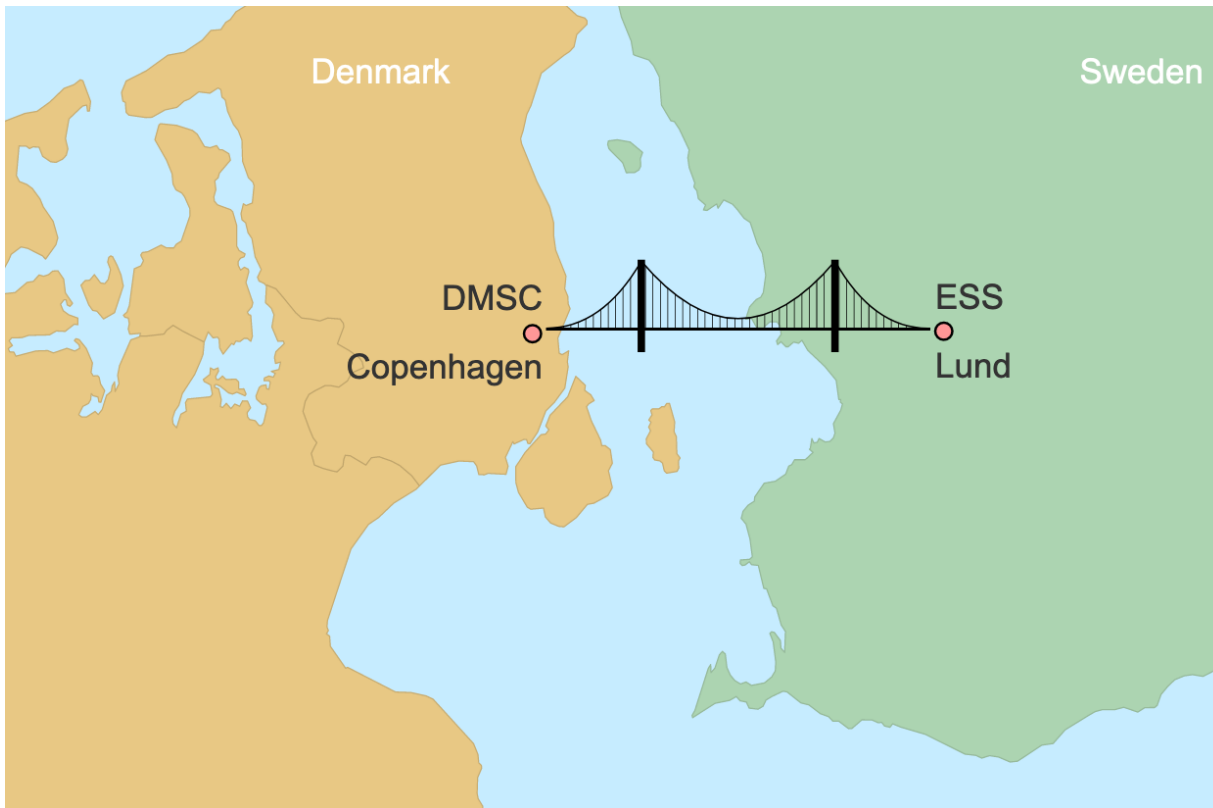
2023-09-19

Agenda



- 1 Introduction to DMSC
- 2 General updates from DMSC
- 3 Specifically for reflectometry

DMSC 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)

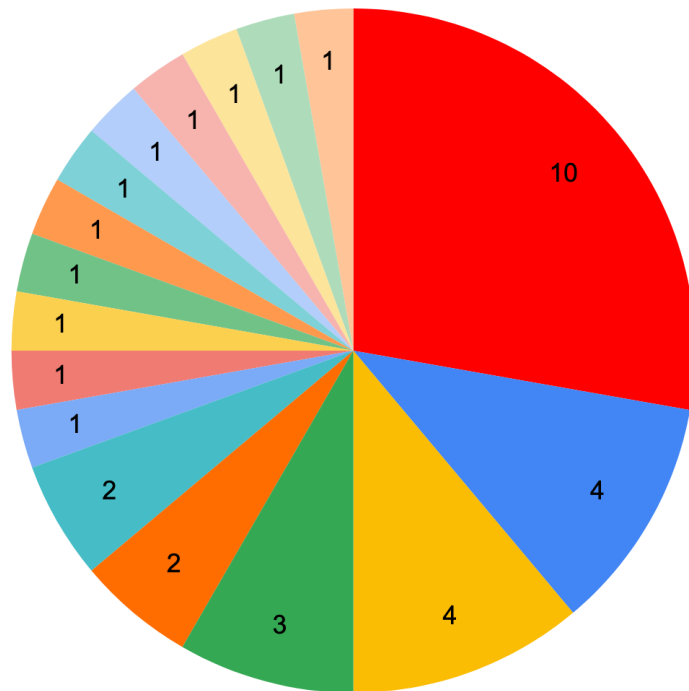
Staffing



DMSC DK staff April 2023

Distribution of nationalities currently at DMSC

- Denmark
- UK
- Germany
- Sweden
- France
- Poland
- Romania
- USA
- Australia
- Bulgaria
- Iceland
- South Korea
- Belarus
- Italy
- China
- Brazil
- Spain

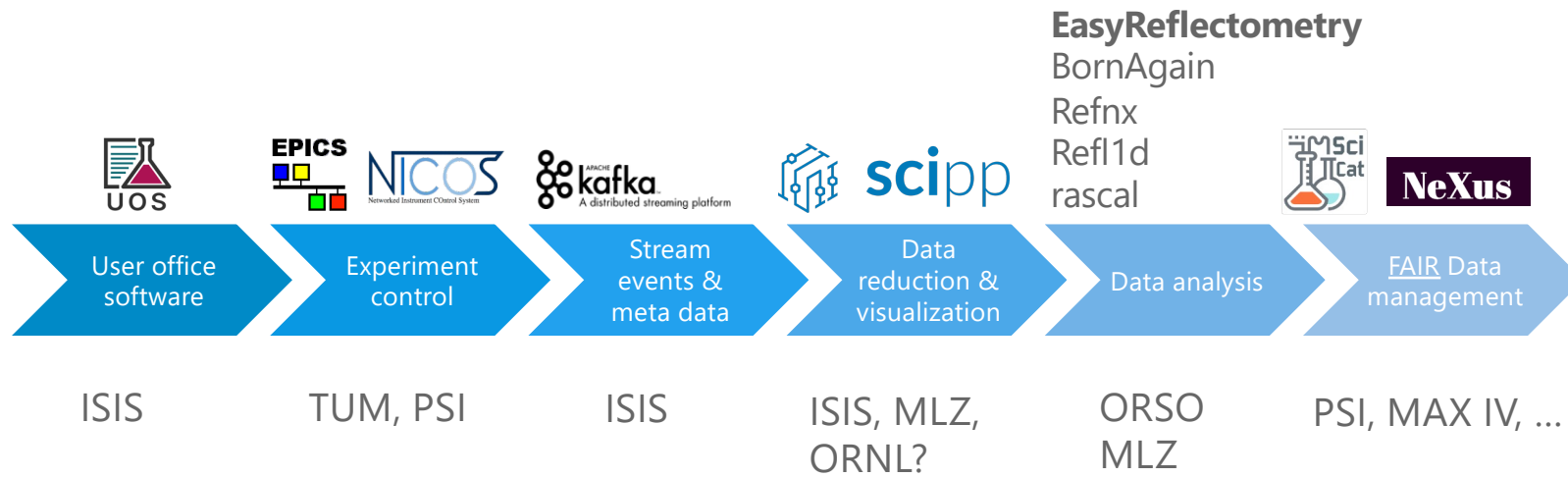


42 staff members in DK + 4 in SE

18 / 19 nationalities

66% has a PhD degree

Integrated data pipeline



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>



The screenshot shows a Jupyter notebook interface. On the left is a sidebar with a search bar and a navigation menu. The main area contains text and code cells. A dropdown menu is open over the code cell, listing related projects: scipp, plopp, scippnexus, scippneutron, and ess. The right sidebar shows a table of contents.

GETTING STARTED
Installation

INSTRUMENTS
Amor
 Divergent data reduction for Amor
Reference
Loki
External Instruments

TECHNIQUES
Diffraction
Reflectometry
SANS
Wavelength frame multiplication

UTILITIES
Modules

DEVELOPER DOCUMENTATION
Style guide
Getting Started

Divergent data reduction for Amor

In this notebook, we will look at the reduction of reflectometry data collected from the PSI instrument Amor in divergent geometry. This notebook is a living document and there are plans to update this as necessary with changes in the data reduction methodology and code.

We will begin by importing the modules that are necessary for this notebook.

```
[1]: import scipp as sc
import plopp as pp
from ess import amor, reflectometry
import ess

pp.patch_scipp()
```

```
[2]: logger = ess.logging.configure_workflow('amor_reduction', filename='amor_...')
[2023-04-20T12:29:08] INFO Software Versions: <scipp.ess.amor>
ess: 23.4.0
(https://scipp.github.io/ess)
scippneutron: 23.4.0
(https://scipp.github.io/scippneutron)
scipp: 23.03.2
(https://scipp.github.io)
Mantid: 6.6.0
(https://www.mantidproject.org)
[2023-04-20T12:29:08] INFO Constructing AMOR beamline from default parameters <scipp.ess.amor>
```

The Amor beamline

Before we can load the data, we need to define the parameters of the beamline and briefly discuss the measurement philosophy. We begin by defining the convention for

Contents
The Amor beamline
 The supermirror reference
Setting the experiment metadata
Loading the data
 Correcting the position of the detector pixels
Coordinate transformation graph
Computing the wavelength
Compute the angle and perform the footprint correction
Resolution function
Compute the Q vector
Calibration of the super-mirror
Normalization by the super-mirror
Writing to a file
Make a (λ, θ) map
References

Data analysis with easyReflectometry



easyreflectometry

Home Features Docs Contact

Making reflectometry data analysis and modelling easy

An intuitive and user-friendly application which integrates multiple popular reflectometry data analysis libraries such as [refnx](#) and [refl1d](#). Allowing for the simulation of reflectometry profiles based on layered structures and refinement against experimental data.

Version 0.0.6-beta (27 Mar 2023)

Download for Windows | Download for macOS | Get it from the Snap Store

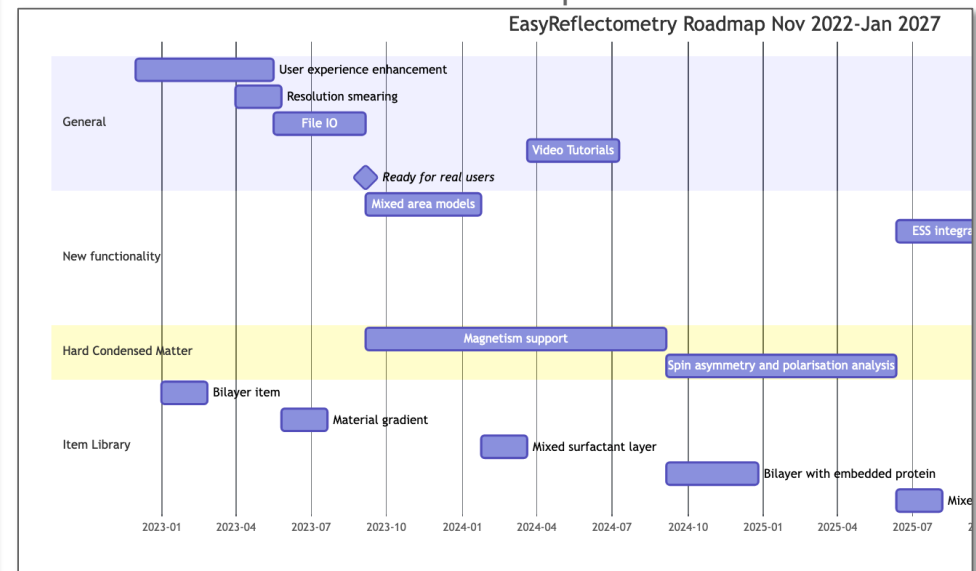
You can also [build it from source](#).

No.	Label	Value	Error	Fit
1	Vacuum SLD	0.0000	1/Å ²	<input type="checkbox"/>
2	Vacuum ISLD	0.0000	1/Å ²	<input type="checkbox"/>
6	D2O SLD	6.3350	1/Å ²	<input type="checkbox"/>
7	D2O ISLD	0.0000	1/Å ²	<input type="checkbox"/>
8	D2O Layer Thickness	100.0000	Å	<input type="checkbox"/>
9	D2O Layer Upper Roughness	3.0000	Å	<input type="checkbox"/>
11	Si SLD	2.0740	1/Å ²	<input type="checkbox"/>
12	Si ISLD	0.0000	1/Å ²	<input type="checkbox"/>

Calculation: refnx Minimization: lmfit (leastsq)

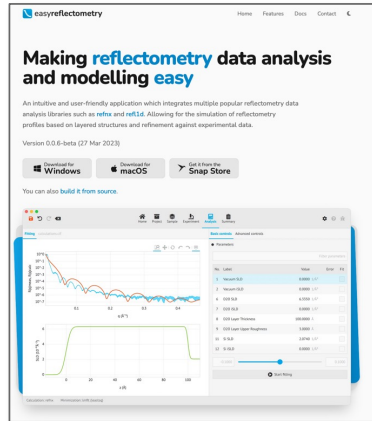
<https://easyreflectometry.org>

Roadmap

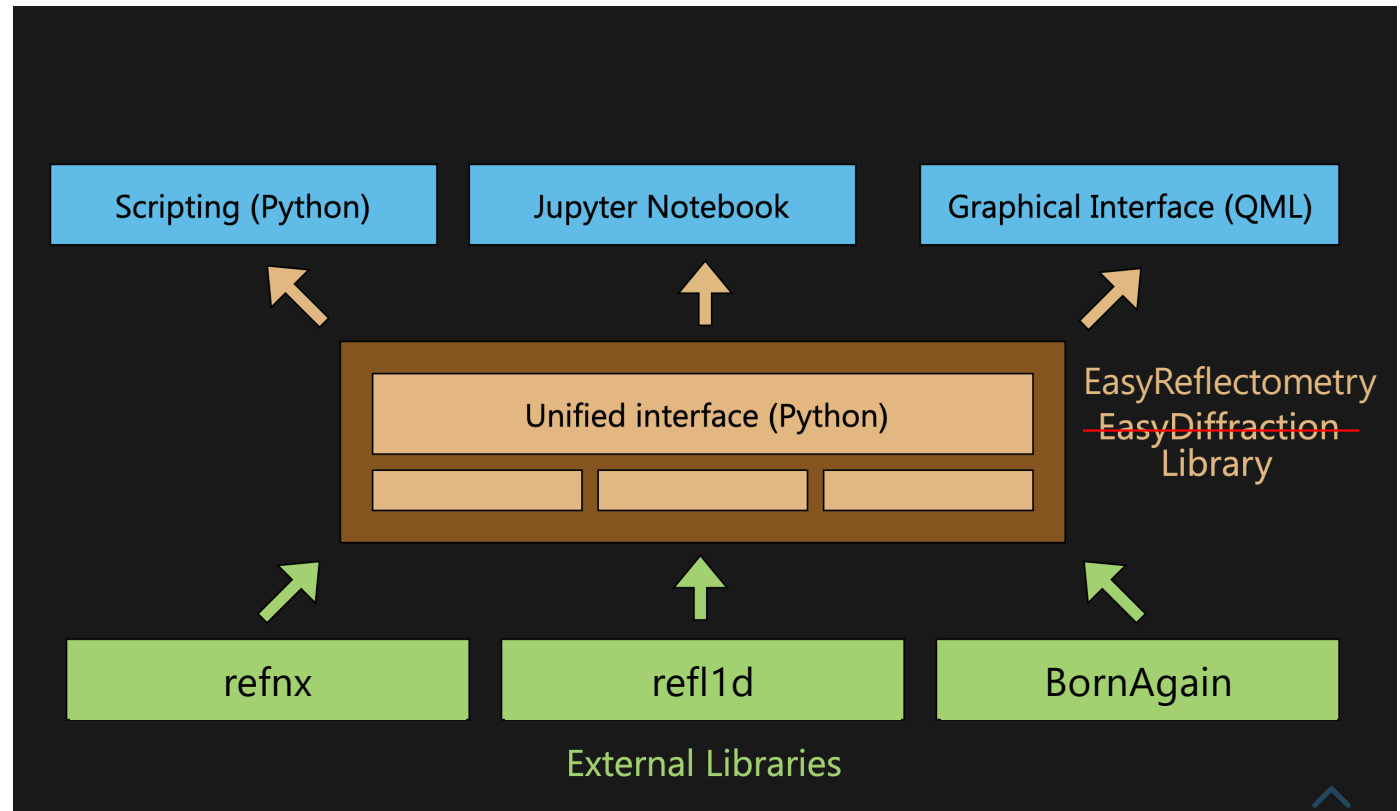


(needs to be updated)

Data analysis with easyReflectometry



<https://easyreflectometry.org>



Courtesy: Andrew Sazonov

Data analysis with EasyReflectometry



The screenshot shows the EasyReflectometry website and its software interface. The website header includes the logo and navigation links: Home, Features, Docs, Contact. The main heading is "Making reflectometry data analysis and modelling easy". Below this, a paragraph describes the application as intuitive and user-friendly, integrating libraries like `refnx` and `refl1d`. It also mentions the version 0.0.6-beta (27 Mar 2023) and provides download buttons for Windows, macOS, and the Snap Store. A link to "build it from source" is also present.

The software interface shows a "Fitting" window with two plots. The top plot shows "Rigorous R_gcalc" vs "q (Å⁻¹)" on a log scale. The bottom plot shows "SLD (10¹⁰ Å⁻³)" vs "z (Å)". To the right, a "Parameters" table is visible:

No.	Label	Value	Error	Fit
1	Vacuum SLD	0.0000	1/Å ³	<input type="checkbox"/>
2	Vacuum ISLD	0.0000	1/Å ³	<input type="checkbox"/>
6	D20 SLD	6.3350	1/Å ³	<input type="checkbox"/>
7	D20 ISLD	0.0000	1/Å ³	<input type="checkbox"/>
8	D20 Layer Thickness	100.0000	Å	<input type="checkbox"/>
9	D20 Layer Upper Roughness	3.0000	Å	<input type="checkbox"/>
11	Si SLD	2.0740	1/Å ³	<input type="checkbox"/>
12	Si ISLD	0.0000	1/Å ³	<input type="checkbox"/>

At the bottom of the parameters table, there is a slider for "Filter parameters" ranging from -0.1000 to 0.1000, and a "Start fitting" button.

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



The image shows two side-by-side screenshots. The left screenshot is an email from Rune Nørager to Andrew Sazonov, dated 09/11/2021. The email content is as follows:

RN Rune Nørager 09/11/2021
Re: easyDiffraction feedback
To: Andrew Sazonov

Yes I have had a look at it - and it looks amazing.
A lot of great thoughts and effort put into it.
I would like to use it as a reference case for our Thursday session.
Would that be ok with you ?

Kind regards.
Rune Nørager, PhD
Adfærds- & designpsykolog, CEO

DESIGN PSYCHOLOGY

The right screenshot shows the 2023 version of the EasyDiffraction software interface. The title bar reads "2023 version of EasyDiffraction". The interface includes a menu bar (Home, Project, Model, Experiment, Analysis, Summary), a toolbar, and a main workspace. The workspace is divided into a plot area and a control panel. The plot area shows a diffraction pattern with the following legend:

- Measured (lmeas) - blue line with markers
- Total calculated (lcalc) - red line with markers
- Background (lbkg) - green line
- Residual (lmeas - lcalc) - green line
- Bragg peaks (lbcg) - yellow vertical bars

The control panel on the right has tabs for "Basic controls", "Advanced controls", and "Text mode". It displays a list of parameters:

name	value	error	min	max	vary
1 a	3.8909 Å	0.0001	-inf	inf	<input checked="" type="checkbox"/>
2 La occ	0.5		-inf	inf	<input type="checkbox"/>
3 La iso	0.496 Å ²		-inf	inf	<input type="checkbox"/>
4 Ba occ	0.5		-inf	inf	<input type="checkbox"/>
5 Ba iso	0.494 Å ²		-inf	inf	<input type="checkbox"/>
6 Co occ	1		-inf	inf	<input type="checkbox"/>
7 Co iso	0.257 Å ²		-inf	inf	<input type="checkbox"/>

Below the table is a slider for the 'a' parameter, ranging from 3.7900 to 3.9900. There are "Start fitting" and "Continue" buttons at the bottom of the control panel. The status bar at the bottom of the software window shows: "La0.5Ba0.5CoO3 1 1 CrysPy Lmfit (BFGS) 31 (3 free, 28 fixed) 1.25 → 1.25".

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)



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

DMSC Summer school

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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 (1/2 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



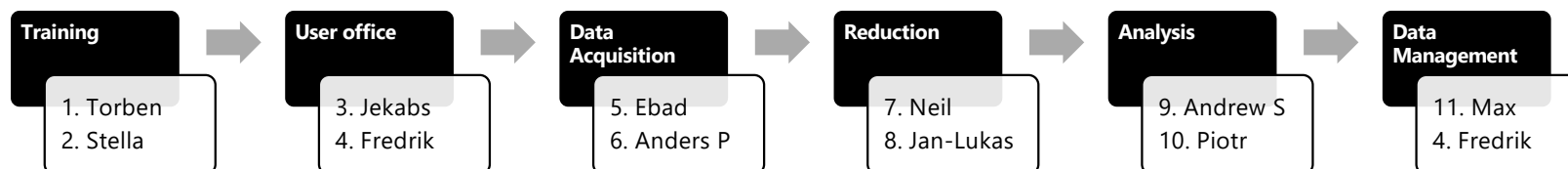
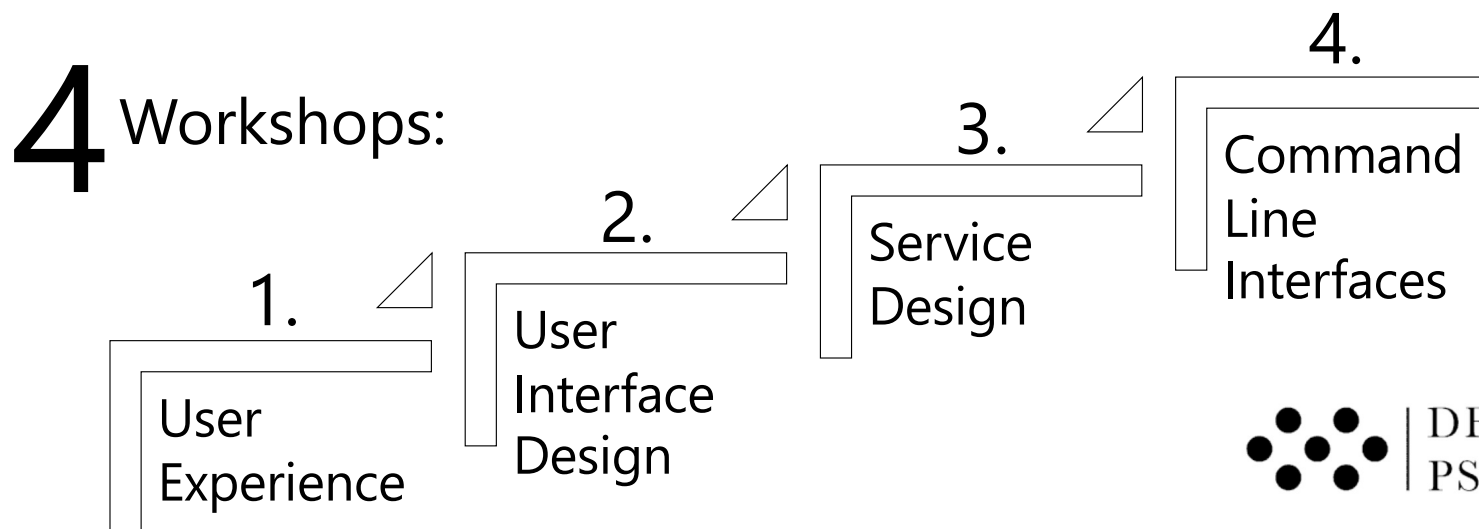
Data analysis core development

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>

