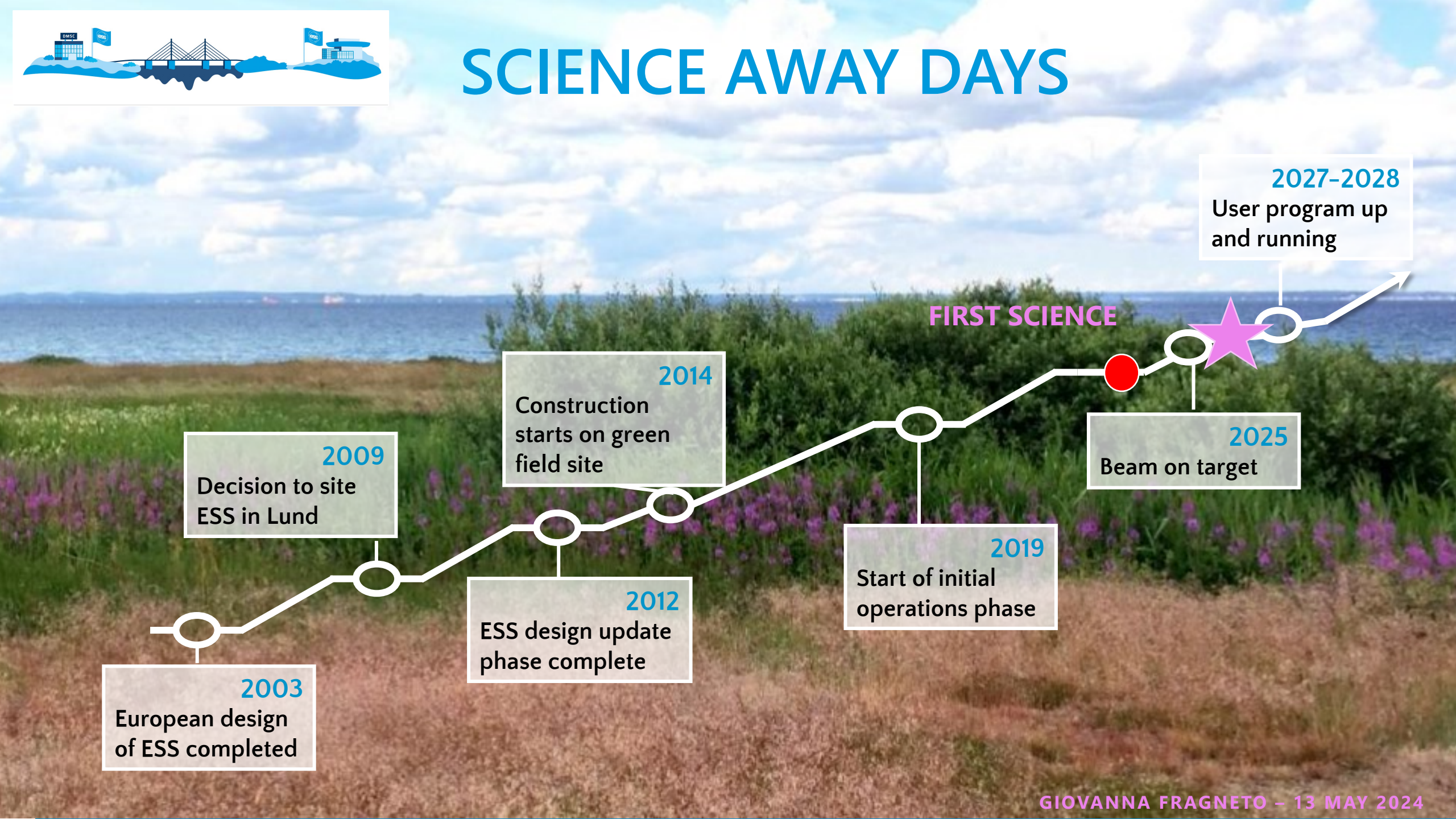
SCIENCE AWAY DAYS



Scope fo these two days

- Get acquainted with new (still evolving…) directorate structure
- Instruments and support equally important for successful scientific output:

  Discuss optimisation of synergies between divisions/groups *Unity is Strength*
- Discuss speeding up of activities towards first neutron science
- Raise issues needing attention as from now

Agenda

Morning day 1

- Presentations from instrument divisions

Afternooon day 1

- Science talk
- Discussion: how we work in SD
- Leisure activity

- *Please leave time for discussion*
- *It is not a formal meeting, we can rearrange schedule if needed*
- *Make science talks pedagogical and enjoyable by all!*

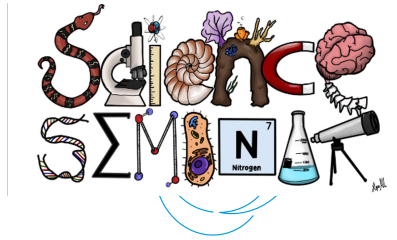
Morning day 2

- Science talk
- Presentations from DMSC
- Technical and Science talks
- Presentations from support labs and sample environment

Afternoon day 2

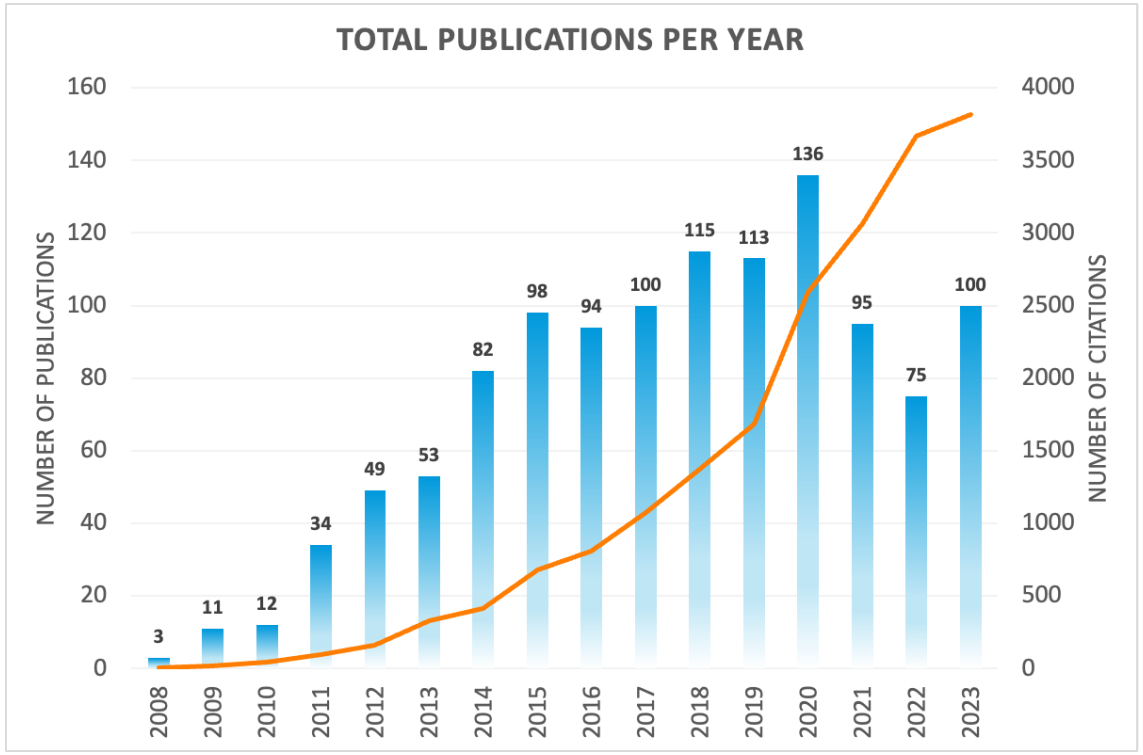
- Hot commissioning, Rescoping, Call for next instruments
- Closing discussion

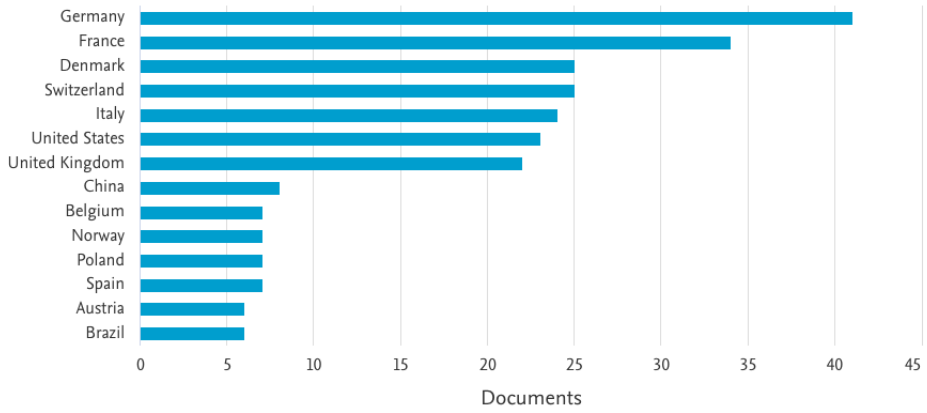
Scientific activities in the last few months

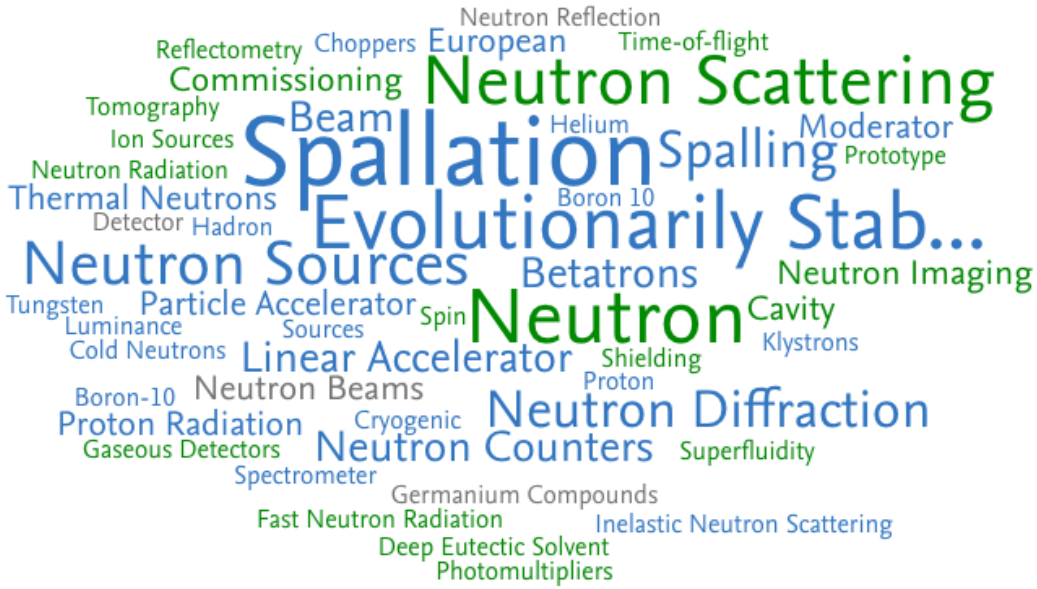


- Good attendance to internal seminars (still room for improvement….), conferences, experiments at other facilities
- First instrument operation engineers arrived to strengthen instrument teams *Welcome!*
- Deuteration laboratories on-site and promoting internal science
- Successful organisation of DMSC and FASEM schools, quantum materials workshop,…
- Fair attendance at UK user meeting, better than in previous years but ESS contribution still weak, need to be visible at national meetings
- Update website/scientists' webpages done – PLEASE PUT SOME CONTENT in the pages
- Publication portal open

Publications with ESS affiliation since 2008

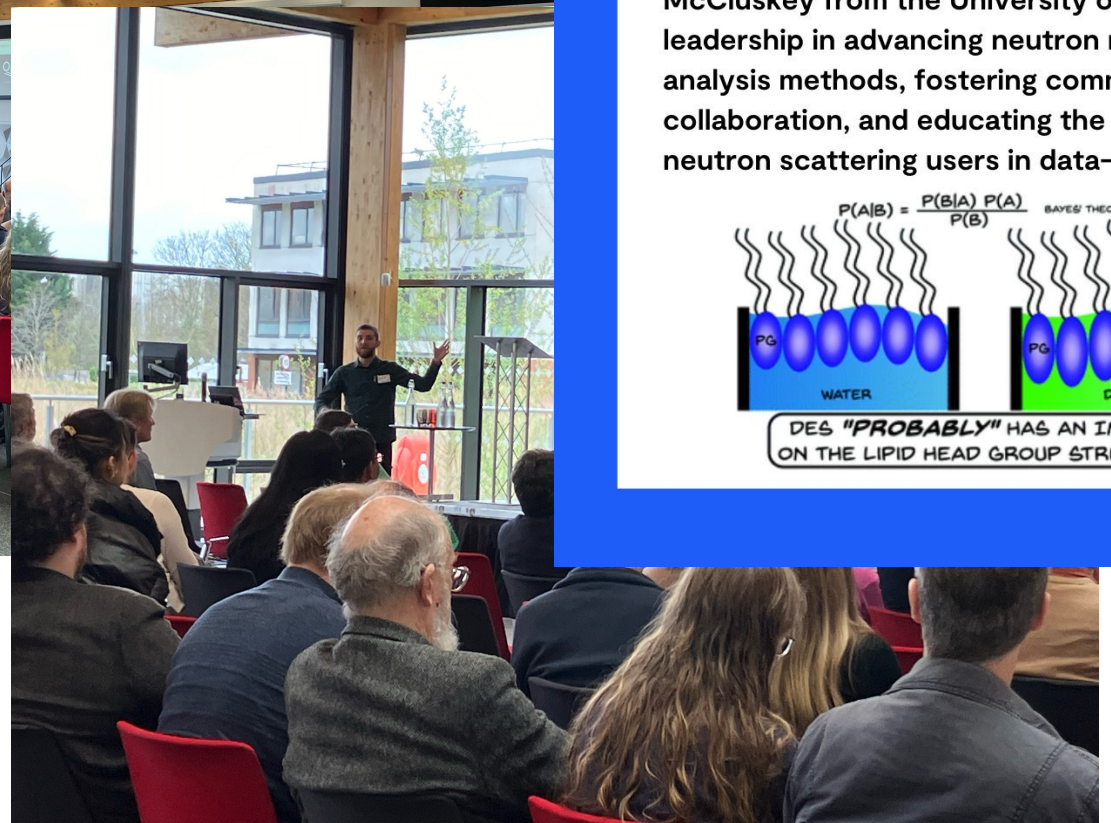






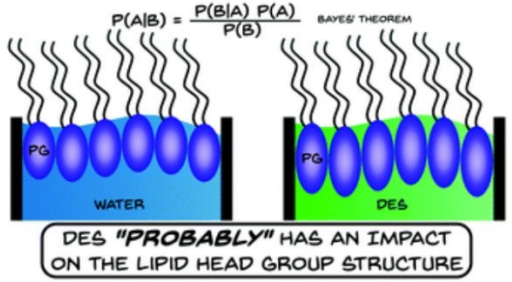
Keyphrase analysis gives an idea of content in our publications during 2023 by identifying the most frequently used keywords and their trends year to year. In the figure, size indicates relevance, **blue indicates declining usage**, **green indicates growing usage** and grey indicates stability.

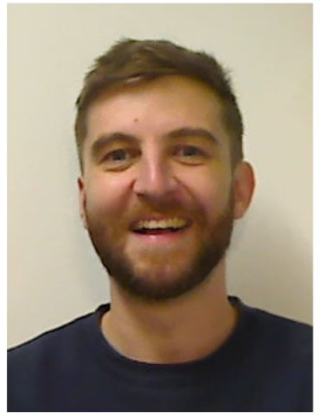
Andrew McCluskey recipient of the 2024 BTM Willis prize – received at the UK NMUM



BTM Willis Prize 2024

The winner of the BTM Willis Prize is Dr Andrew McCluskey from the University of Bristol for leadership in advancing neutron reflectometry analysis methods, fostering community standards and collaboration, and educating the next generation of neutron scattering users in data-centric science.





40 Years of ISIS Neutron and Muon Source

Science and Technology Facilities Council

ISIS Neutron and Muon Source

Delivering world class neutron science is ESS primary goal. The science directorate is in the spotlight much more than other ESS directorates and expectations from stakeholders and user community are steadily increasing.

Not everyone in the organisation has a clear understanding of our end goal. We have the responsibility to make sure that this changes and need a strong voice from a strong directorate evolving towards steady state operation.

Science Directorate current organogram

- *User office*
- *Grants team*
- *Library*
- *Scientific outreach*
- *Industrial liaison activities*
- *Students' programmes*

Science Director

Researh Coordination Office

Beate under direct supervision of SD and assisting all divisions (except DMSC) and RCO

Diffraction and Imaging Division

BEER
DREAM
HEIMDAL
MAGIC
ODIN
TBL

Large Scale Structure Division

ESTIA
FREIA
LOKI
NMX
SKADI

Spectroscopy Division

BIFROST
CSPEC
MIRACLES
T-REX
VESPA

Data Management and Software Center

- Instrument Data Reduction & Data Analysis
- DMSC Computer Center/System Operations
- Instrument Data Scientists
- Scientific Web Applications

Scientific Support Division

On-interim head of division internal position open until end of the week

- Chemistry and Life Science Support Group — *Decision to stop optics activities for the time being and until end of project*
- Materials Science and Physics Support Group — *Polarisation activities moved to NSS – contract for MeOP filling station signed with ILL*

Instrument scientists (hiring at least one scientist per instrument in progress)
Instrument operations engineers (6 hirings in progress)
Post-docs, students (to come)

SSO review:

exercise carried out in last quarter of 2023; external committee met 5-6 November; chair J. Daillant

***Panel 2, Science Directorate**, chaired by Z. Bowden (STFC) with Hans Christen (SNS-ORNL), Toby Perring (ISIS-STFC), Karen Edler (Lund University), Regine Willumeit-Römer (Hereon), Mark Johnson (ILL), Russell Ewings (ISIS- STFC), Elizabeth Blackburn (Lund University).*

Final report presented to Council 36; ESS will work taking into account the panel advice; SSO organisation to be validated by end of 2024 in order to establish operation budget; science directorate proposed model will need optimisation especially in support activities planning (sample environment, laboratories, technical support). Better benchmarking with existing facilities is requested and a reduction of staff numbers (avoiding doubling of roles in the facilities - silos).

Steady State Review

We need to work through use cases

- To come to a better understanding of steady state operations the review urged us to dig into a variety of use cases

- This work aims to:
  - Increase understanding of what operations looks like for those in user facing roles
  - Increase understanding of ownership of equipment and responsibility
  - Improve uniformity of service offered within the science directorate
  - Decrease duplication of labour and non-labour costs within and beyond the science directorate

Courtesy C. Lobley

Employees on the User Journey

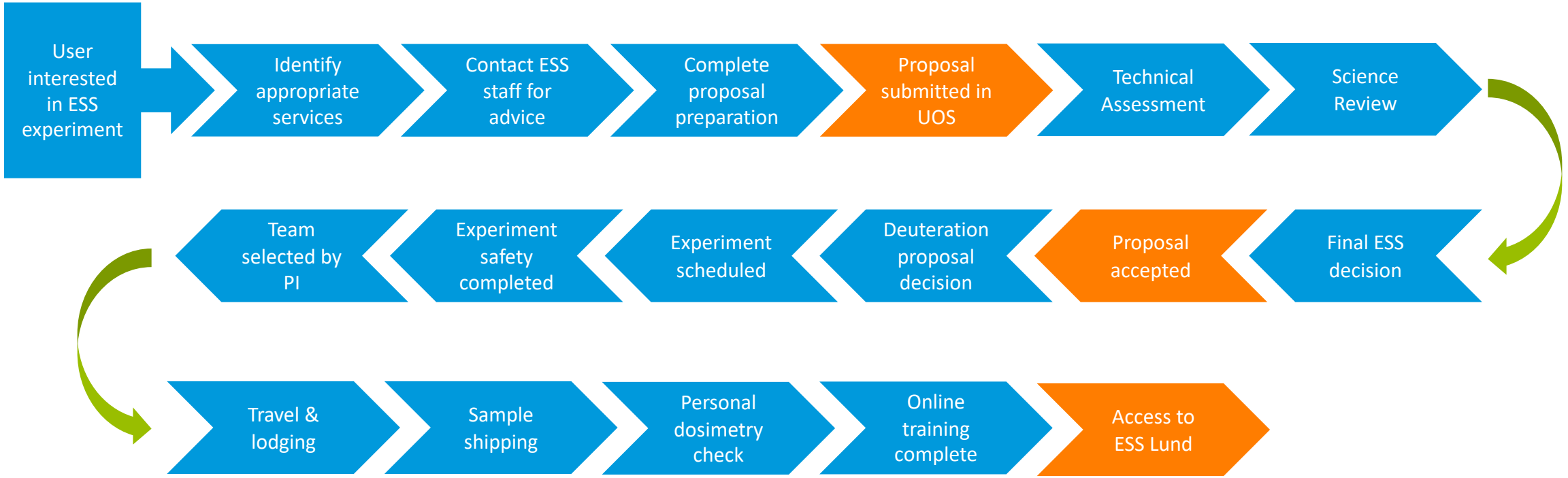
There are a number of ESS staff who interact with the users

- One key part of the use cases work on-going is to understand the ‘types’ of people involved in user facing roles
  - Instrument scientist (local contact/panel secretary)
  - Instrument data scientist (local contact)
  - Instrument operational engineer
  - Sample environment scientist
  - Sample environment engineer
  - Sample environment technician
  - Laboratory scientist
  - Laboratory technician
  - Deuteration scientist
  - Occupational health and safety (OHS)
  - Radiation protection (RP)
  - Hall coordinator
  - User officer

Courtesy C. Lobley

Detailing the user journey - 1

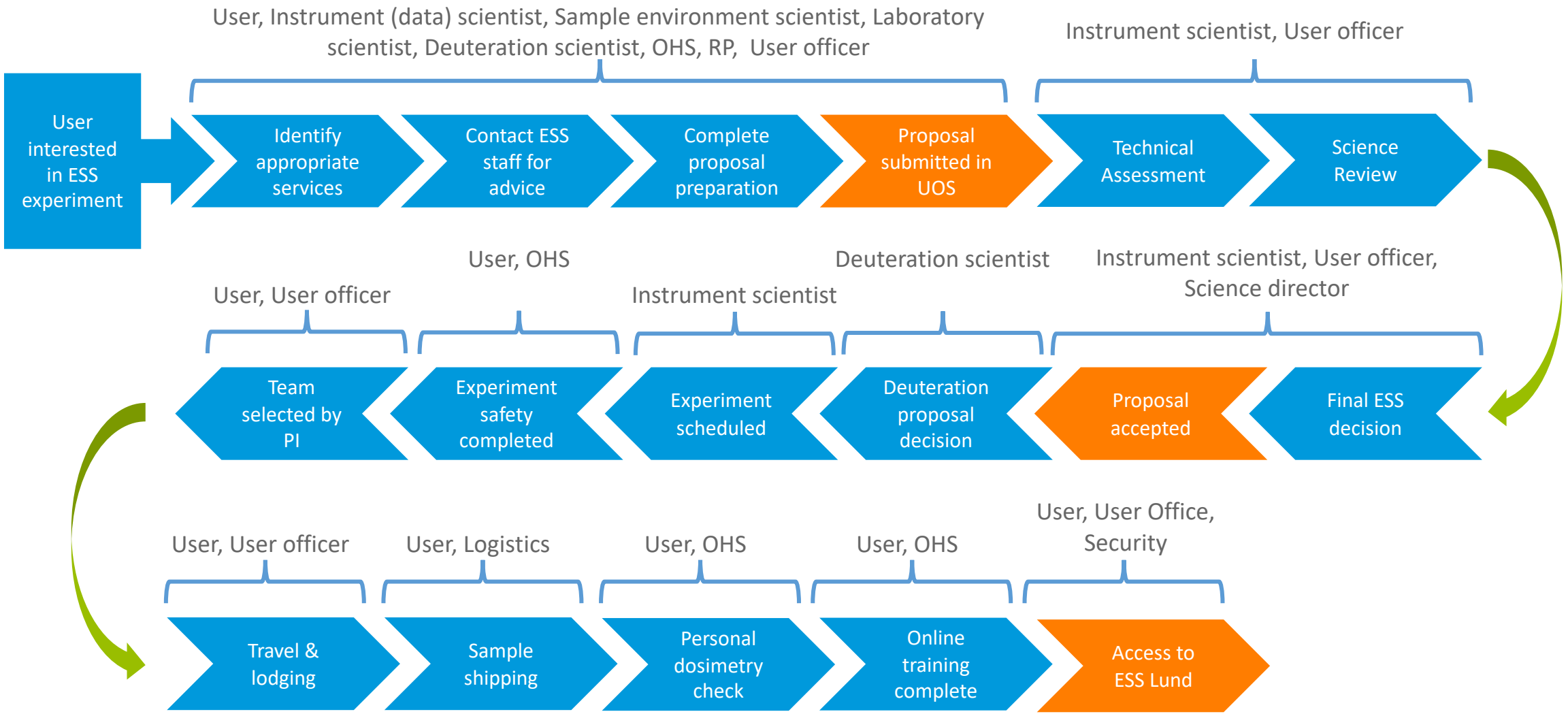
Before ‘coming’ to ESS



Courtesy C. Lobley

Detailing the user journey - 2

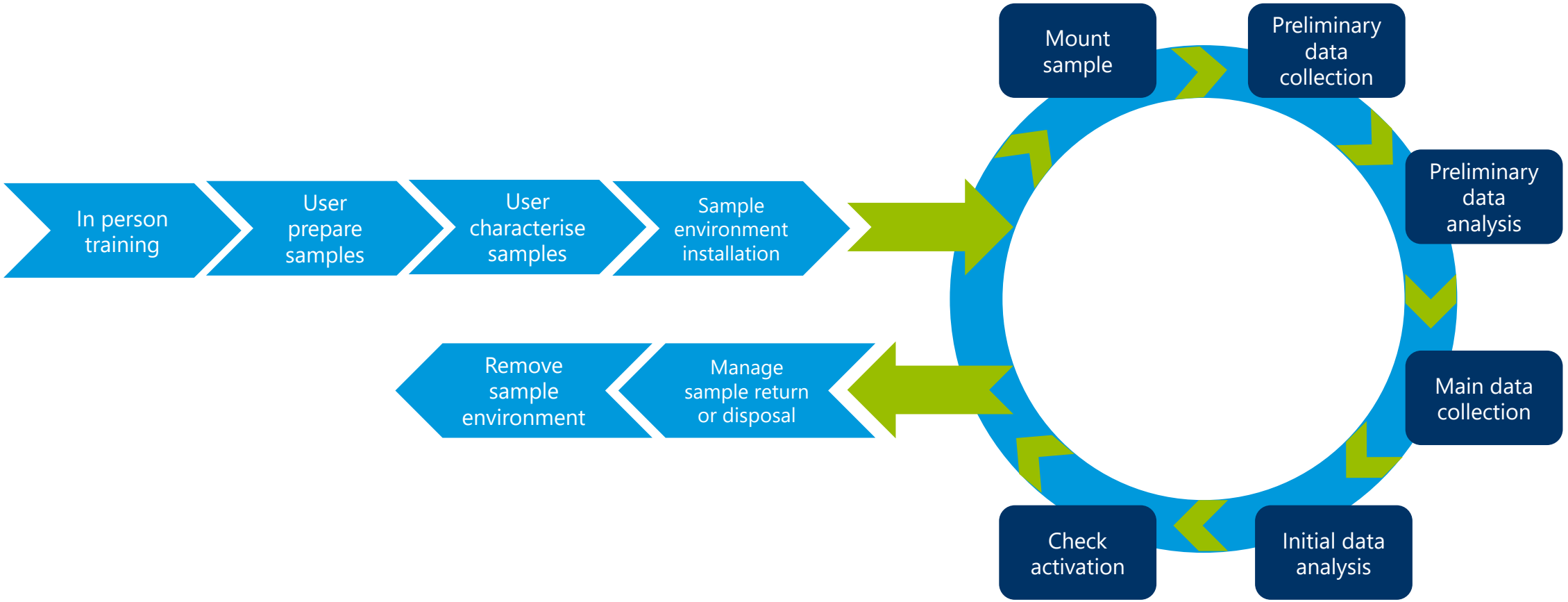
Before 'coming' to ESS



Courtesy C. Lobley

Detailing the user journey - 2

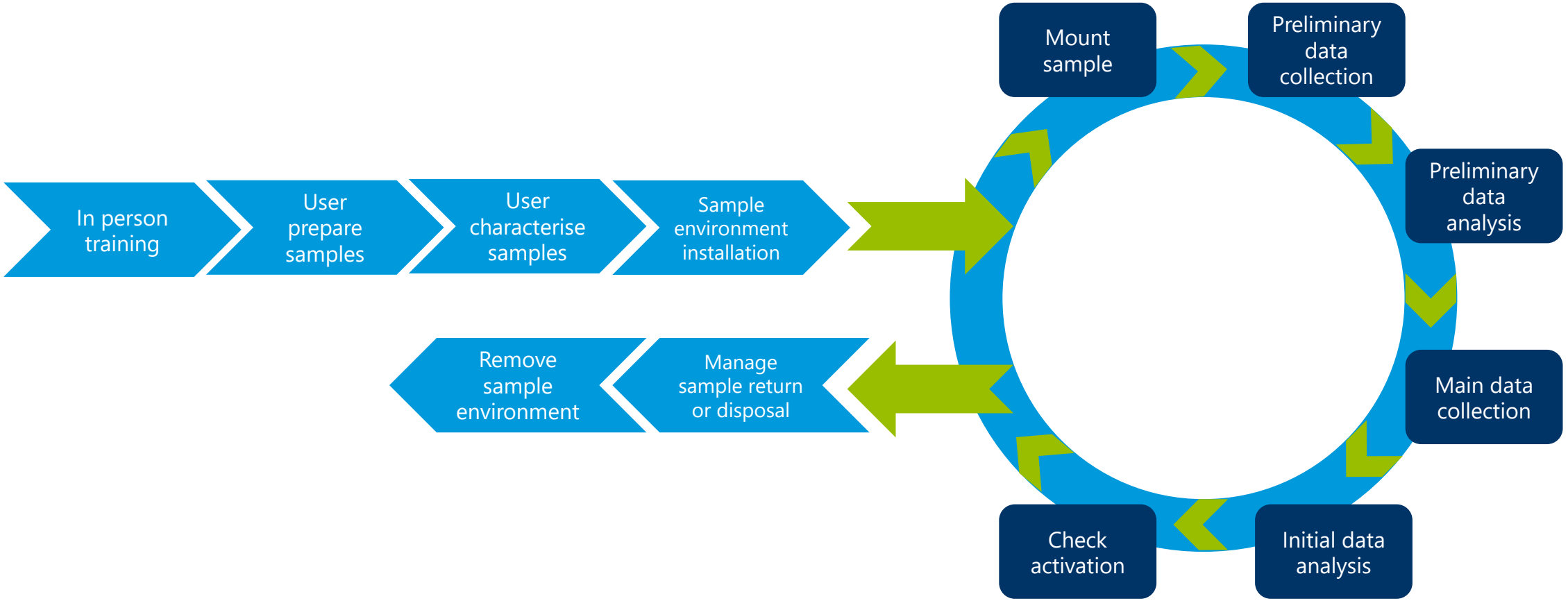
'At' ESS



Courtesy C. Lobley

Use Case 1

Powder diffraction experiment on DREAM
Metal doped alumina & *in situ* gas loading with H_2

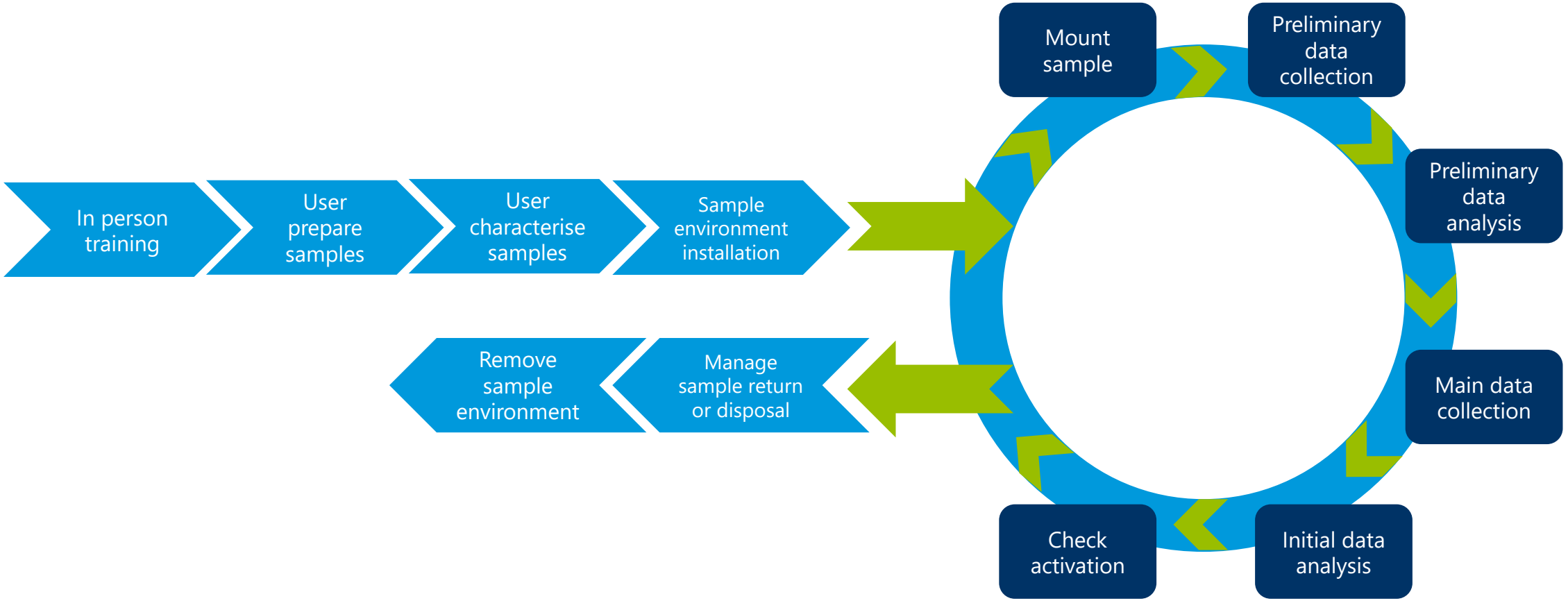


Courtesy C. Lobley

Use Case 2

NB: This case is unrealistically simple - update in progress

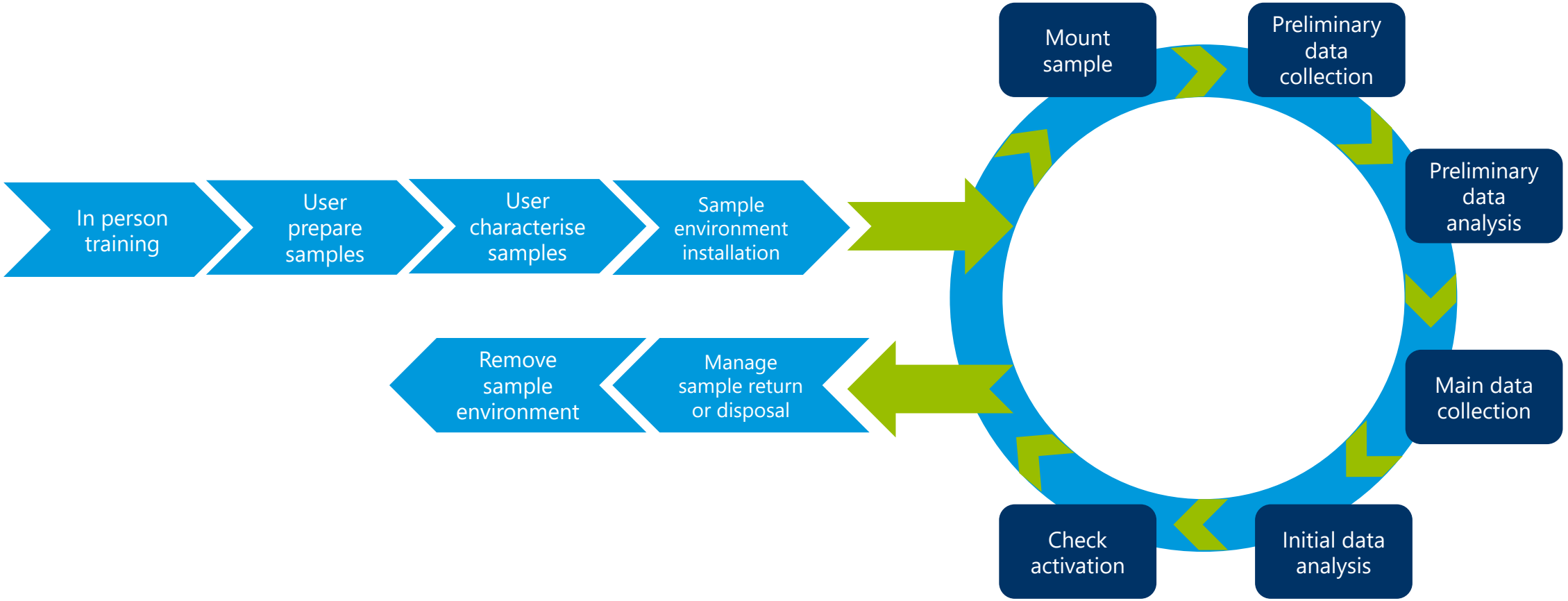
Small angle neutron scattering on LOKI
Deuterated liquid sample with sample changer



Courtesy C. Lobley

Use Case 3

Single crystal magnetic material on CSPEC
Magnet, rotation stage and dilution fridge



Courtesy C. Lobley

Detailing the user journey - 3

After ‘leaving’ ESS

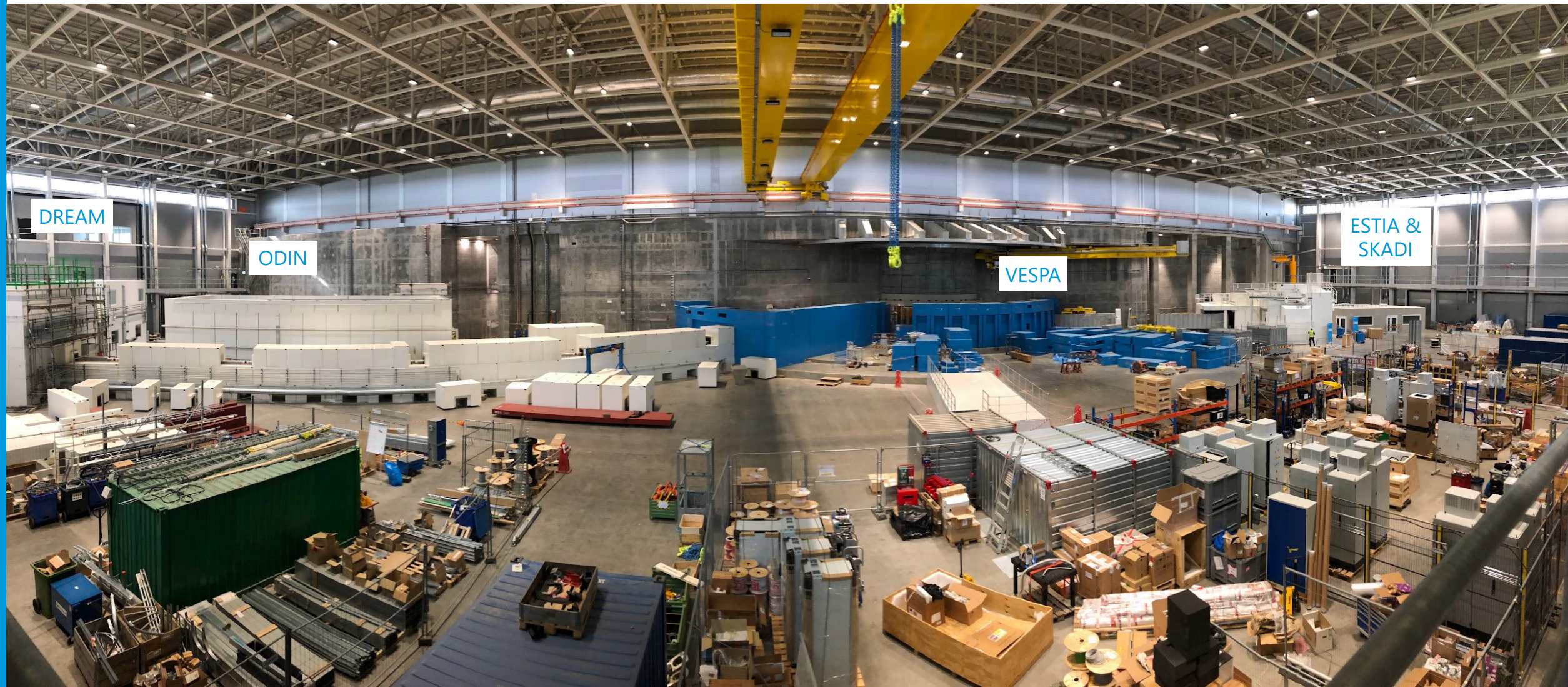
Courtesy C. Lobley

Moving towards first science

INSTRUMENTS READINESS

Neutron Instruments

D01 side



Neutron Instruments

D03 side

Neutron Instruments

Week 6: The in-bunker neutron guide section for LOKI is being assembled and aligned in an area next to the cave.

Tranche 1 is progressing:

The current focus is getting LOKI, BIFROST, ODIN, DREAM, NMX and TBL ready for BOT

In bunker components for later instruments are also being prioritized to limit future bunker work

Cave installations for ESTIA, SKADI and MAGIC ongoing

Re-planning of later instruments

Reflecting reality

The majority of instrument plans at the time of the re-baseline were unrealistic

- Still in design phase
- Contracts still to be placed
- Commissioning plans yet to be defined
- Schedules held by partners and not linked sufficiently (or at all) with ESS master schedule

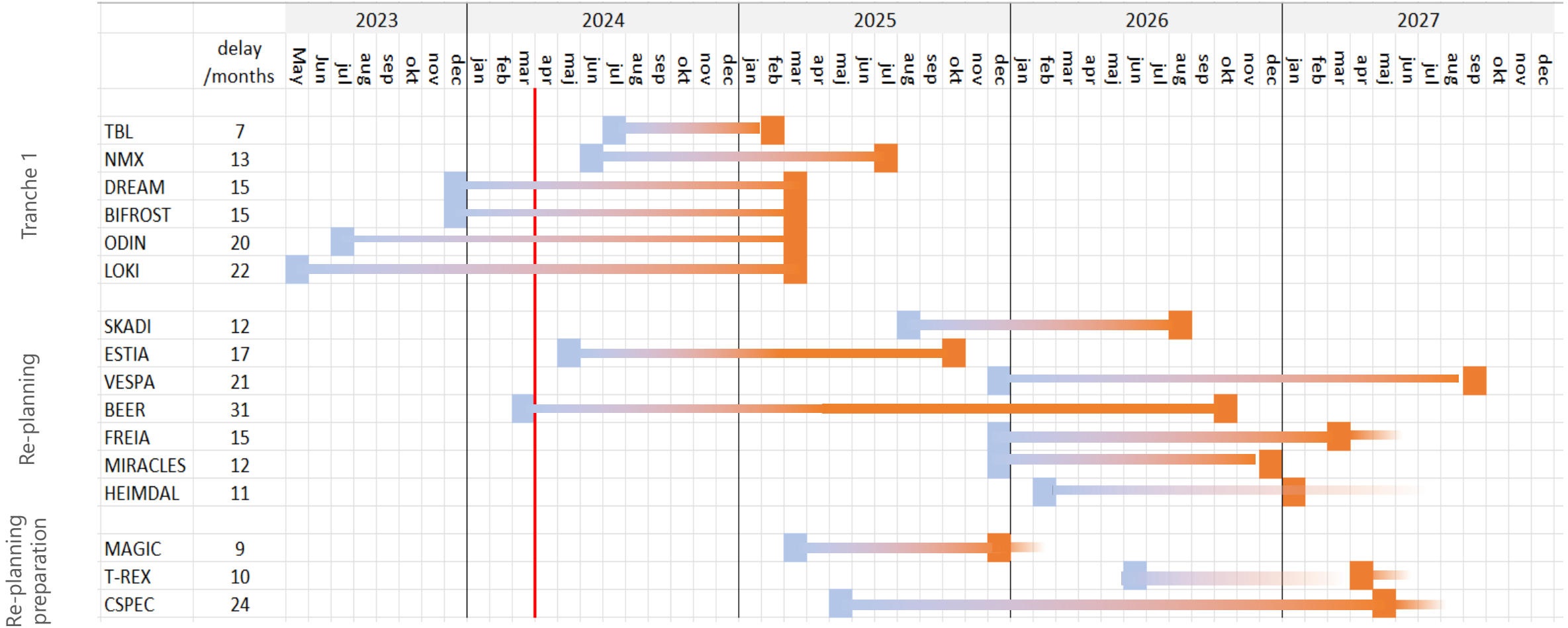
Re-planning of tranche 2&3 instruments to reflect reality:

- Massively improved durations and logic, now integrated into master schedule
- Understanding of constraints, issues and risks
- Acceleration measures (additional resources for instance)
- Dedicated planning resources being made available
- Detailed week-long workshops for each instrument

Courtesy R. Connatser

Re-planning of later instruments

Delay of TG5 milestone for all instruments



Courtesy S. Ossowski

Rebaseline of T2-T3 instruments: danger

Our Governance bodies as well as ESS management alerted by the slippage of dates for T2 and T3 instruments

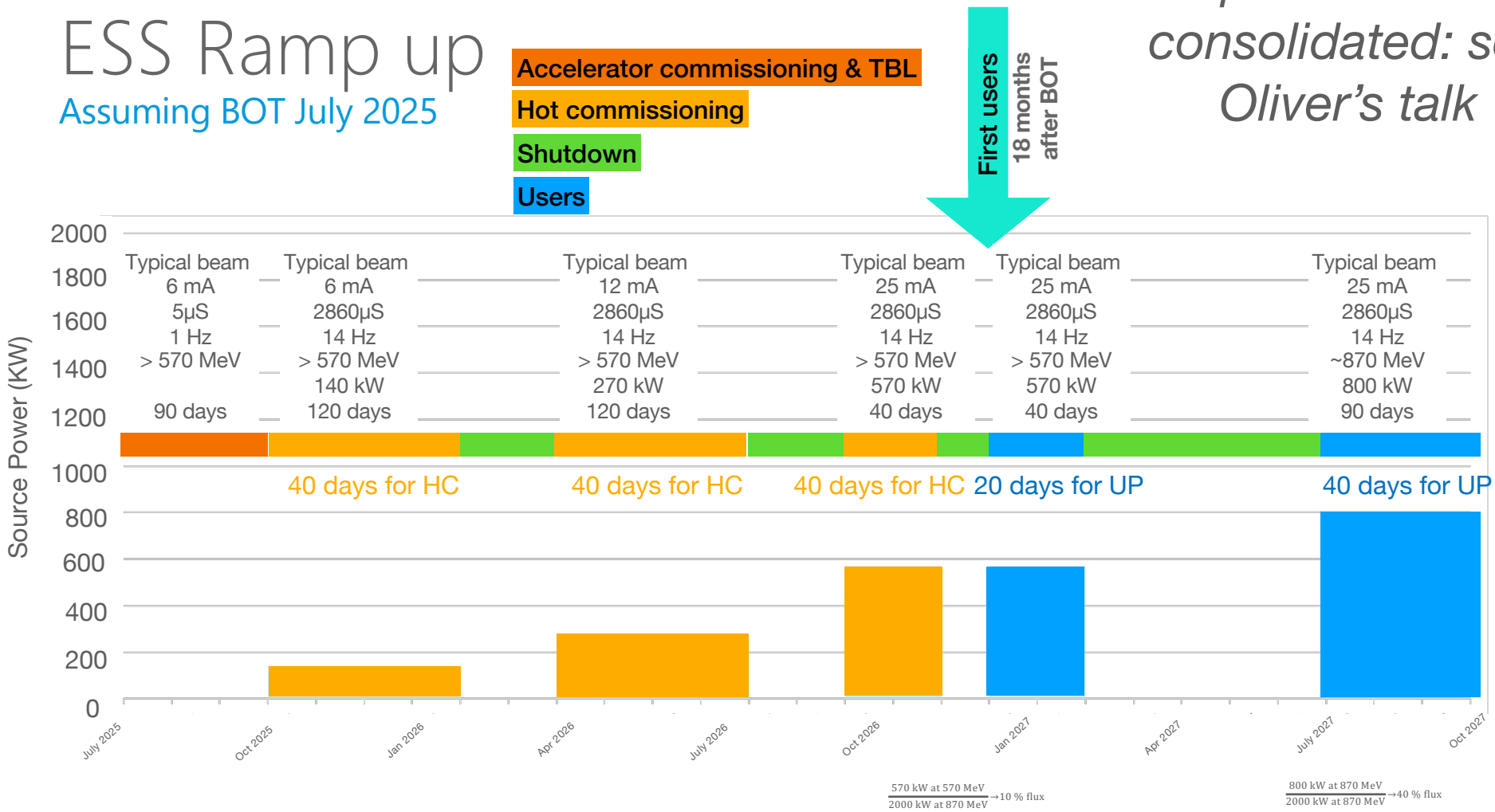
A fast reaction is requested to minimise harm and risk of not delivering 15 instruments by end of projects:

- ✓ Reorganisation of some activities are being planned
- ✓ An improved instrument project structure in progress (more news to come soon)
- ✓ New actions with in-kind partners planned to discuss *ownership* of late instruments

ESS Ramp up

Assuming BOT July 2025

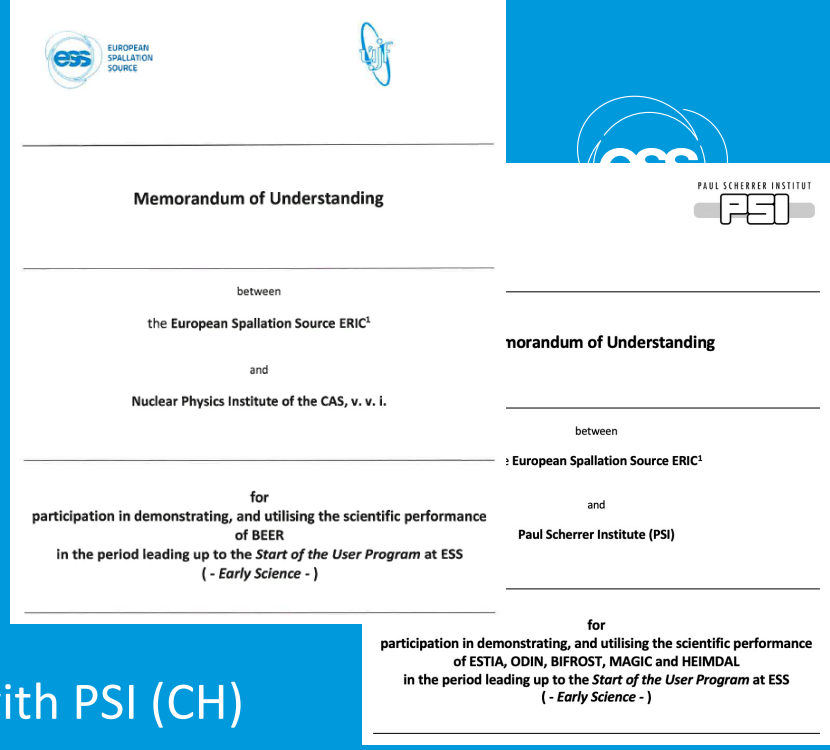
Hot commissioning plans to be consolidated: see Oliver's talk



See ESS-0420218 "Early operations of ESS and prerequisites for first scientific results" for more details

Courtesy P. Deen

Moving towards first science



- MoU with in-kind partners signed with NPI (CZ) and to be signed with PSI (CH)
- 6 Post-docs for first science included in costbook
- Workshops and brainstorm with user community organised throughout 2024
- Participation to grants' applications
- Benchmarking; rescoping; use cases study; reorganisation of STAPs; …
- Access policy

ESS Initiatives for HORIZON 2024 INFRA Calls

SAKURA MOBILITY PROGRAMME

Acronym	Coordinator	ESS Role	ESS Contact	Notes
BOBINE: Bettering Our B-field Infrastructure for Neutrons in Europe	ILL	Partner	Alex Holmes	
AI4SI: Artificial Intelligence for Science and Innovation	ILL	Partner	Thomas Holm Rod	Resubmission
SPLENDID: Single Photon Localization Event-based Neutron Detectors for Imaging and Diffraction	TUM	Partner	Manuel Morgano Robin Woracek	Resubmission
NEMO: Development of NEsted Mirror Optics for European Neutron Research	ESS	Coordinator	Valentina Santoro	
ARTIFACT: ARTifical Intelligence For Accelerators, user Communities and associated Technologies	GANIL	Partner	Thomas Shea	
ACTNEXT: Advanced Characterization of Technical components for NEw power-to-X Technologies	DTI	Letter of Support	Robin Woracek Manuel Morgano	
THEIA: Modular Tribometer for Hydrogen Environment In operando Analysis of Materials with Synchrotron and Neutron Beamlines for Research Infrastructures	AC2T	Partner	Caroline Curfs	
DICE: Development of an Infrastructure for colder neutrons without Carbon Emissions at the ESS	ESS	Coordinator	Valentina Santoro	Continuation of HighNESS project

INFRATECH

INFRADEV

Courtesy S. Ucer

ESS meetings organisation & first science brainstorm

NMX – ECM 34 – (Padova)

SANS - ECIS 2024 satellite – (Copenhagen)

IMAGING – NEUWAVE 12 (Lund)

DIFFRACTION - IUCr High Pressure (Lund)

REFLECTOMETRY – SXNS & ORSO (Grenoble)

ILL/ESS USER MEETING – Grenoble

ORSO

STAPs role and organisation currently under discussion

Current STAPs and Responsibles:

Diffraction – Werner Schweika
NMX – Esko Oksanen
Spectroscopy – Pascale Deen
Imaging – Robin Woracek
MSPS – Caroline Curfs
CLS – Monika Hartl
Reflectometry – Tom Arnold
DMSC - Thomas H Rod
Fundamental and Particle Physics – Valentina Santoro
SANS – Andrew Jackson

Proposal for future STAPs:

Diffraction
Spectroscopy
Imaging
LSS
Sample environment
Support Laboratories
DMSC
Fundamental and Particle Physics

Start move towards an advisory committee for first neutron experiments and evolve slowly towards beamtime proposal panels

Current organisational changes

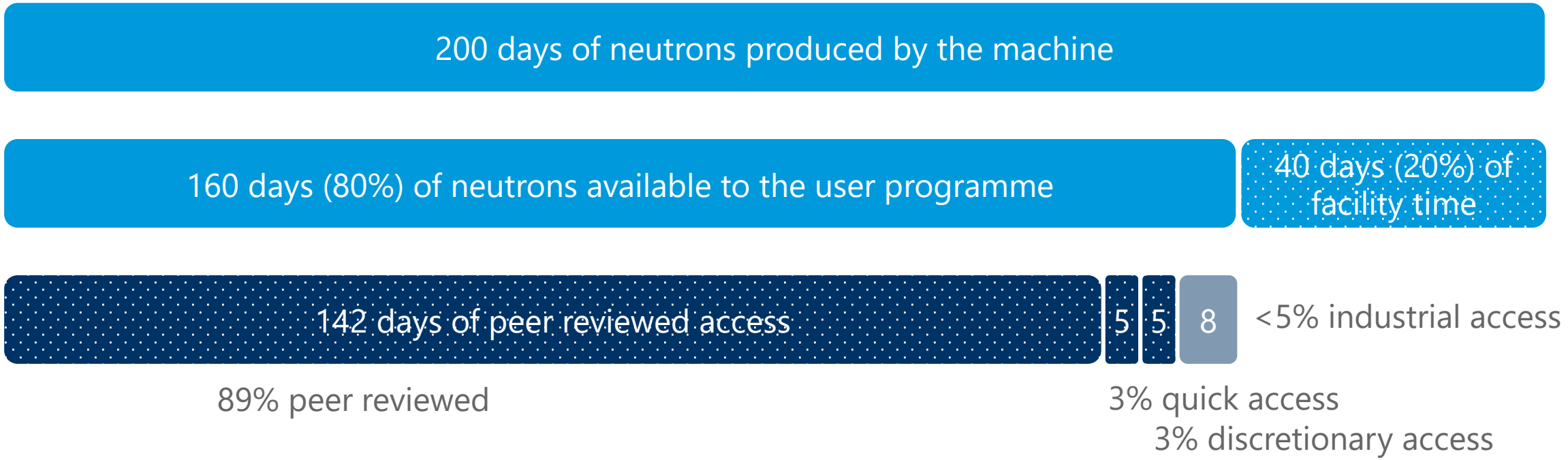
- Organisation and budget centralised in Research Coordination Office
- On-site meetings to be held the same week as SAC with common introductory session
- *On-site* support activities STAPs' meetings to take place in spring and instrument STAPs' meetings in autumn
- Where appropriate replace overseas with European members (can include people from in-kind partners)

Scientific Evaluation and Access Policy

COURTESY CARINA LOBLEY

2024-04-18

ESS Access to Neutron Instruments



- ESS staff have access to any facility time not needed for other work
- ESS staff are invited to use the peer review process
- ESS can apply for quick or discretionary access

Current Status

The Access Policy is currently under scrutiny by ESS Council

Issues to address:

- The policy should reference the European Charter — Done
- Define modes of access and % for public beamtime — Done
- Clarify the use of the in-house 20% — Done
- Clarify that % are expected averages across instruments/years — Done
- Add new options e.g. programmatic access, EU access
- Define the modes of industry access — Done
- Decide on the cost for proprietary access
- Define the algorithm for calculation of usage
- Prepare a paper on the advantages/disadvantages of T&S funding — Done
- Decide on whether to have an institutional user agreement

Travel and Subsistence

2.25 researchers funded per experiment

User Office Funded

Travel:

- A return flight between airport nearest the user home institute and Copenhagen
- Train travel from Copenhagen to Lund
- Unlimited tram travel in Lund

Accommodation:

- For the experiment duration plus one night
- Forskarhotellet, Motel L, Hotel Concordia
- (separately preparing a document/case for user accommodation at ESS)

Meals and Refreshments:

- Daily allowance, assuming breakfast is taken at the accommodation

Not User Office Funded

Travel:

- Travel to and from home airport
- Taxi/hire car between Copenhagen and Lund
- Food or drink on the journey
- Insurance e.g., travel, health

Visas or passport fees

Sample Shipping

Lab Consumables

Future science at ESS

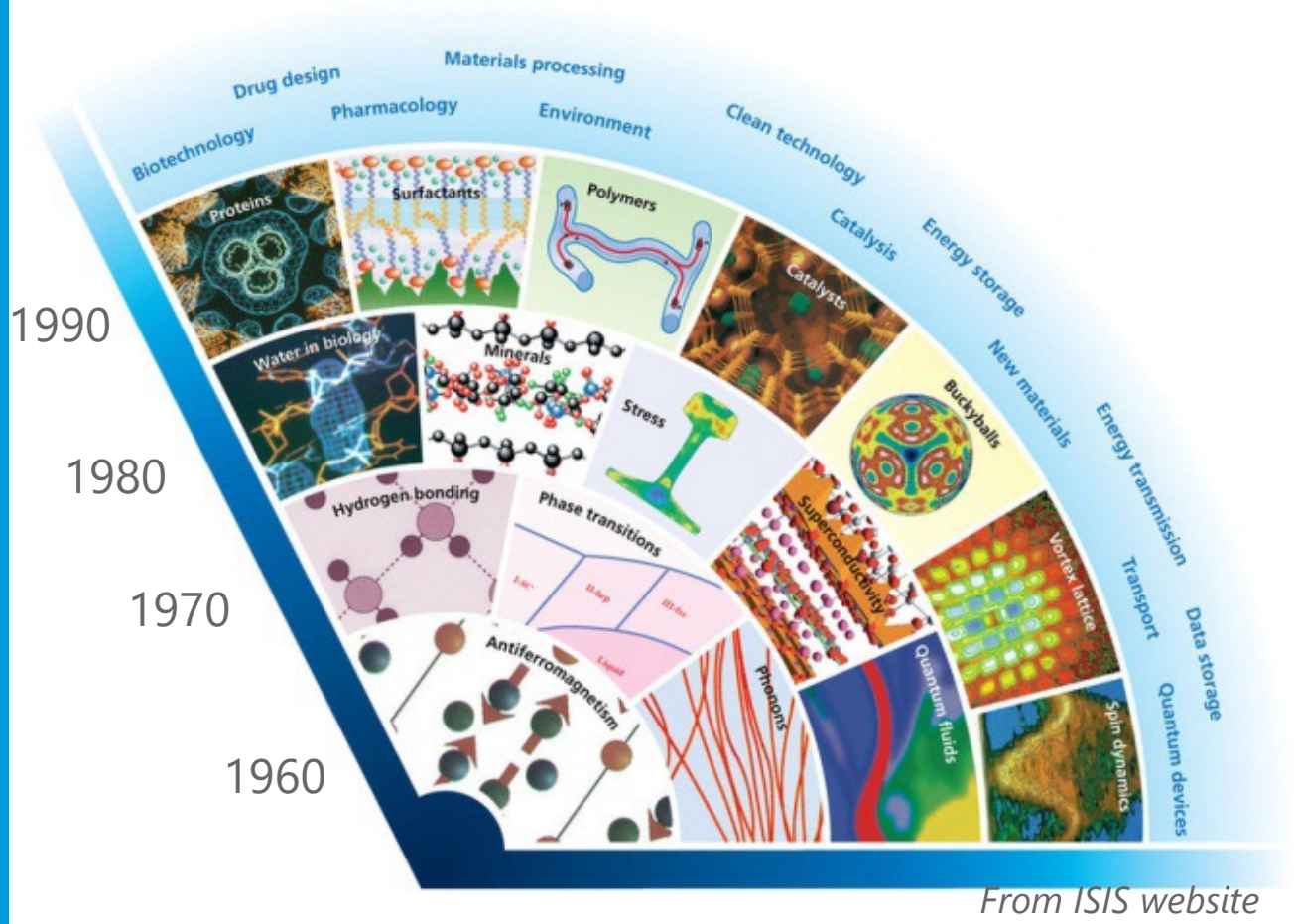
Courtesy H. Wacklin-Knecht

Advances expected in capabilities at ESS:

- Rapid data collection / short counting times to enable kinetics and high-throughput studies
- Probe broad size range to examine hierarchical structures
- Small samples for scanning, biological and complex samples
- Integrated flexible sample environment for non-equilibrium studies
- Integration of complementary techniques experimentally and in data analysis

Future scientific challenges:

How can the advantages of ESS be used to meet societal challenges?



From ISIS website

- Improved understanding of materials and production processes
- Elucidating disease processes and improving medical treatments
- Helping the green energy transition
- Developing the next generation of smart materials and IT
- Furthering our understanding of the universe

How, why and when should different scientific challenges be prioritised at ESS?

Market analysis

- What are the topical questions?
- What creates high impact?
- What does industry need?
- What could be addressed using neutrons?
- What other techniques are used?
- Who is doing this research and what do they expect?
- What are the future trends?

How: STAPs, First science workshops, Literature, Conferences

Science case

- Which ESS experiments can address the scientific market?
- What is unique about the information obtained from neutron experiments?
- How will ESS advance the field?
- What does ESS need in order to support the research?

From: Instrument science cases, Scientific support cases

Business case

- Benchmarking to other facilities
- *Scientific performance and*
  - source power
  - instrument scope
  - science support facilities
- ESS strategy to support the science

By: Continued benchmarking, Following developments

⇒ Scientific scope and prioritisation for supporting high impact research

(cf. capability gap analysis for instruments)

Many thanks to Bea and Carina for the organisation of these days

Looking forward to constructive discussion and improved cooperation among all parts of the directorate