



Update ESS and Science Directorate

STAP meetings April 2021

PRESENTED BY ANDREAS SCHREYER, DIRECTOR FOR SCIENCE

14 April 2021



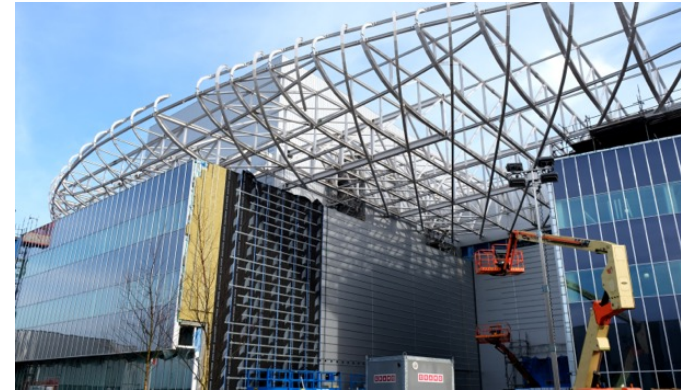
Outline

1. **ESS Project Highlights**
2. **Progress in the Science Directorate**
3. **Move to Campus**
4. **Ensuring ESS plans and resources are aligned**
5. **Conclusions**

Project Highlights



Project Highlights – CF



Structural steel and cantilever roof takes shape as well as final building cladding

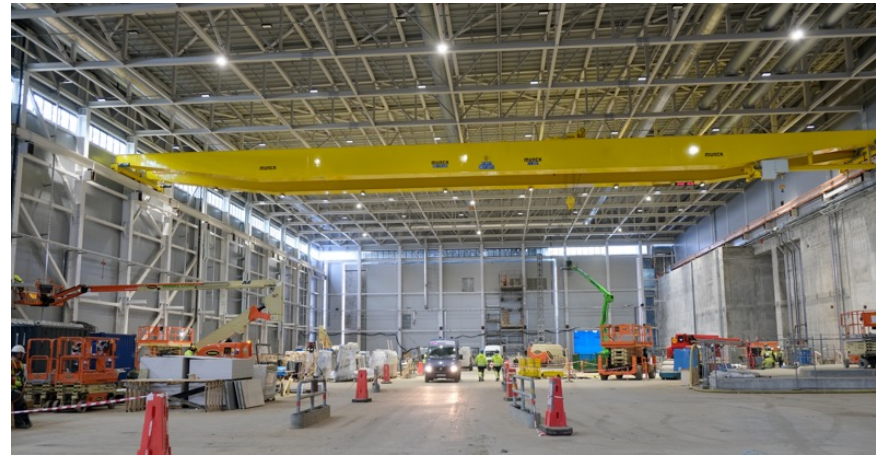


CF External Review completed.
Skanska is at 85% staffing due to second wave

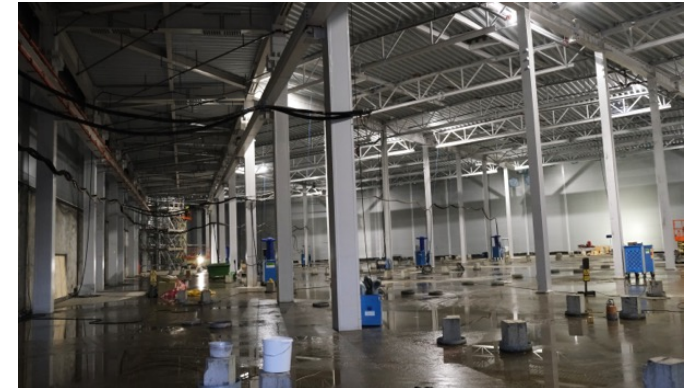
Project Highlights – CF



D03 overhead crane commissioned, and bunker crane installed

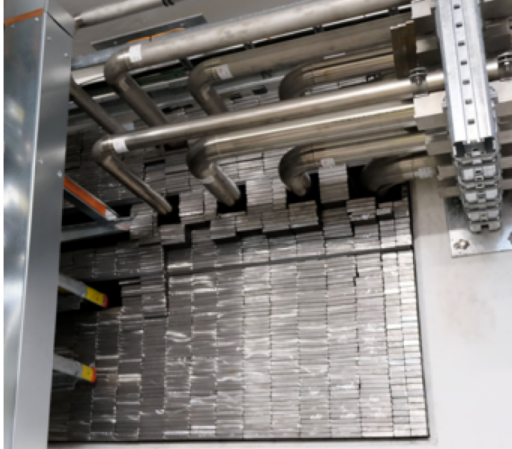


The 50m D01 overhead crane is welded and lifted in place, testing ongoing.



D01 crane consoles welded in place; D02 Transport Hall entrance gates; E02 part 2 installations.

Project Highlights - Accelerator



NCL Shielding: front end penetrations, front end chicane wall and drop hatch shielding.



Temporary shielding wall.



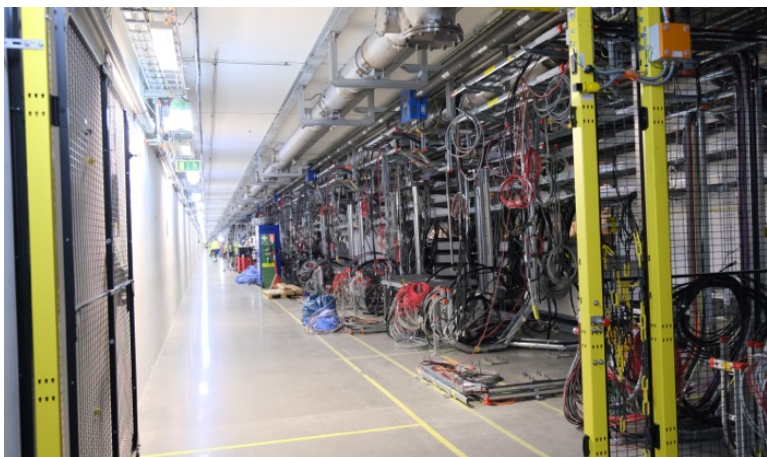
Stands for LWUs.

Project Highlights - Accelerator



First MB Modulator tested and in place.

NCL Modulator #1 and Klystron operated at full power, 5 of 6 NCL Klystrons in place.



Electrical installation in Gallery and Tunnel (cable pulling) continues now in SPK, MBL and HBL.

Project Highlights - Target



16 NBPPs on site, with only 10 to come this year



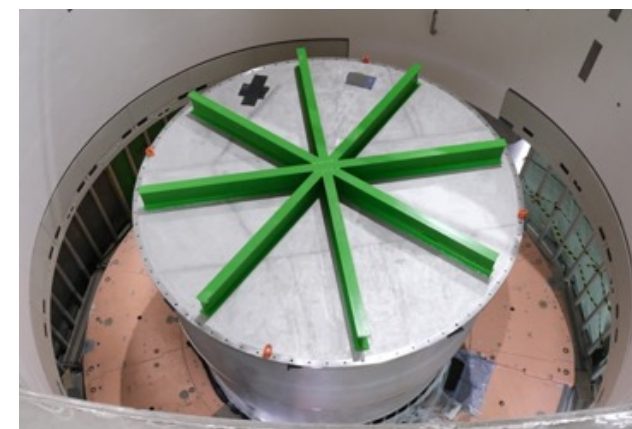
Proton Beam Window Vessel and port block parts ready to ship to ESS



Mockup and test stand assembled in Transport hall



<-Final Machining of wheel



Vessel lower & mid installed

Project Highlights - Target



Active Cell: RACE infrastructure works.



High bay: Ventilation ducting and piping.



Utility installations.

Project Highlights - ICS



Activities for NCL ongoing projects are progressing according to plan
Good and steady progress with the PSS1-a iteration of the personnel safety system, focus now on integrated testing the associated access stations



Network and computing equipment in the H01 server hall, 1.3Pb of backup storage

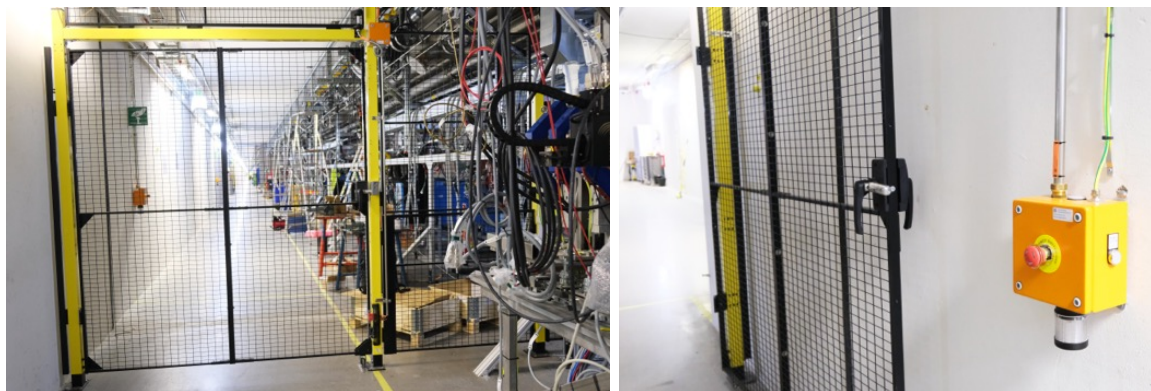


Equipment installed and deployed by the ICS infrastructure group ESS firewalls

Project Highlights - ICS



Personnel Safety Systems installed in Front End Building.



Project Highlights - NSS



Bunker Pillar system installing in D03, outer west wall shielding 95% assembled.



Bunker North sector (D03) and East and South sector (D01 side)

Project Highlights - NSS



E04 labs fitted out and operational.

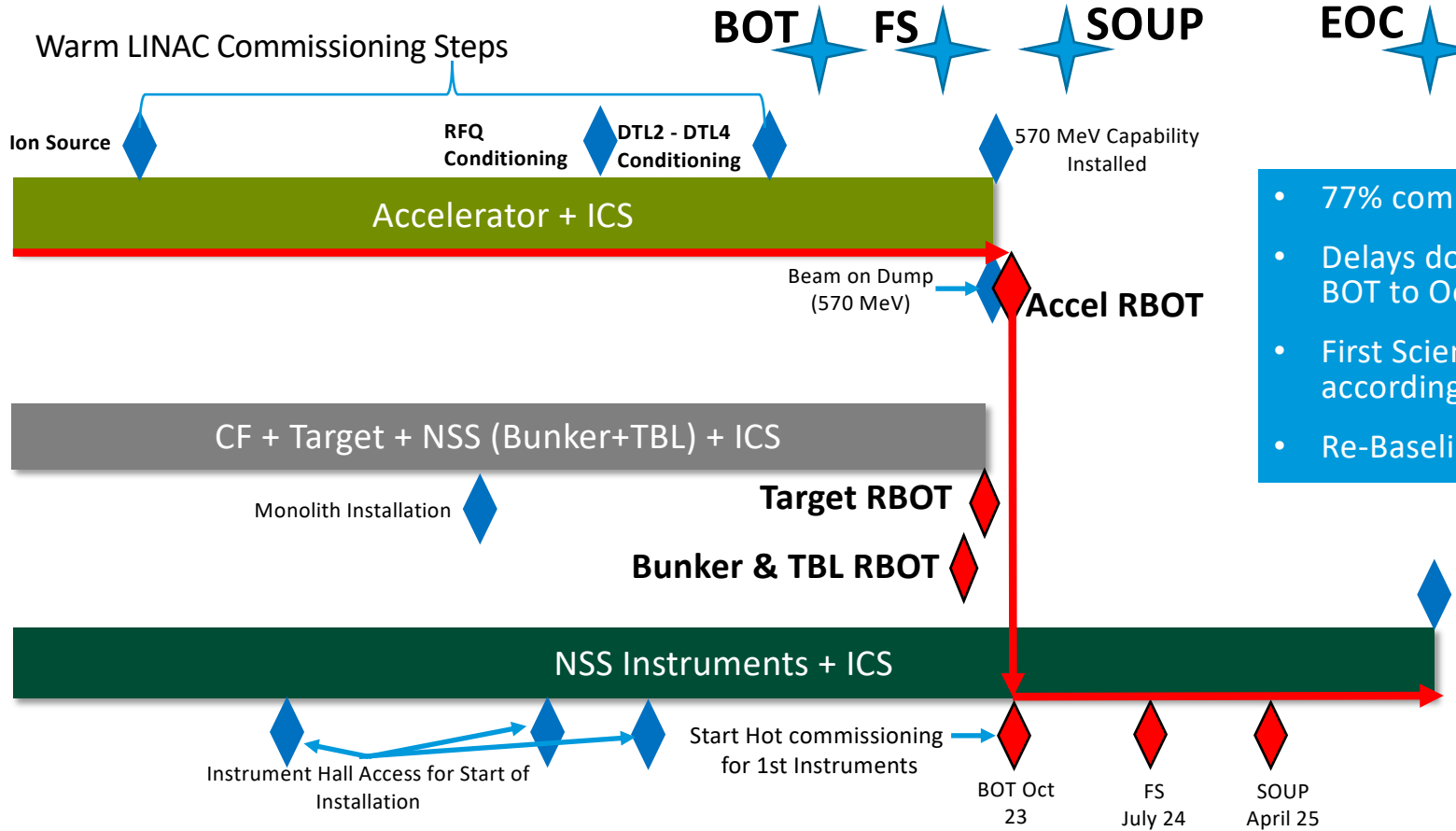
Summary Schedule and Critical Path for Remaining Work (Zero Float Schedule)



2018 2019 2020 2021 2022 2023 2024 2025

Baseline Dates

- BOT - Beam on Target July 22
- FS - First Science March 23
- SOUP - Start of User Prog Dec 23
- EOC - End of Construction Dec25



- 77% complete
- Delays dominantly due to pandemic move BOT to October 2023
- First Science and SOUP delayed accordingly
- Re-Baselng planned for Fall

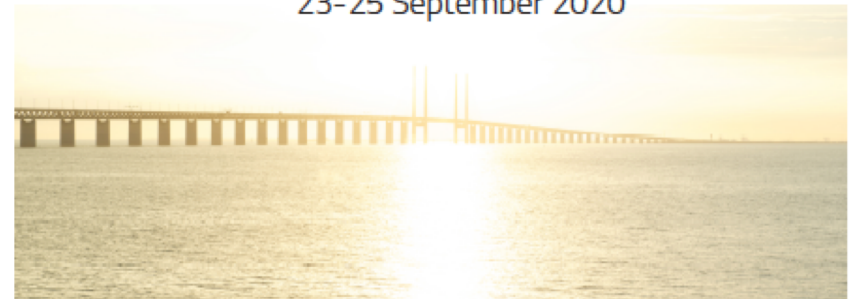
Red line indicates critical path

Progress in the Science Directorate



ESS ILL User Meeting 2020

Lund, Sweden
23-25 September 2020



Welcome to the second ESS ILL User Meeting

- Plenary talks about using neutron science to meet societal challenges
- Reports on recent achievements and ongoing work at ESS and ILL
- Focused parallel sessions on specific areas of neutron science

neutrons4europe.com



ESS/ILL Topical Workshop on Chemistry and Magnetism



13. October 2020,
<https://indico.esss.lu.se/event/1542/>

Zoom Webinar

a quantum liquid of magnetic octupoles

s, comparison to predictions for QSI monopoles ('two spinon contin...

212 registrants

A

Lingjia Shen (Lund Univ...)

Page 15

2021-04-14 PRESENTATION TITLE FOOTER

Introduction: Link to the meeting; https://ill.zoom.us/j/94763977623?pwd=V2REeW5QOXFkZkUxV1JlVkdQUVNFQT09 Please note that the zoom public link directs you to a page where - if you don't already have a Zoom account in use - yo...	
	Manila Songvilay, Institut Neel, CNRS, Grenoble. From one- to two-magnon excitations in the S = 3/2 magnet β -CaCr2O4
10:00	Lingjia Shen (Lund University). Hidden quantum critical point in SrCo2V2O8
	Break
11:00	Romain Sibille (PSI). Octupole ice in Ce2Sn2O7 quantum spin liquid
	Matthew Coak (Warwick University). Tuning dimensionality, magnetism and conduction in van-der-Waals Mott insulators
12:00	Lunch Break
13:00	
14:00	Matthew Rosseinsky, (Liverpool University) . Design of Advanced Materials?
	Eleonora Vottero, (University of Turin). Inelastic neutron scattering spectroscopy applied to supported metal nanoparticles in catalysis.
15:00	Break
	Werner Paulus, (Institut Charles Gerhardt Montpellier). LOW-T OXYGEN DIFFUSION PATHWAYS EXPLORED BY SINGLE CRYSTAL NEUTRON DIFFRACTION METHODS IN NON-STOICHIOMETRIC OXIDES.
16:00	Pascal Launois, (University of Paris Sud). SPECIFIC WATER STRUCTURE IN A GEO-INSPIRED NANOTUBE AND INTERRELATED DYNAMICS.

ESS/ILL Topical Workshop on Imaging, Materials and Engineering



14./15. October 2020, <https://indico.ess.lu.se/event/1506/>

WEDNESDAY, 14 OCTOBER

13:30 → 13:45 Instrument Updates: Engineering Diffractometers

- 13:30 SALS Update** (10m)
Speaker: Thilo Pirling
SALS@ILL.2020
- 13:40 BEER Update** (5m)
Speaker: Premek Beran
BEER@ESS reminder

13:45 → 14:45 Materials Science and Engineering - Overviews & General

- 13:45 Neutron diffraction in material science** (30m)
Speaker: Martin Sahlberg
- 14:15 The Common Calibration Protocol and Neutron Quality Label for Neutron Strain Scanning instrumentation** (30m)
Speaker: Ranggi S. Rhamadan
Common Calibratio...

14:45 → 14:55 BREAK (10m)

14:55 → 16:25 Materials Science and Engineering - Studies & Applications

- 14:55 Measurement of strain during fatigue crack growth by stroboscopic neutron diffraction** (20m)
Speaker: Molly Probert
- 15:15 Development of new approaches for neutron diffraction 3D strain mapping in aluminium additive manufactured materials** (20m)
Speaker: Anastasia Mikheenkova
- 15:35 Residual stress measurement in dissimilar metal joints using neutron diffraction** (20m)
Speaker: Taneshan Sapanathan
Stress in metal joints
- 15:55 Studying granular mechanics with neutron diffraction** (20m)
Speaker: Stefanos Athanasopoulos
Granular mechanics

THURSDAY, 15 OCTOBER

13:00 → 13:20 Instrument Updates: Imaging Beamlines

- 13:00 NEXT Update** (10m)
Speaker: Alessandro Tengattini
- 13:10 ODIN Update** (10m)
Speaker: Aureliano Tartaglione, Manuel Morgano

13:20 → 14:50 Neutron Imaging - Overviews & General

- 13:20 Advanced imaging methods** (30m)
Speaker: Nikolay Kardjilov
- 13:50 Cultural heritage metal artefacts tackled by neutron imaging and scattering** (30m)
Speaker: Francesco Grazi
- 14:20 Open source neutron imaging software** (30m)
Speaker: Anders Kaestner
Analyzing_NI_Data_...

14:50 → 15:00 BREAK (10m)

15:00 → 16:30 Neutron Imaging and Diffraction - Studies & Applications

- 15:00 Bragg-edge imaging reveals local texture variations in additive manufactured samples** (20m)
Speaker: Victor Manuel Pacheco Gimón
- 15:20 Neutron diffraction and imaging on battery systems** (20m)
Speaker: Anatolij Senyshyn
- 15:40 Monitoring Li-ion batteries by advanced operando neutron techniques** (30m)
Speakers: Claire Villevieille, Sandrine Lyonnard
- 16:10 Results from the GeoArchaeology try-out workshop** (20m)
Speakers: Björn Nilsson, Burkhard Schillinger

ESS/ILL Topical Workshop on Imaging, Materials and Engineering



14./15. October 2020, <https://indico.ess.lu.se/event/1506/>

Recording

Participants (129)
Panelists (12) Attendees (117)

Find a panelist

Introduction

Contrast mechanisms + Time + Multi-Modes

Diffraction Phase Magnetic Attenuation

Hydrogen in metals

Water uptake in plants

Li transport in batteries

Corrosion

Device inspection: particle filters

Monolith Soot

Strains

Phase transitions

Internal defects

Magnetic fields

Magnetic domains

Microstructure in artefacts

Contrast mechanisms length scales

Å nm μm mm cm

Applic. Energy Storage Cultural Heritage Hydrogen Magnetism Metals

356 registrants!

Q&A

Open Answered(1) Dismissed

Alan HEWAT 01:28 PM
Two very nice summaries of instruments that should start work in 2022. It is fascinating to see ILL competing with the two leading imaging labs, PSI and TUM at ESS. Thank you Alessandro and Aureliano. What will be the main advantages and disadvantages of ODIN vs NeXT-2? Constant wavelength vs Pulsed operation? Intensity? Resolution? Special techniques with wavelength selection?

Alessandro 01:34 PM
The flux should be essentially comparable between the two instruments (since the ESS flux is thus far only simulated, so the exact comparison is not available yet), and as you say the main difference is pulsed vs constant flux, with the usual pros and cons of both. As for the spatial resolution I can answer for the ILL part, we are below 4μm and pushing for more in the upgrade, and temporal resolution ~1s tomography, and also pushing for more (in low resolution mode, of course)

Nikolay Kardjilov, ESS - ILL Topical Workshop on Imaging, Materials and Engineering

entertaining! Just saying.

From Robin to Panelists:
Burkhard, Bjorn: You indicated before that you are limited in time. We are about 10 minutes late. Is it ok for you to start 16.20?

To: Panelists

Type message here...

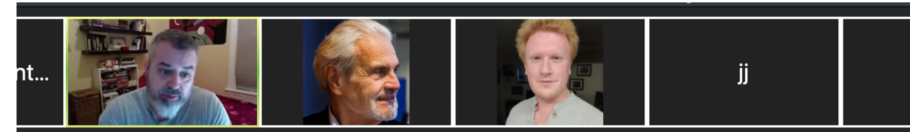
ESS/ILL Topical Workshop about Fundamental Physics



14. October 2020, <https://indico.ess.lu.se/event/1507/>

13:00	→ 13:10	Introduction Speaker: Valentina Santoro santoro.pdf	10m	2
13:30	→ 13:35	The ESS neutrino Super Beam Design Study (ESSnuSB) and the High Intensity Frontier Initiative (HIFI) Speaker: Tord Ekelof (Uppsala University) ESSnuSB-HIFI pres...	25m	2
13:35	→ 14:00	Coherent Elastic Neutrino-Nucleus Scattering at the European Spallation Source Speaker: Juan Collar ESS_CEvNS_Collar...	25m	2
14:00	→ 14:25	New platforms for ultra cold neutron production: SuperSUN and beyond Speaker: Skyler Degenkolb 20201014_ILL-ESS...	25m	2
14:25	→ 14:50	Neutron Beam EDM Experiment Speaker: Florian Piegsa piegsa_ess+ill.pdf	25m	2
14:50	→ 15:05	Virtual Coffee Break	15m	
15:05	→ 15:30	Sterile Neutron Searches at ORNL Speaker: Leah Brossard ESS-ILL workshop ...	25m	2
15:30	→ 15:55	The HIBEAM and NNBAR experiment Speaker: David Milstead (Stockholms Universitet) hibeam-ess-ill-ws-s...	25m	2
15:55	→ 16:20	Antineutron optics Speaker: William Snow (Indiana University) nbartalkWMESS...	25m	2
16:20	→ 16:35	A combined paper on fundamental physics possibilities at ESS? Speakers: David Milstead (Stockholms Universitet), Valery Nesvizhevsky 2021-04-14 ESS overview paper...	15m	2

66 registrants

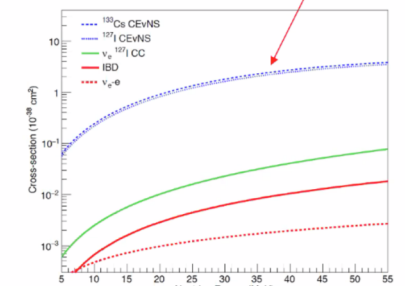


CEvNS: the advent of "miniature" neutrino detectors



CEvNS has largest ν x-section

The catch: low-E NRs are the only detectable signature



ESS/ILL topical workshop on Atomic-scale simulations in NS



20./21 January 2021 (<https://indico.ess.lu.se/event/2411/>)

Wed 20/1

13:00	Welcome	13:00 - 13:15
	Unraveling water dynamics and restructuring upon α -synuclein fibril formation by neutron spectroscopy and molecular dynamics simulations	Dr. Kevin Pounot
	Short-time diffusive dynamics of proteins in a naturally crowded environment	Hender Lopez-Silva
14:00	Sucrose and trehalose as agents of dynamic molecular dynamics simulations	Dr. Inna Ermilova
	Structure and Dynamics of Huntingtin. A Segmental Labelling Approach	Mr. Xamuel Loft Lund
15:00	Solution Structure of the Gloeobacter violaceus Ligand-Gated Ion Channel Probed by Small Angle Neutron Scattering	Marie Ly
	Coffee Break	15:20 - 16:00
16:00	An investigation of 3He in C60: A DFT, theoretical and INS study	Mohamed Aouane
	Neutron scattering and MD simulation of water dynamics in carbon nitride	Arianna D'Angelo
	Water dynamics in carbon nitride	Karolina Lisowska
17:00	THE STRUCTURE OF WATER IN CALCIUM-SILICATE-HYDRATES STUDIED BY NEUTRON DIFFRACTION WITH ISOTOPIC SUBSTITUTION.	Mrs. Zhanar Zhakiyeva
	Neutron reflectivity and MD simulation study of ionic liquids and deep eutectic solvents at a solid electrode	Nebojsa Zec
18:00		

Biology

Nano-particles & liquids

Thu 21/1

13:00	Enhancing refinement with quantum mechanics in neutron protein crystallography	Octav Caldararu
	New on-line DFT approach to analyse neutron diffraction crystallography and SANS data	Luigi Genovese et al.
	Diffusive motions in a solvent free myoglobin-polymer hybrid revealed by neutron scattering and MD simulation	Yann Fichou
14:00	OpenMP Parallelized Neutron Scattering Experiments	Yanqin Zhai
	Molecular modeling and neutron scattering experiments to investigate F127-PM microgels	Letizia Tavagnacco
	Coffee Break	15:05 - 16:00
16:00	A combined computational and experimental approach to studying structure-property relationships in complex oxide ion conductors	Chloe Fuller
	Lattice dynamics and thermal conductivity in complex metallic alloys with atomic simulations in neutron scattering	Pierre-Francois Lory
17:00	Reproducing Anharmonicity in INS Measurements	Stella d'Ambrumenil
	Tunable bonding in the incipient metal thermoelectric GeTe	Dr. Simon Kimber
	Persistent homology for magnetism	Mr. Bart Olsthoorn
18:00	Closeout	18:05 - 18:30

Soft matter incl. Biology

Hard condensed matter

221 registrants

Neutron Instruments Division



Outreach, Research, & Community Interactions

In addition to instrument project duties, which take up most of the time, NID/ISG has responsibilities in outreach, user and community development, and undertaking scientific research activities.

Grants & Supervision

- Swedness, Tillväxtverket, Vinnova, Sakura, VR, 7 PhD students

Teaching

- LU, KU, UU courses

Reviewing, Advisory Boards & Community Groups

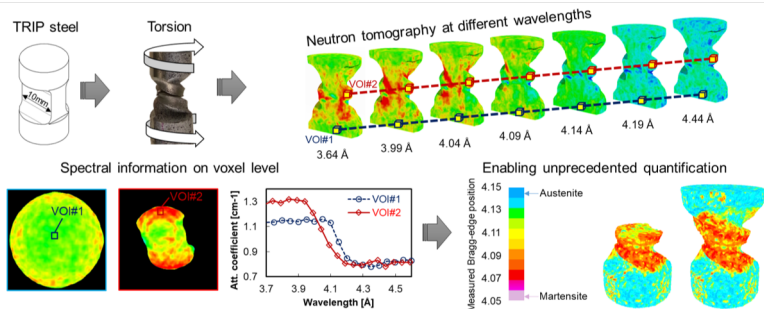
- SuperAdam Board; Mantid Board; ISIS SAC; CSNS Instrument Advisory Panels; Reviewing for ILL, MLZ, NIST, ANSTO, SNS, J-PARC; ORSO; canSAS;

Conferences & Community Interactions

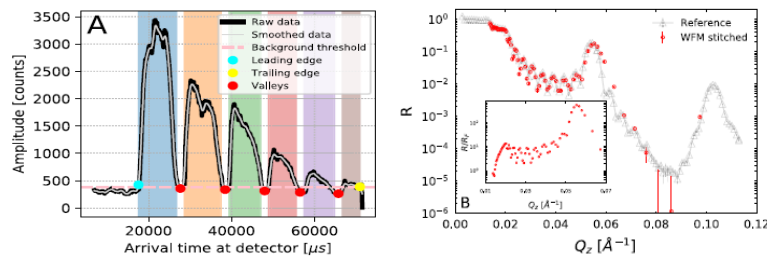
- Accelerate Webinars in Nov 2020 – Andrew, Judith, Zöe and Robin
- CanSAS Workshop on Resolution – March 25th and 26th (Judith and Wojciech organising)

Neutron Instruments Di

Papers, PhDs, and Prizes!



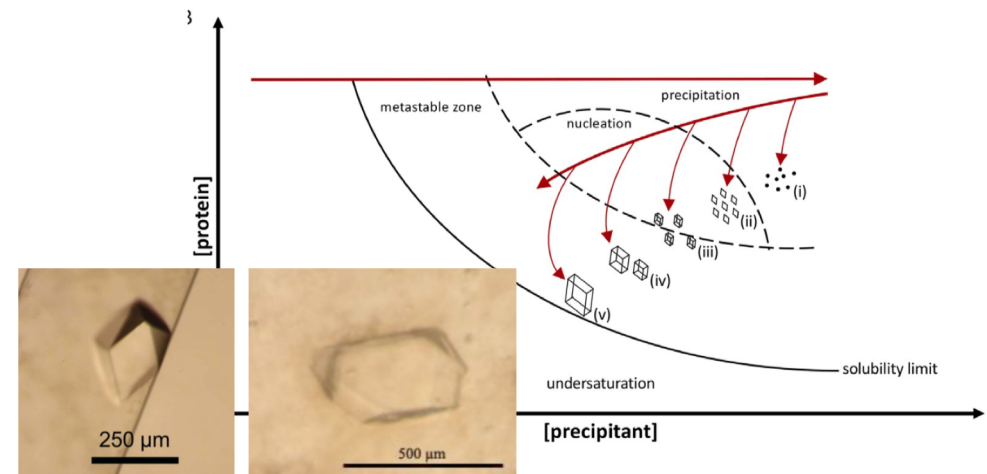
“Spectral neutron tomography” Tran, Woracek, et al, *Materials Today Advances*, 9 (2021)



“Wavelength frame multiplication for reflectometry at long-pulse neutron sources.” Löhmann, et al, *Review of Scientific Instruments* 91 (2020)



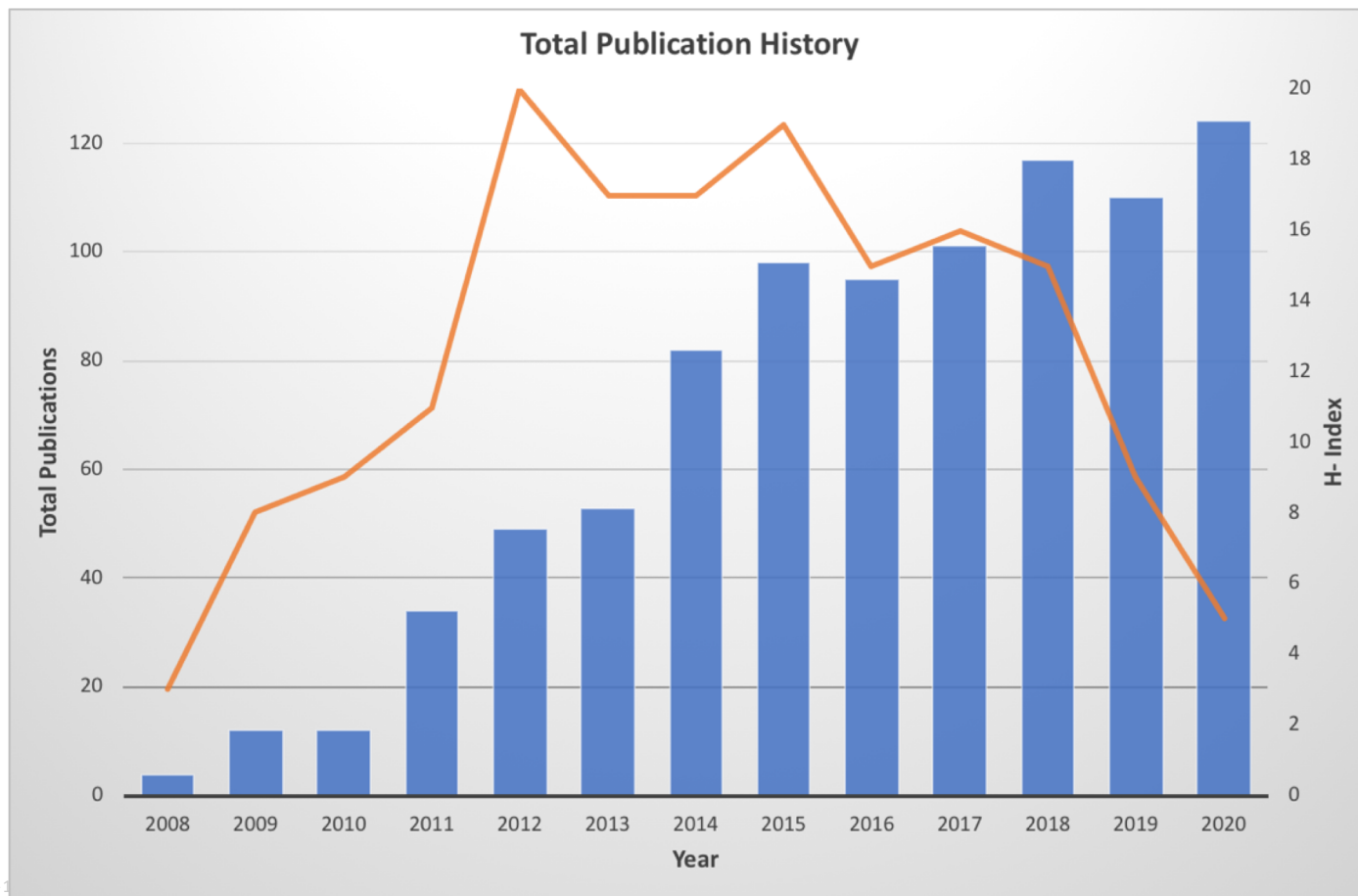
German Materials Society Werner Köster Prize
Premek Beran



Sam Hjorth-Jensen PhD defence - Co-supervisor Esko Oksanen

ESS Publications

All Directorates



2021-04-1

Scientific Activities Division – towards operations



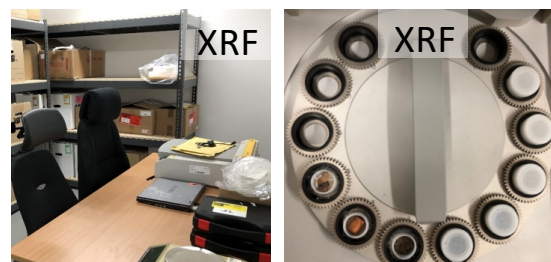
chemistry (SULF) & deuteration (DEMAX) services support ESS construction & users

Buildings E03/E04 used daily! **SULF** & part of sample env. moved on-site using labs & office spaces

SULF starts support services for ESS from E04 – in temporary spots as labs are being finished

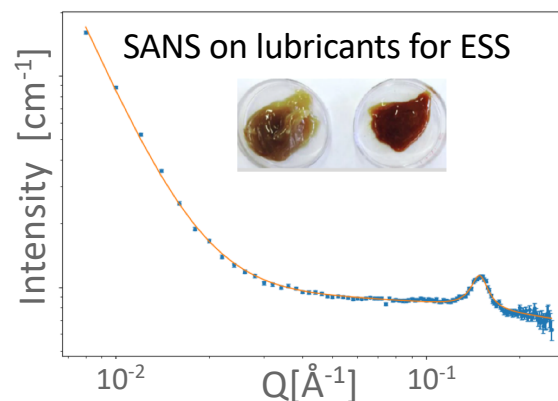
DEMAX delivering 2nd pilot & Covid-19 related projects;

DEMAX demonstrates enzyme capabilities supported by grants (publication ACS omega)



2021-04-14

Electrochemistry



<https://pubs.acs.org/journal/acscod> Article

Enzyme-Assisted Synthesis of High-Purity, Chain-Deuterated 1-Palmitoyl-2-oleoyl-*sn*-glycero-3-phosphocholine
Oliver Bogojevic and Anna E. Leung*

Cite This: <https://dx.doi.org/10.1021/acscomega.0c02823> Read Online

ACCESS | Metrics & More | Article Recommendations | Supporting Information

1. chemical esterification
2. regioselective enzymatic hydrolysis
3. regioselective enzymatic esterification

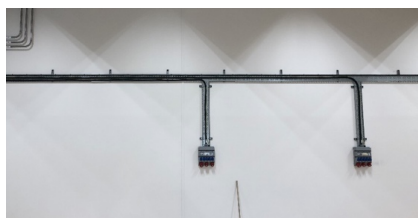
R = C₁₅H₃₁

Scientific Activities Division – towards operations



Sample Environment (SE) moving on-site and commissioning first systems

E03 electrical installation is 90% complete – testing/commissioning phase ongoing (with QA team)



2021-04-14

B02 campus workshop nearing completion & SE fit-out starts

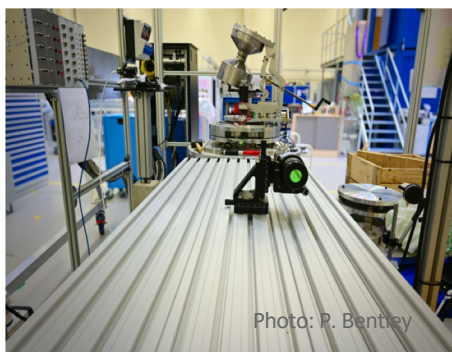
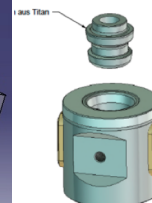
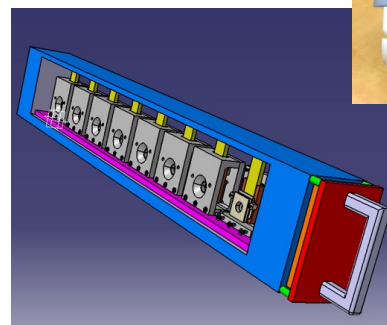
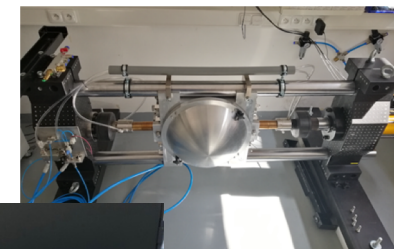


Photo: P. Bentley

First **SE systems** arriving to ESS & constructed at ESS being mechanical / control integrated & commissioned.



Photo: P. Bentley



E03 / E04 labs and workshops from 2019 to 2020



Basic chemistry lab E04.110.2021



Cutting & polishing lab



kitchen & conference room 'first lunch'



Dec/20 almost ready

Nov/20 nearly complete

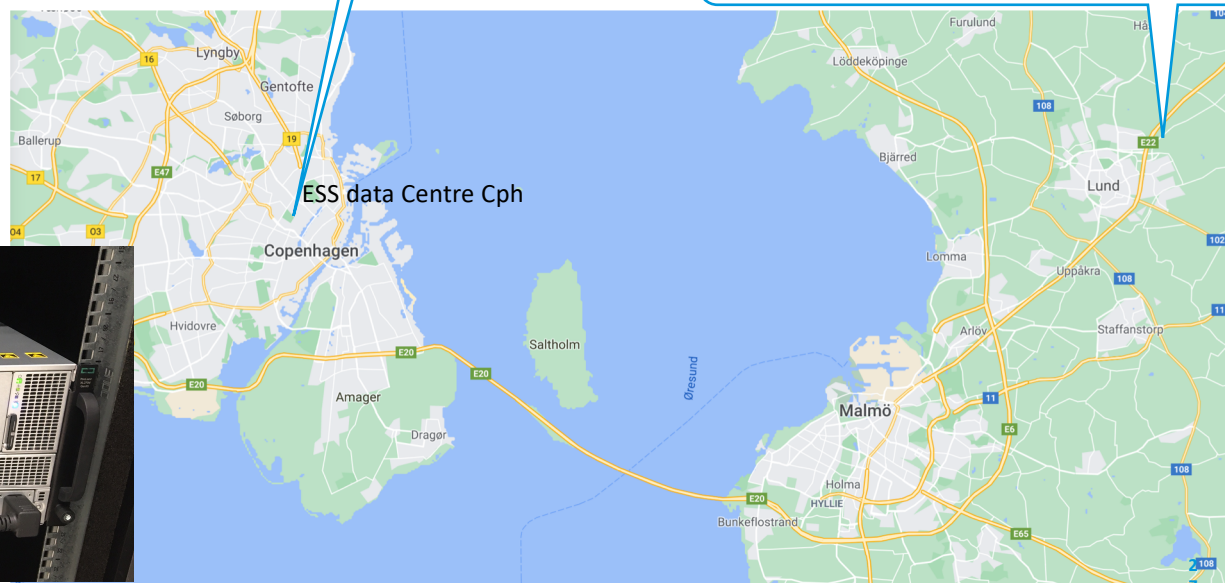
November 2020

DMSC: Hardware procurement

Storage and Compute for H01 & Copenhagen 1M€.



ESS Data Centre Lund



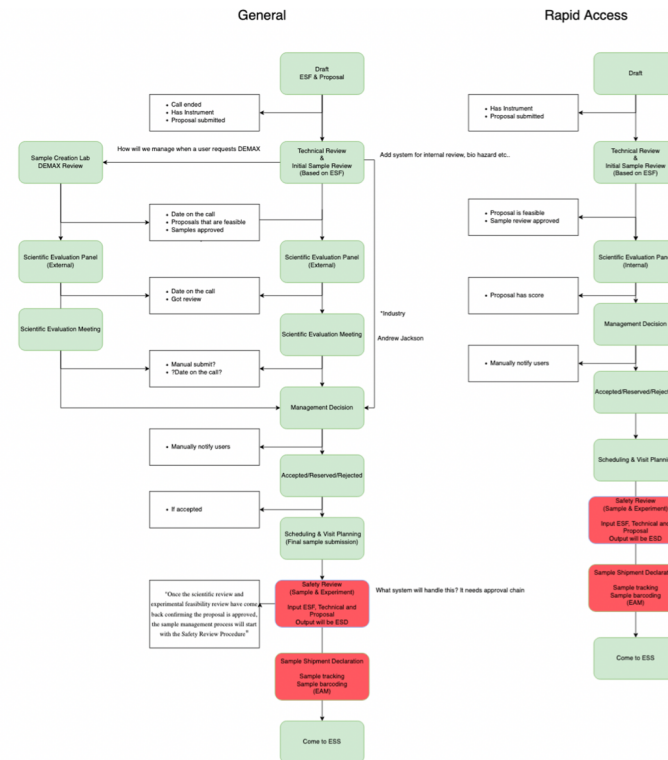
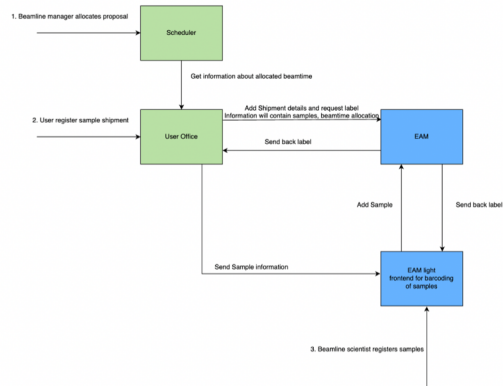
DMSC/SAD: User Office Software Development

Significant progress has been made



Ongoing

- Proposal submission with sample
- Sample safety review
- Proposal scheduling
- Visit declaration
- Shipment declaration
- Sample shipment handling
- Sample barcoding

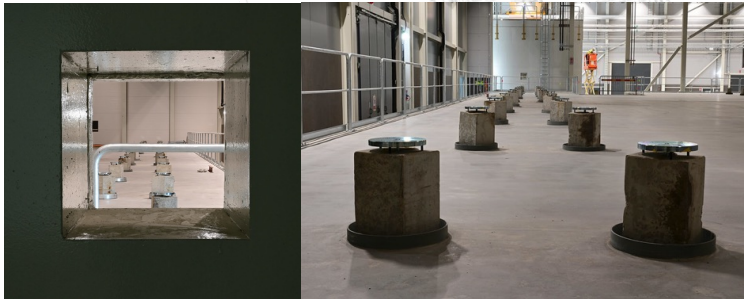
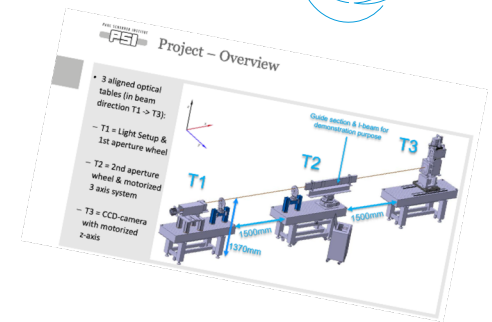


Instrument Technologies Division

Optics lab, collaboration with PSI & installation support



...from an empty room to equipment being installed in E03.100.1002 (thanks to SAD team & SANBER); continuing into early 2021. PSI on Optical Test Bench System collaboration progressing well...



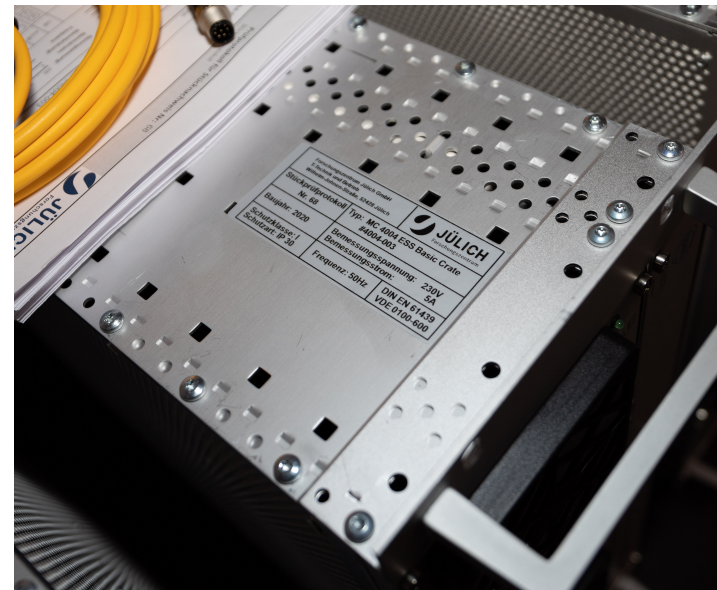
09/12/20



Instrument Technologies Division

Motion Control & Automation

Jülich delivered 3 MCU 4004 test crates to ESS in February (fully tested, documented and CE marked) ready for deployment at partner labs.

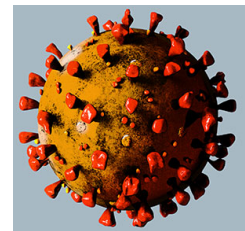


MCA lab installation in E04.100.2025 progressing....

17/03/2021



...despite...



Instrument Technologies Division: Polarisation



Aim to have Scientific Case and plan at the end of 2020



Joint ESS ILL User Meeting



Report on ESS Polarisation Workshop 21-22 September, 2020

Wai Tung (Hal) Lee, European Spallation Source
Arantxa Arbe, Materials Physics Center, CSIC-UPV/EHU, Spain
Tom Arnold, European Spallation Source
Elizabeth Blackburn, Lund University, Sweden
Stefano Carretta, Università di Parma, Italy
Pascale Deen, European Spallation Source
Eddy Lelièvre-Berna, Institut Laue-Langevin, France
Stefan Mattauch, Forschungszentrum Jülich, Germany
Göran Nilén, ISIS Neutron and Muon Facility, UK
Katia Pappas, Delft University of Technology, The Netherlands
Sören Schmidt, European Spallation Source
Xin Tong, China Spallation Source, China



From a workshop postponed due to Corona pandemic to a report and plan for discussion with the Director for Science and NSS project leads on 15 December 2020

SS intends
ron capab
12 instr
) We are
3) Work
measurement
(4) The priority is based
Scientific Advisory Committee, October 2020
in order for it to be available by 2025."
ESS Workshop on Polarisation will be held on 26th-27th of March at
<https://indico.ess.lu.se/event/1390/>
Participation fee payment

Move to Campus



Campus handed over to ESS



The ESS Campus, consists of three buildings:

- an entrance building,
- an office complex including a canteen and an auditorium,
- a labs & workshop building.

ESS staff is moving into the new buildings, slowed down by pandemic/work from home



Office Building

B01

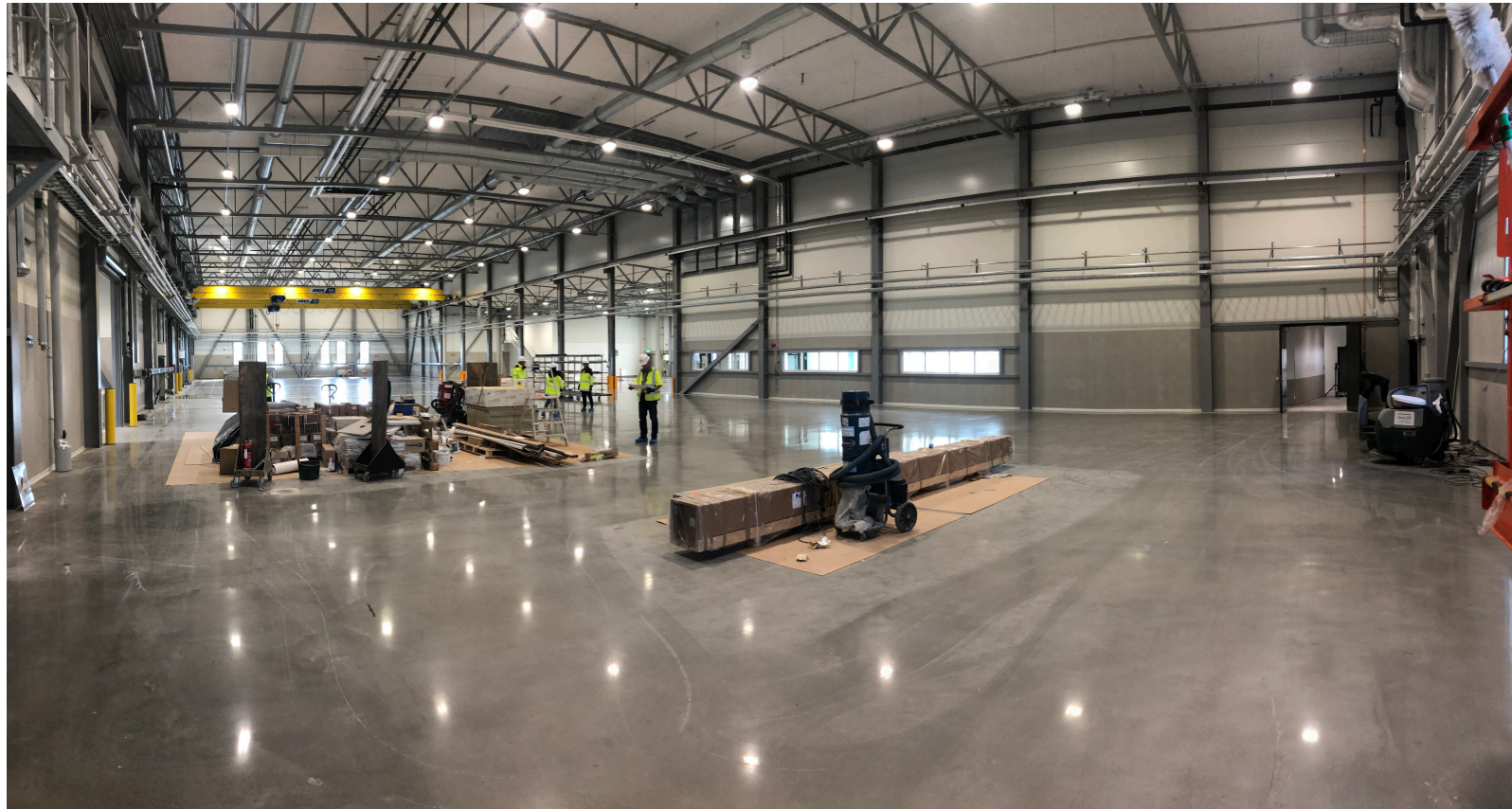


2021-04-14 PRESENTATION TITLE/FOOTER



Lab and Workshop Building

B02, High Bay Area, Oct. 2020



Lab and Workshop Building

B02, High Bay Area, April 2021



Ensuring ESS
plans and
resources are
aligned



We are at a critical point for ESS



- Both Construction and Initial Operations resources are highly constrained
- Construction contingency remaining is very limited and costs increase
- IO funding secured only at the level of 763M€₂₀₁₃ – under additional pressure
 - 124M€₂₀₁₃ lower than our initial plans and 43M€₂₀₁₃ below the level in the ESS statutes
- Additional costs and delays from Covid-19 – not yet contained
- Hiring freeze at ESS
- Way forward discussed with Council:
 - **Focus remains to complete scope of 15 Instruments, 2MW source capability**
 - Might have go from technically limited to resource limited schedule
 - Acceptable delay would require additional funding (< 10% of approved Construction funding)
- Rebaselining planned for later this year

What does this mean for the instruments?

and for the path towards an operational facility?



- BOT now at Oct 2023
- BOT will be delayed further due to technical/delivery issues in Acc./Target and potentially due to changing to a resource limited schedule
- Instruments projects are NOT driving these delays
- End of Construction (EOC) milestone is December 2025
- The reduction of the time between BOT and EOC makes it impossible to achieve FS, SOUP and complete the construction of all 15 instruments by the end of 2025, delay of EOC is required and being discussed
- Instrument schedule needs to be adjusted



- FS on the first three instruments is one key priority
- Delivering all 15 instruments into operation as fast as possible is another priority
- Discussions with in-kind partners started

Conclusions



- Successful user meeting, next one in Lund in 2022
- We have been able to make good progress despite the pandemic.
- Schedule delays also due to Covid-19
- Full picture only when combined with financial boundary conditions
- Re-optimization of the instrument schedule is needed
- Close collaboration and open discussion with in-kind partners is key to success
- Issues will be focus of the upcoming SAC meeting

➤ **Ensure that within the emerging financial limitations we get the best Science Output for the Euro**

