



Science Update

IKON 21

PRESENTED BY ANDREAS SCHREYER, DIRECTOR FOR SCIENCE

27. September 2021

NID/ISG

Growing the Team

- Tom Arnold (FREIA + LSS Co-ordinator)
- Premek Beran (BEER)
- Pascale Deen (CSPEC + Spectroscopy Co-ordinator)
- Judith Houston (LoKI)
- Dan Mannix (HEIMDAL)
- Daria Noferini (CSPEC)
- Esko Oksanen (NMX)
- Werner Schweika (Diffraction Co-ordinator)
- Rasmus Toft-Petersen (BIFROST + Spectroscopy Co-ordinator)
- Robin Woracek (Test Beamline + Imaging/Engineering Co-ordinator)



Manuel Morgano
Instrument Scientist ODIN



Mikhail Feygenson
Instrument Scientist DREAM



Alessandra Luchini
Instrument Scientist Estia
Currently at PSI
Will join ESS in January

Focus on scientific activities here (Science Directorate scope, not NSS scope)



Activities

Outreach, Research, & Community Interactions

Grants, Supervision, Examination

- Swedness, Tillväxtverket, VR, RÅC
- 8 PhD students
- Opponents and Examiners for PhD and Masters students at various universities

Teaching

- LU, KU, UU courses

Reviewing, Advisory Boards & Community Groups

- SuperAdam Board; Mantid Board; ISIS SAC & ISIS II advisory panel; SNS Instrument Advisory Panels; CSNS Instrument Advisory Panels (SANS, Spectroscopy);
- Review of NCNR; Reviewing for ILL, MLZ, NIST, ANSTO, SNS, J-PARC;
- ORSO; canSAS;



Activities

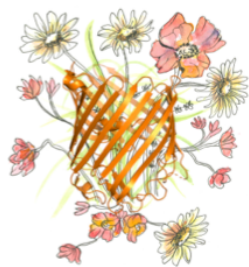
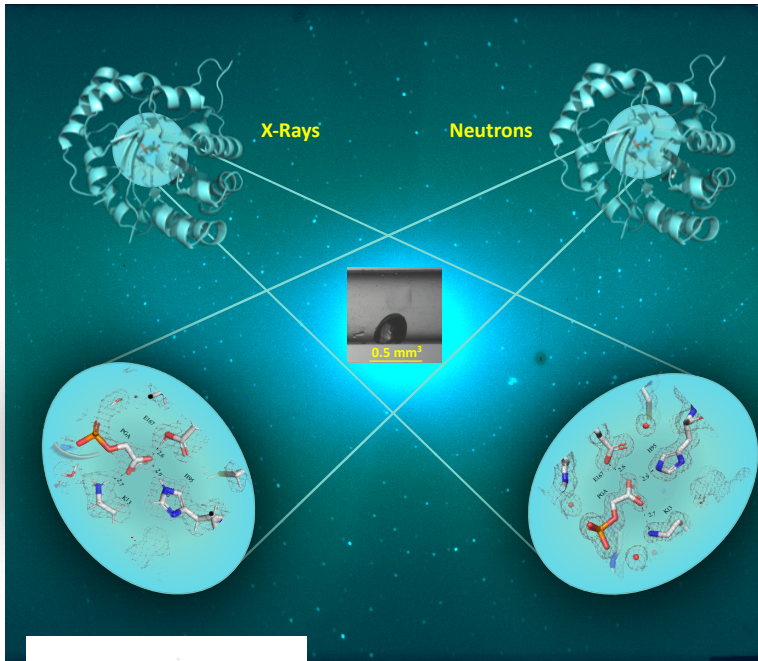
Outreach, Research, & Community Interactions

Conferences & Community Interactions

- Nordic Physics Days (Premek)
- CanSAS Workshop on Resolution – March 25th and 26th (Judith and Wojciech + Andrew, Henrich, Sebastian)
- Session chair at IUCr meeting (Esko)
- QENS/WINS conference (Pascale, Arno)
- Northern Lights on Food (Judith, Andrew)
- LINX themes
- Teaching FullProf workshop at UU (Premek)
- ...

Activities

PhDs and Prizes



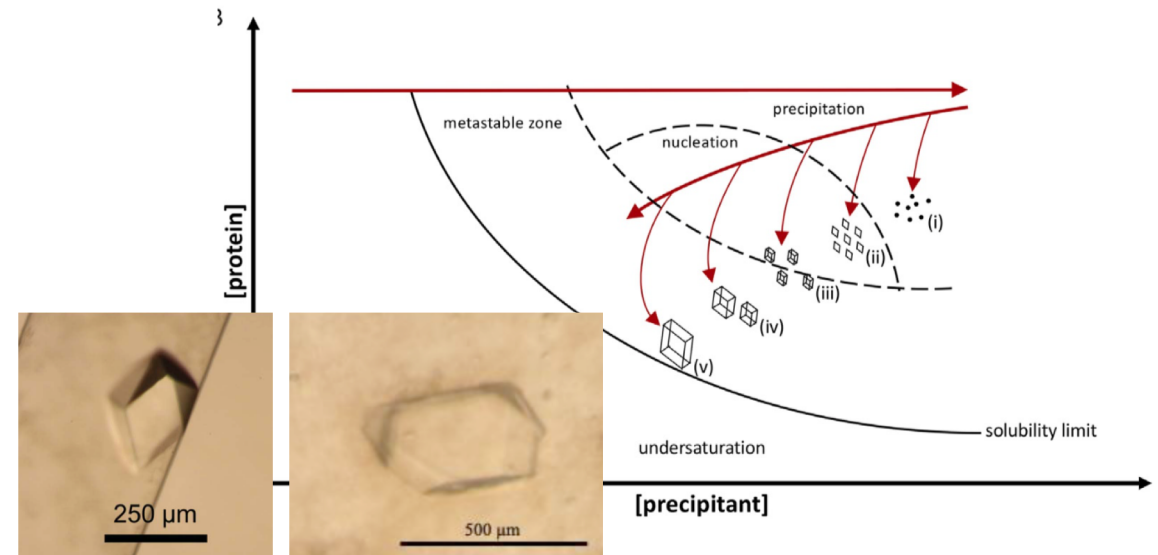
"Elucidating the function of proton pumps with neutron crystallography"

Swati Aggarwal from Neutron Instruments Division is defending her PhD thesis 28th September

MSCA ITN RAMP project
Supervisor Esko



German Materials Society Werner Köster Prize
Premek Beran



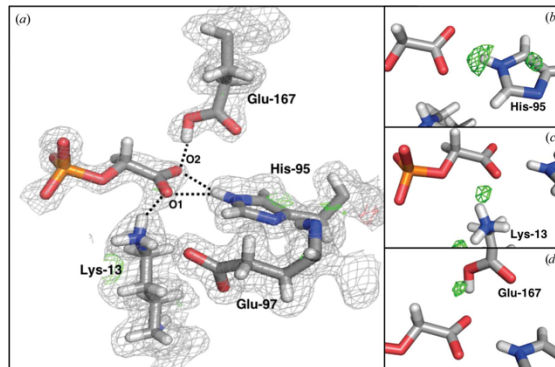
Sam Hjorth-Jensen PhD defence - Co-supervisor Esko

Activities

Publication Highlights ...



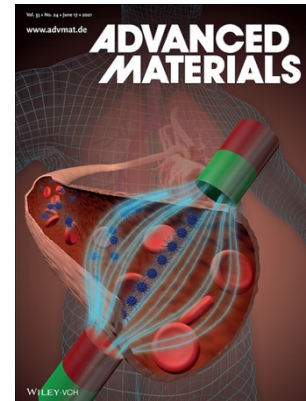
Examining reaction mechanism of triosephosphate isomerase



Esko and collaborators
IUCrJ 8 (2021)

<https://doi.org/10.1107/S2052252521004619>

Chaining of Magnetic Nanoparticles with in-vivo applications



Mikhail and collaborators

Advanced Materials 2008683 (2021)

<https://doi.org/10.1002/adma.202170189>

CSPEC Instrument Paper

CSPEC: The cold chopper spectrometer of the ESS, a detailed overview prior to commissioning.

CSPEC: The cold chopper spectrometer of the ESS, a detailed overview prior to commissioning.

P.P. Deen,^{1,2} S. Longeville,³ W. Lohstroh,⁴ F. Moreira,¹ G. Fabrèges,³ L. Loaiza,⁴ and D. Noferini¹

¹European Spallation Source, Tunavägen 24, 223 63 Lund, Sweden

²Nanoscience Center, Niels Bohr Institute, University of Copenhagen, 2100 Copenhagen Ø, Denmark^{a1}

³Laboratoire Léon Brillouin, Université de Paris-Saclay, CEA/CNRS UMR 12, CEA-Saclay, 91191 Gif-sur-Yvette cedex, France

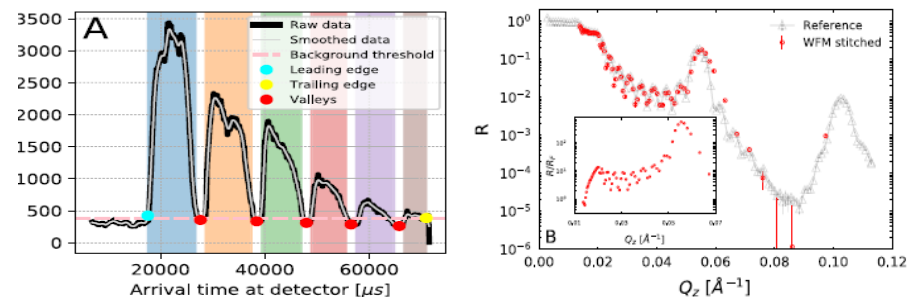
⁴Heinz Maier-Leibnitz Zentrum, Technische Universität München, 85748 Garching, Germany

(Dated: 20 September 2021)

CSPEC is the cold chopper spectrometer of the European Spallation Source (ESS) and will come on-line with the ESS beam on target. CSPEC will be the first cold chopper spectrometer on a long pulsed spallation source which provides great opportunities in terms of signal to noise and novel measuring schemes. We provide a detailed overview of the instrument, scientific design considerations and engineering requirements.

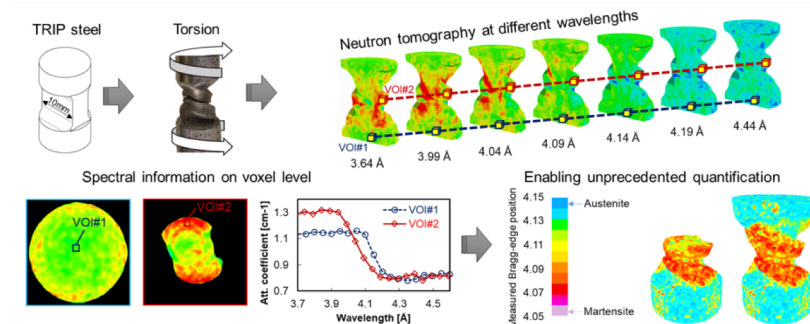
Pascale and CSPEC Team
Review of Scientific Instruments
In Press

Results from V20 on wavelength frame multiplication



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

TOF/Wavelength dependent tomography



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

Activities

Publication Highlights



PHYSICAL REVIEW B

covering condensed matter and materials physics

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Emergent magnetic behavior in the frustrated $\text{Yb}_3\text{Ga}_5\text{O}_{12}$ garnet

Lise Ørdu Sandberg, Richard Edberg, Ingrid-Marie Berg Bakke, Kasper S. Pedersen, Monica Ciomaga Hatnean, Geetha Balakrishnan, Lucile Mangin-Thro, Andrew Wildes, B. Fåk, Georg Ehlers, Gabriele Sala, Patrik Henelius, Kim Lefmann, and Pascale P. Deen
Phys. Rev. B **104**, 064425 – Published 13 August 2021



Article References Citing Articles (1) PDF HTML Export Citation

ABSTRACT

We report neutron scattering, magnetic susceptibility and Monte Carlo theoretical analysis to verify the short-range nature of the magnetic structure and spin-spin correlations in a $\text{Yb}_3\text{Ga}_5\text{O}_{12}$ single crystal. The quantum spin state of Yb^{3+} in $\text{Yb}_3\text{Ga}_5\text{O}_{12}$ is verified. The quantum spins organize into a short-ranged emergent director state for $T < 0.6$ K derived from anisotropy and near-neighbor exchange. We derive the magnitude of the near-neighbor exchange interactions

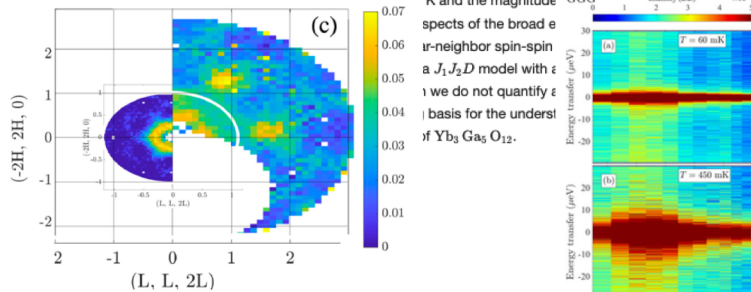
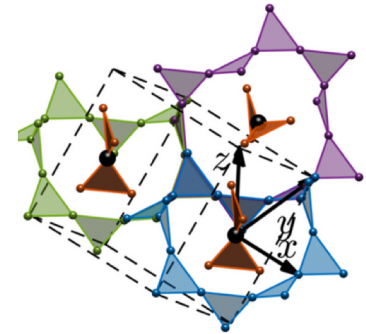
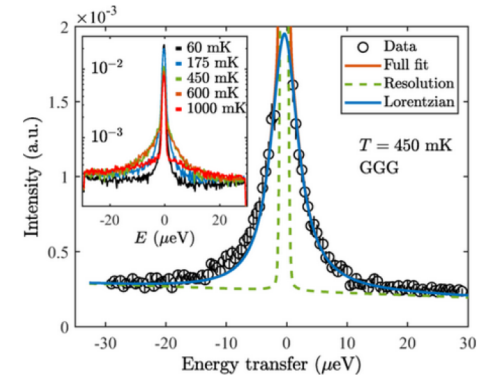


FIG. 4. (a) $S_{\text{mag}}(\mathbf{Q})$, $E_i = 1.55$ meV, derived from a high-temperature subtraction. (b) $S_{\text{mag}}(\mathbf{Q})$, $E_i = 8.11$ meV. We estimate the sample temperature to be $0.1 < T < 0.2$ K. (c) Relative regions of reciprocal space probed in $S_{\text{mag}}(\mathbf{Q})$, $E_i = 1.55$ meV (CNCS) (a) and $S_{\text{mag}}(\mathbf{Q})$, $E_i = 8.11$ meV (D7) (b).



PHYSICAL REVIEW B

covering condensed matter and materials physics

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Spin dynamics of the director state in frustrated hyperkagome systems

Henrik Jacobsen, Ovidiu Florea, Elsa Lhotel, Kim Lefmann, Oleg A. Petrenko, Chris S. Knee, Tilo Seydel, Paul F. Henry, Robert Bewley, David Voneshen, Andrew Wildes, Garan Nilsen, and Pascale P. Deen
Phys. Rev. B **104**, 054440 – Published 30 August 2021

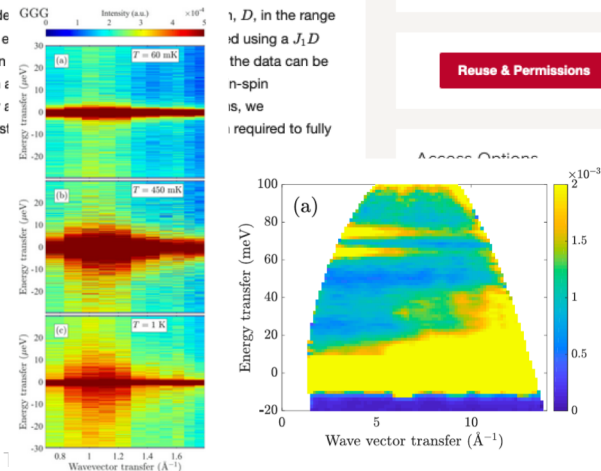


Article References No Citing Articles PDF HTML Export Citation

ABSTRACT

We present an experimental study of the magnetic structure and dynamics of two frustrated hyperkagome compounds, $\text{Gd}_3\text{Ga}_5\text{O}_{12}$ and $\text{Gd}_3\text{Al}_5\text{O}_{12}$. It has previously been shown that $\text{Gd}_3\text{Ga}_5\text{O}_{12}$ exhibits long-range correlations of multipolar directors that are formed from antiferromagnetic spins on loops of ten ions. Using neutron diffraction and reverse Monte Carlo simulations we prove the existence of similar magnetic correlations in $\text{Gd}_3\text{Al}_5\text{O}_{12}$, showing the ubiquity of these complex structures in frustrated hyperkagome materials. Using inelastic neutron scattering we shed further light on the director state and the associated low-lying magnetic excitations. In addition, we have measured quasielastic dynamics that show evidence of spin diffusion. Finally, we present AC susceptibility measurements on both $\text{Gd}_3\text{Ga}_5\text{O}_{12}$ and $\text{Gd}_3\text{Al}_5\text{O}_{12}$, revealing a large difference in the low-frequency dynamics between the two otherwise similar compounds.

Issue
Vol. 104, Iss. 5 – 1 August 2021

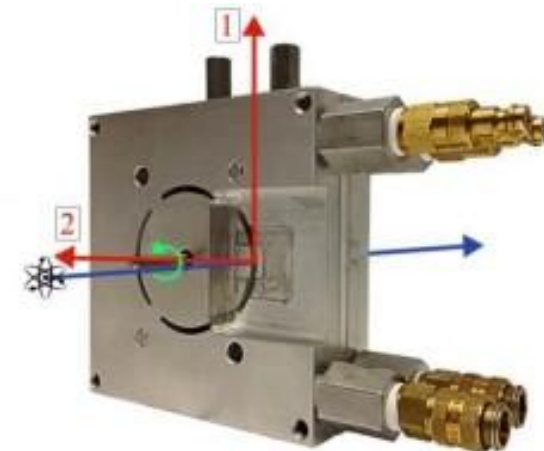


Activities

Grants ...

- ~20 proposals to VR Call "Cooperation with ISIS: instrumentation and methods for ESS" with colleagues from DMSC, SAD and partner labs in collaboration with Swedish university researchers and ISIS staff, including:
 - MuMol: Multi-Modal imaging for materials investigation (Manuel, Søren + collaborators at LU and ISIS)
 - ReHEART: Revealing Hydrogen Embrittlement of Alloys in Real Time (Robin, Søren, Manuel, Premek, Caroline, Alice + collaborators at UU and ISIS)
 - Reaction cell development for *In situ* Studies (Mikhail, Caroline + collaborators at UU and ISIS)
 - Maximizing information content in neutron reflectivity data by optimised magnetic reference layers (Alessandra, Andrew McCluskey + collaborators at LiU, UU, LU and ISIS)
 - Fast processes studied with neutrons (Judith + collaborators at UU and ISIS)
 - Rapid-mixing neutron spectroscopy : molecular dynamics during assembly processes and reactions (Daria, Greg + collaborators from MaU, LU and ISIS)

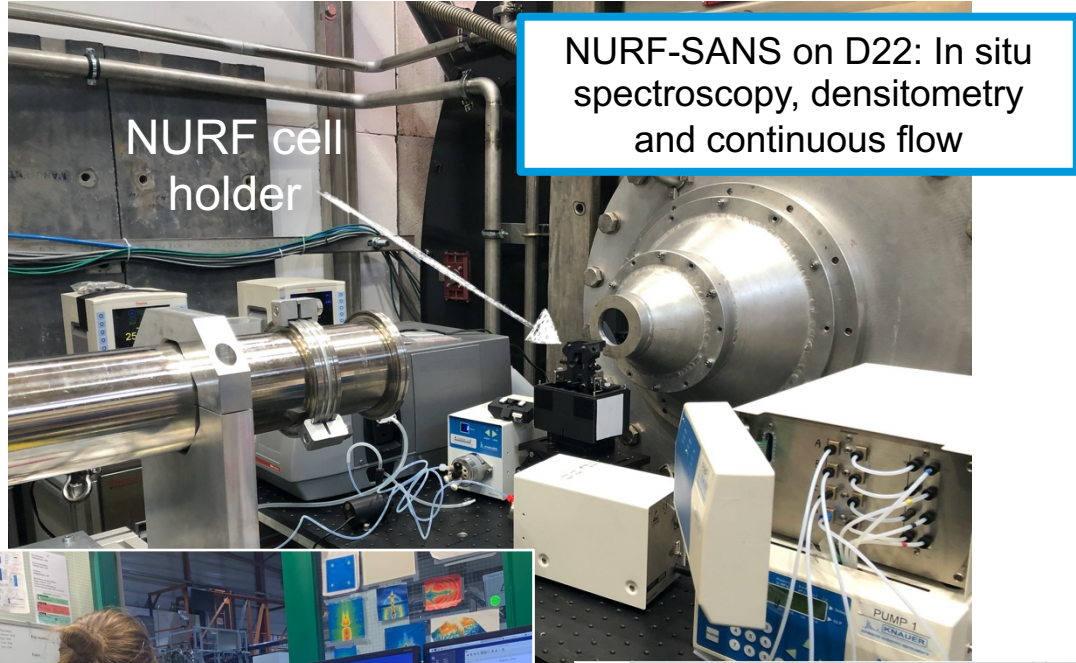
- RÅC proposals including :
 - Enabling early science at ESS for multi-modal in situ studies of solid-liquid interaction using neutron imaging and isothermal calorimetry as sample environment (Manuel and collaborators)
 - New alloys for the hydrogen society; design and realisation, guided by neutrons (Mikhail and collaborators)
 - Probing the structuring of soft matter under flow using a compact and flexible 1,2-shear cell (Judith, Anders and collaborators)



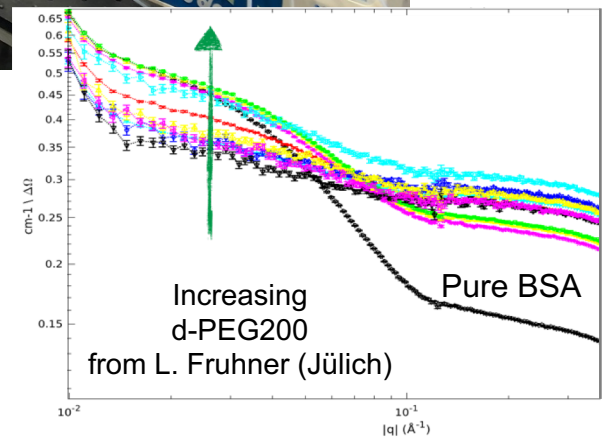
Gratuitous picture of existing 1,2 plane shear cell courtesy of NIST

Activities ...

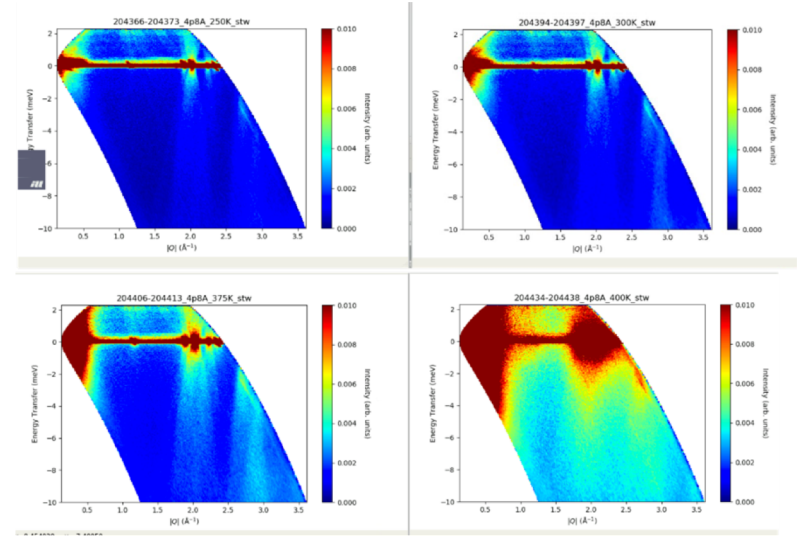
Experiments and Testing ...



NURF-SANS on D22: In situ spectroscopy, densitometry and continuous flow



Phonon-magnon interactions in magnetocaloric materials



Pascale and collaborators from UU

Publication and Sponsoring Guidelines



- ESS Guidelines for **Scientific Publications** from ESS Users and Staff and Associates of the ESS Science Directorate including a Commitment to Scientific Integrity and Research Ethics **ESS-3488883**
- Topics: Scientific Integrity, Publication Requirements (Open Access), Acknowledging Resources and Service, Affiliation Requirements

- ESS Guidelines for **Sponsorship** of Scientific Events by the Science Directorate **ESS-3634448**
- Topics: Types of Eligible and Ineligible Scientific Events, Application and Evaluation Process,

On-site Laboratories and Project Support Services



E04 labs fitted out and operational

On-Site Laboratories and Project Support Services



D08 fume hoods



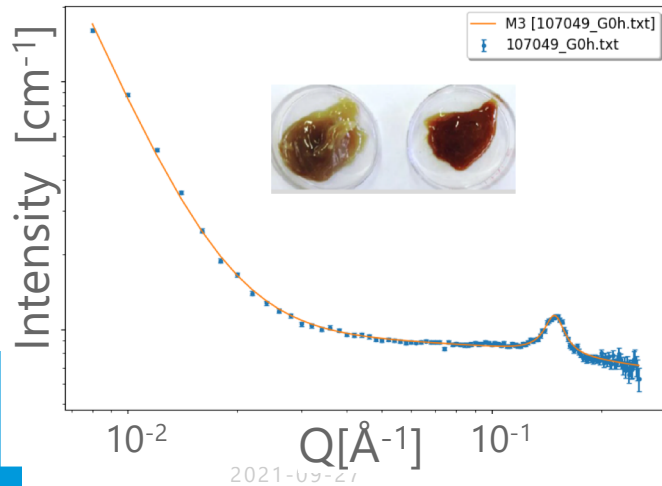
glove box



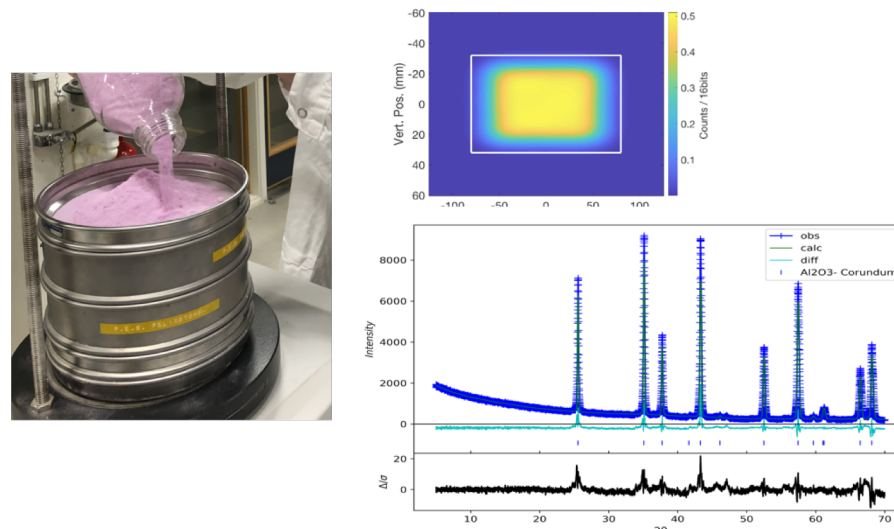
XRD



Testing lubricants



Improving luminescence materials



Water Analysis



Sample Environment

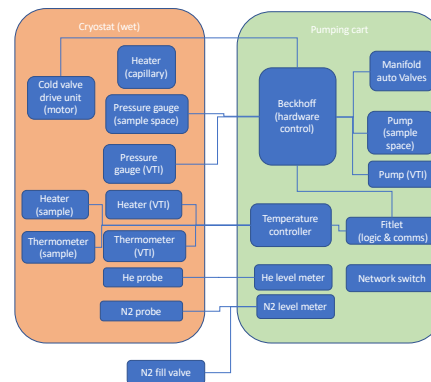
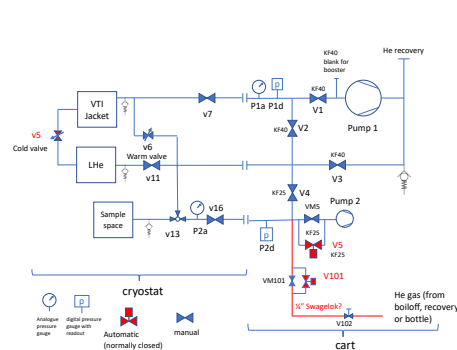
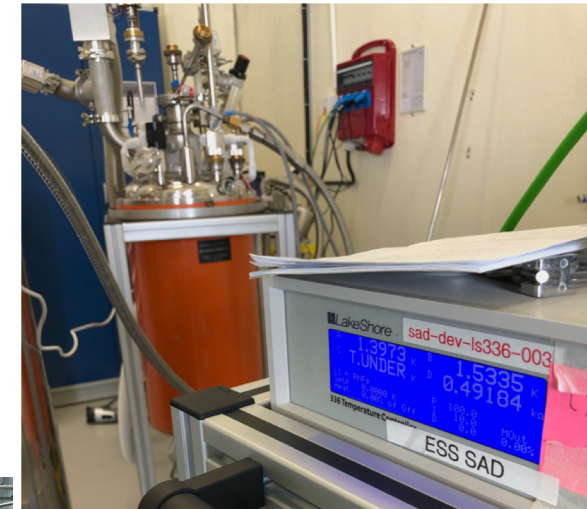
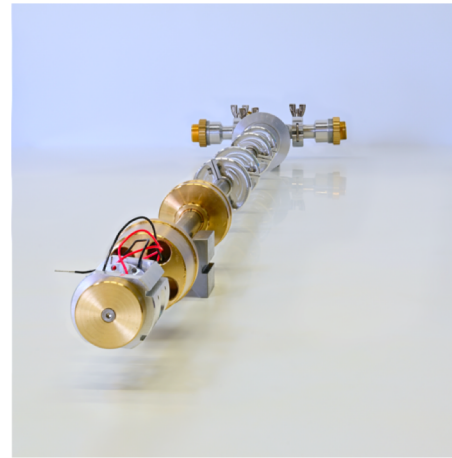
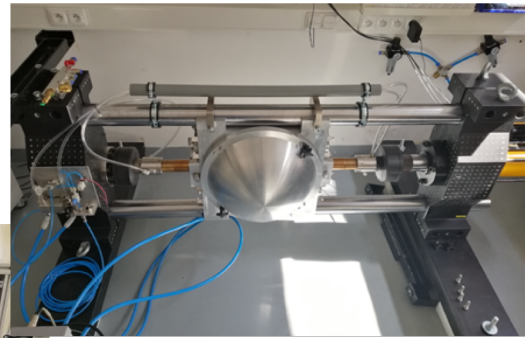
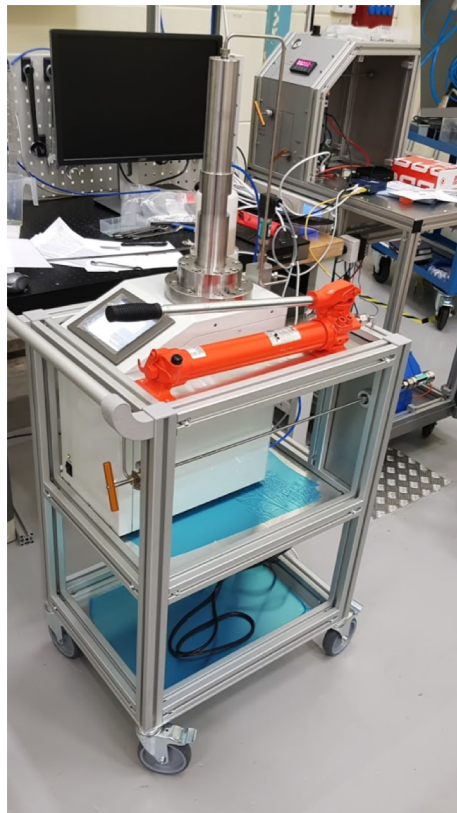


E03 SE main lab and workshop is nearly finished and the SE Team is ready to move in October

High pressure systems

stress rig

cryogenic systems



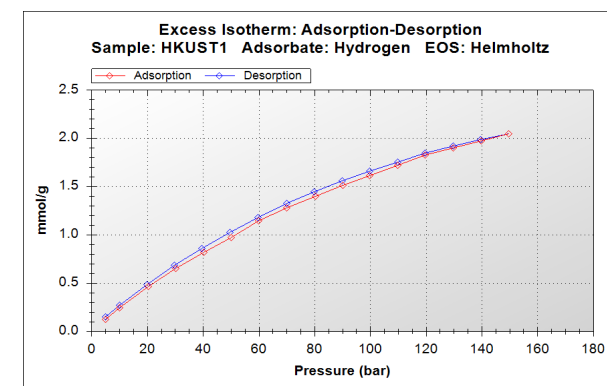
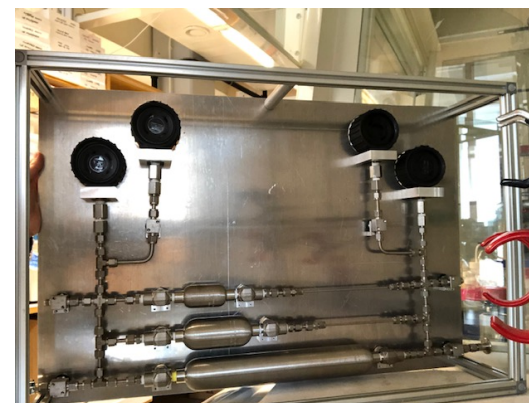
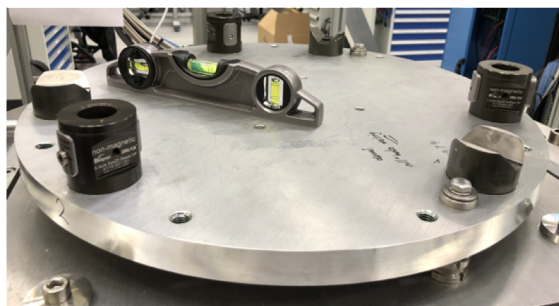
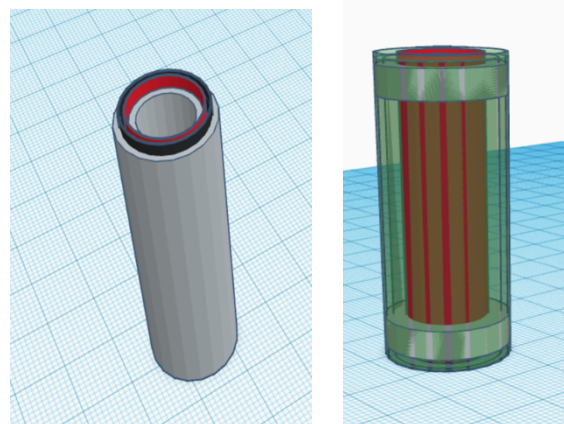
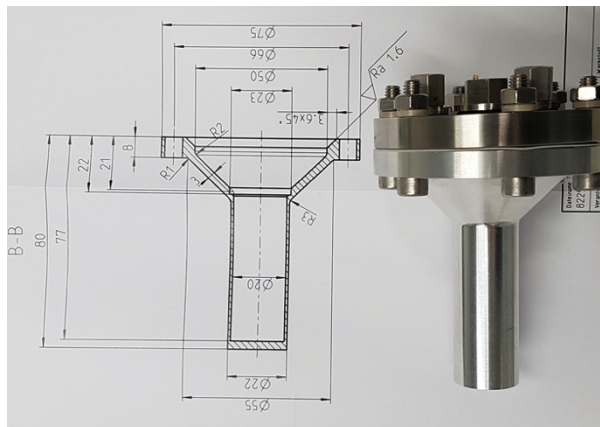
Sample Environment



SE mounting interface
Kinematic mounts about to be delivered
be will be supplied to all instruments

electrochemistry
IK projects (pump-probe, electro chemistry) ongoing

gas handling
automatic gas handling system successfully to
installed and tested.



2021-09-27

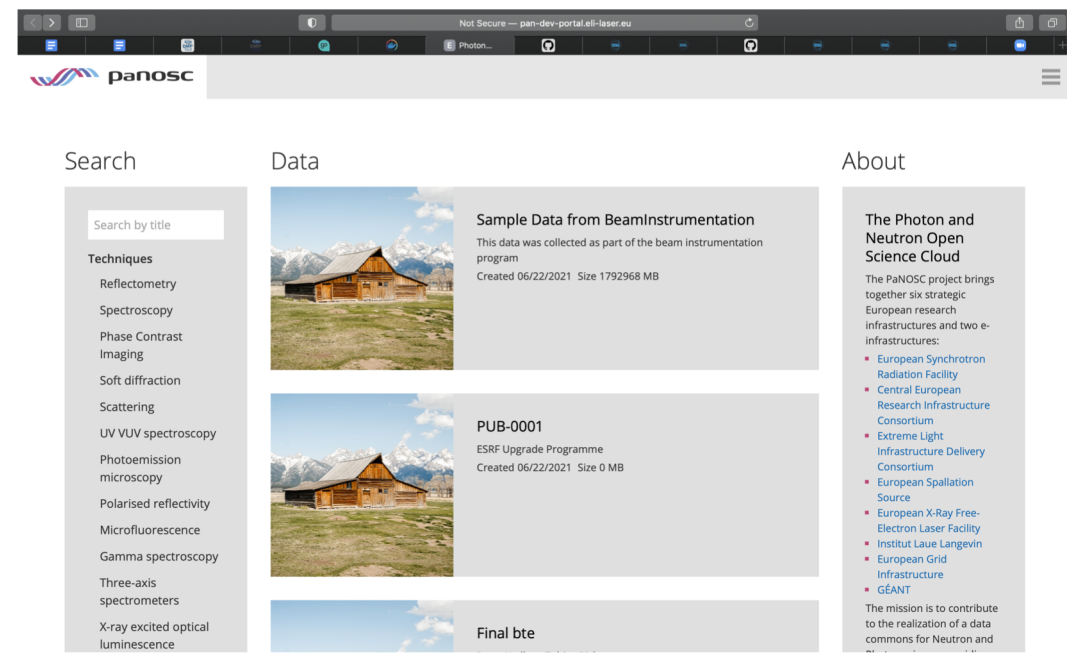
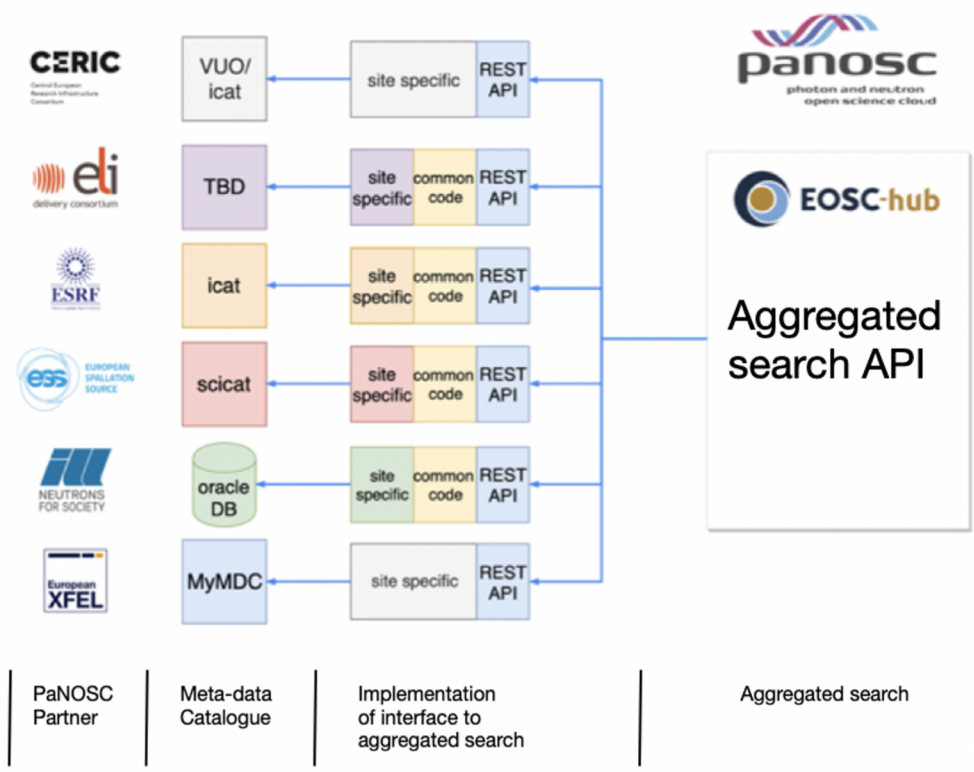
Sample Environment Update by Caroline Curfs , Wednesday 29.9 15:20

Federated search

New PaNOSC developments

- Federated search API deployed at ESS
 - search metadata from ESRF, ILL, ESS and XFEL in one place

<http://pan-dev-portal.eli-laser.eu/>





User office development with ISIS

Collaboration with ISIS ensures testing at operating facility

The screenshot shows a web browser window with the URL 'Welcome to the Users' Office'. The page header includes the UK Research and Innovation logo, 'Science and Technology Facilities Council', and 'User Office'. The user is logged in as '1059527 (User Officer)'. A left-hand navigation menu lists various categories: Proposals, Calls, People, Instruments, SEPs, Pages, Institutions, Templates, Proposal, Sample declaration, Shipment declaration, Visitation, Questions, Sample safety, Sample shipments, and Settings. The main content area is titled 'Templates' and features a search bar and a table with the following data:

Actions	Name	Description	# proposals	# calls
	default template	original template	19	1
	new template		0	0

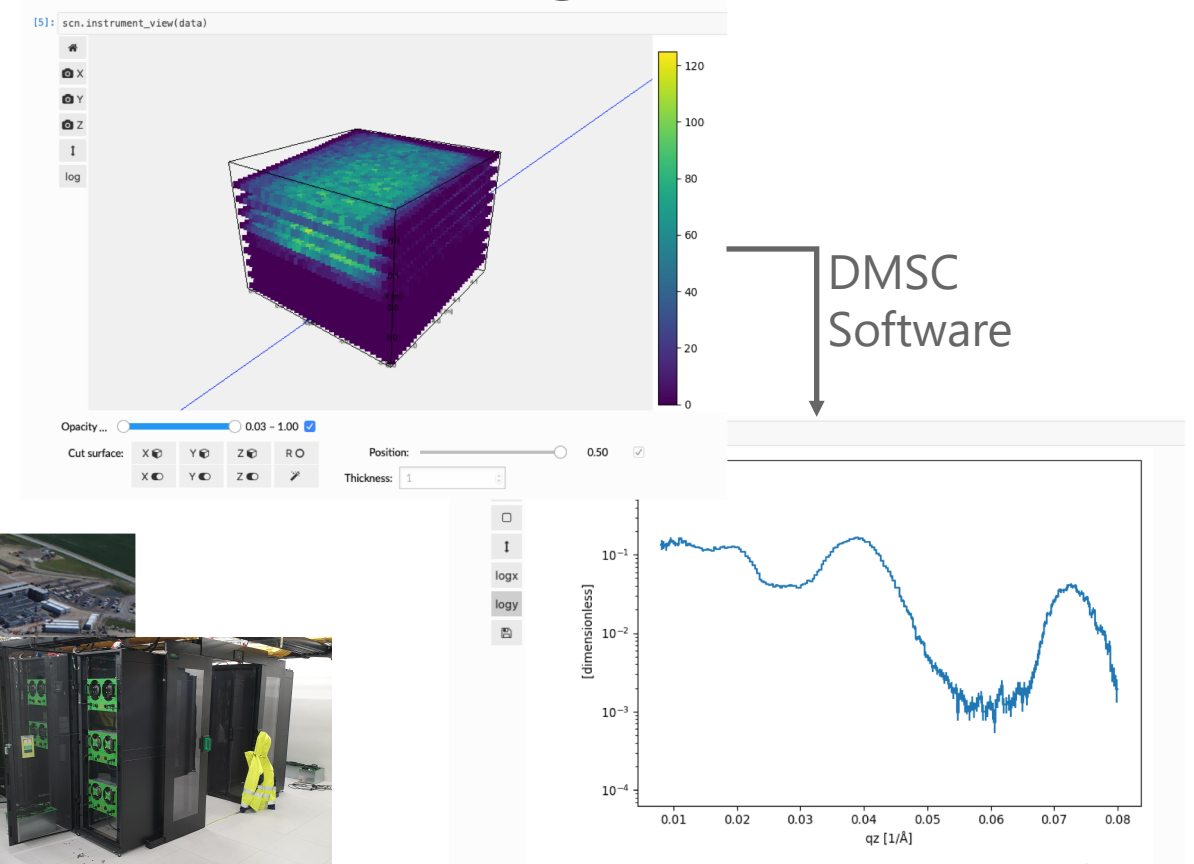
At the bottom right of the table area, there is a 'CREATE TEMPLATE' button. Below the table, there is a pagination control showing '5 rows' and '1-2 of 2'.

(Preparing for) validation of scientific computing infrastructure

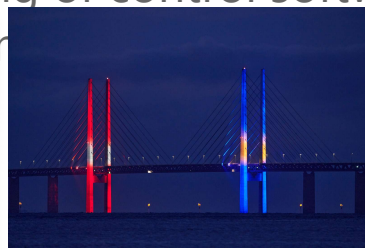


- **Scientific computing infrastructure installed in both Lund and Copenhagen and connected across Sound**
 - enables testing and commissioning of data reduction & analysis software in their production environment
- **Integrating DMSC system with the control systems network for BIFROST tank & YMIR**

- **Validation of scipp based data reduction workflow through commissioning of AMOR @PSI**



– Enables testing of control software



Python training at IKON21

61 registrants



Thursday and Friday afternoon this week!

Will use the training platform pan-learning.org developed in PaNOSC from e-neutrons.org

We will work in smaller groups on the following topics:

- Jupyter notebooks basics
- Python basics
- Using external libraries (numpy, scipy, matplotlib, pandas)
- Code testing
- Using McStas from Python (<https://github.com/PaNOSC-ViNYL/McStasScript>)
- Scipp (<https://scipp.github.io/>)

New scipp release!

The screenshot shows the PaN-learning Moodle interface. At the top, there is a search bar labeled "Search courses" and a user profile for "Thomas Rod". Below the search bar, the section "Available courses" lists several courses with their full names and icons for locking and navigation. The courses listed are:

Full name	Lock icon	Navigation icon
Neutron Scattering Library	🔒	➡
Introduction to Neutron Scattering	🔒	➡
Advanced Topics in Neutron Scattering	🔒	➡
Quasi-Elastic Neutron Scattering		➡
Introduction to Muon Spin Spectroscopy		➡
Muons in Semiconductors		➡
Muons in Magnetism		➡
Muons in Superconductivity		➡
IKON21 Python Workshop		➡
IKON Python Workshop (March 2021)		➡
SasView: Analysis of SAS Data (Swedness)		➡

On the right side of the page, there are three informational boxes:

- Wiki Contribution:** "If you are interested in contributing to the wiki please email admin@pan-learning.org. We are especially looking for articles on photon science."
- Funding:** "This project has received funding from: **EU FP grant No. 283883** **Horizon 2020 grant agreement No. 654000** **Horizon 2020 grant agreement No. 823852**" with the European Union flag below.
- Data Policy:** "PaN-learning is GDPR compliant. Click [here](#) to read the data policy."

easyScience & easyDiffraction & easy...

Working on their PR - (<https://www.easyscience.software>)



es easyscience

Home Features Contact

Projects

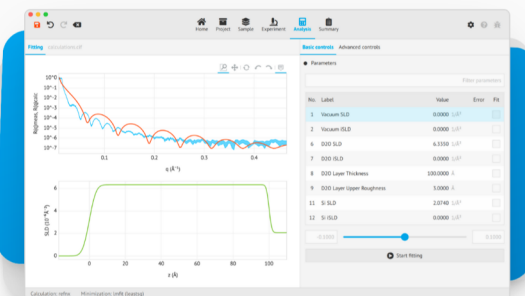
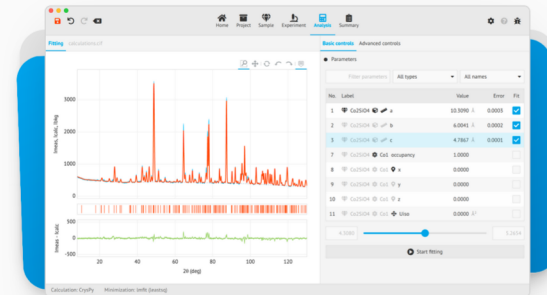


easydiffraction

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

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

Visit 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 [bornagain](#).

Source code on github:

easyScience
A framework for building applications and libraries for data analysis and modelling
Copenhagen, DK <https://easyscience.software/> contact@easyscience.software Verified

Repositories 24 Packages People 3 Projects 2

Find a repository... Type Language Sort

easyDiffractionApp
Making diffraction data analysis and modelling easy
Python GPL-3.0 1 1 40 (1 issue needs help) 3 Updated 2 hours ago

easyCore
The building blocks for science libraries in the easy universe.

Top languages
Python JavaScript QML
Jupyter Notebook

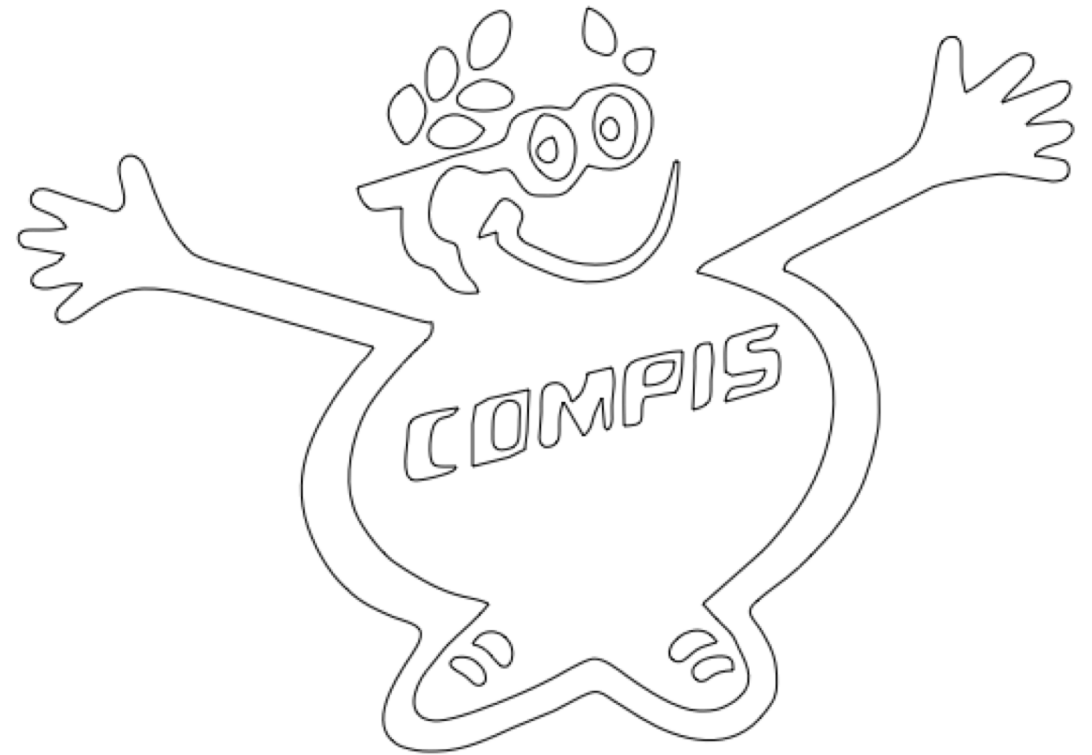
People 3 >

Analysis of ToF data will be available in release beginning of next month (Version 0.8.3)

Easyscience will be used as framework for joint post doc project with Chalmers and MAX IV on statistical learning for diffraction

IDS collaboration with SNS

- Instrument data scientists off to a very good start
 - Søren Schmidt (img & eng)
 - Céline Durniak (diffraction)
 - Wojciech Potrzebowski (SANS)
 - Andrew McCluskey (reflectometry)
 - Gregory Tucker (spectroscopy)
- Frequent (monthly) meetings with SNS Computational Instrument Scientists
- Have created joint forum named COMPIS open to facility staff linking instrument teams with scientific computing



Credit: Gregory Tucker

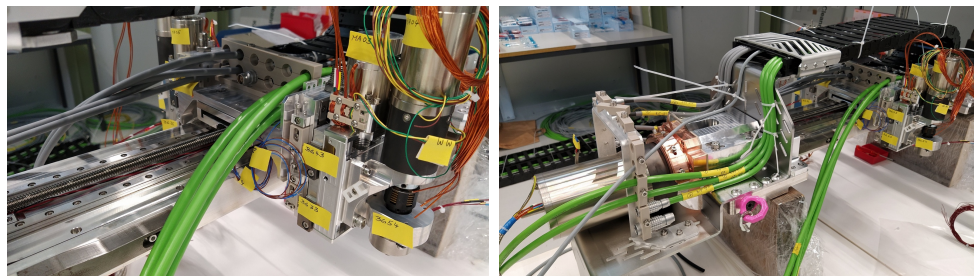
Motion Control & Automation

Commissioning of ESTIA Selene Guide @ PSI

- Commissioning of Selene I successfully done remotely
 - 16Ax. Cabinet design proved successful
 - First large scale implementation of the MCA software on the basis of the TwinCAT collaboration
 - Software includes now new abstraction layer PILS at the interface to EPICS
- Guide housing delivered to ESS



Motion Control cabinet for Estia at PSI



Components used for alignment of the Selene Guide system



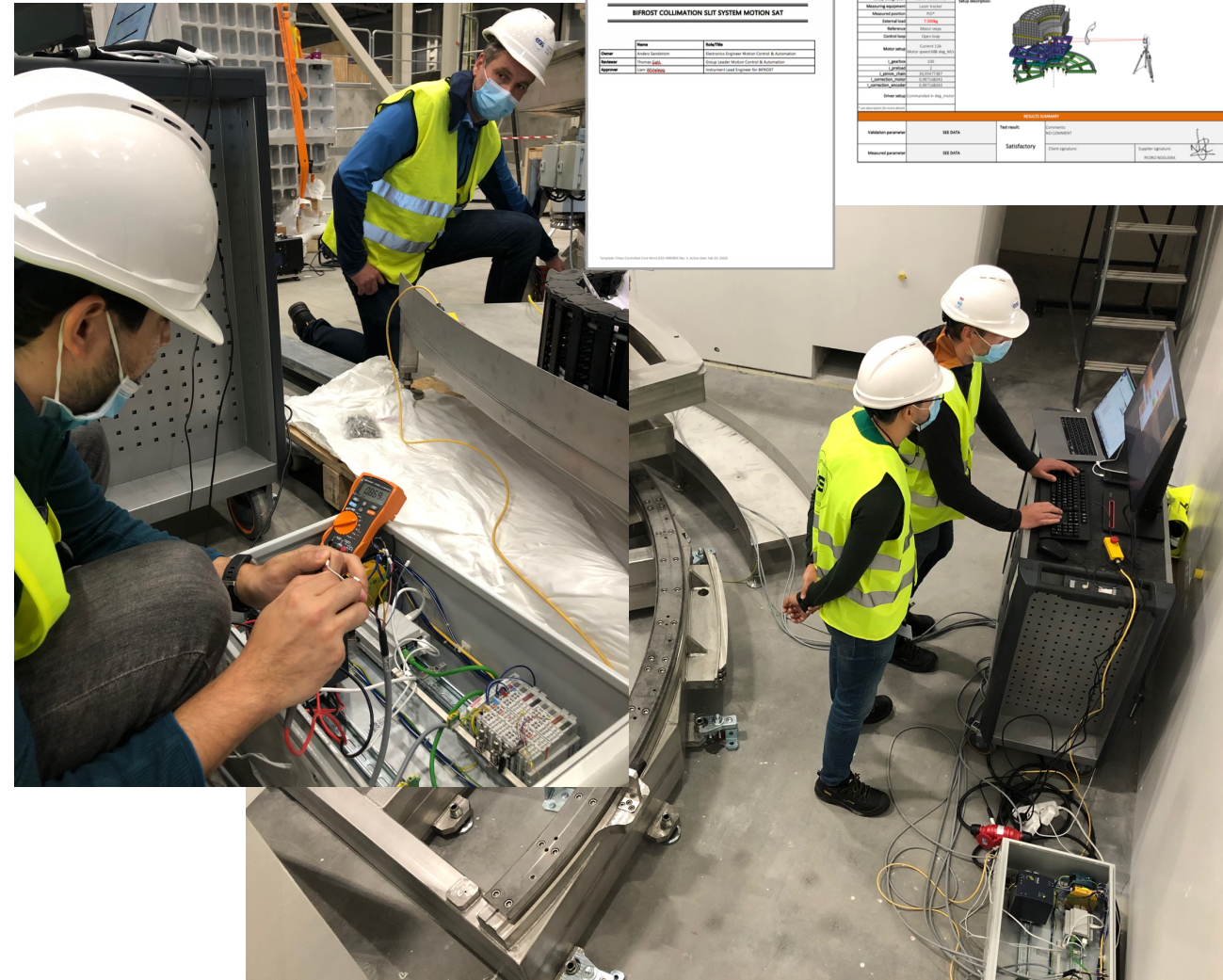
Estia Selene 1 Guide housing delivered to D01

Motion Control & Automation

FAT and SAT for Bifrost



- Pandemic made it difficult to travel and participate on FATs; large delay on production of test equipment
- Focus changed from FAT to SAT
 - Participate remotely in FAT at the supplier; needs good preparation and communication lines
 - Repeat the tests in the SAT in exactly the same way to be able to confirm FAT results.
 - Use identical control hardware for both tests
- Flexibility in hardware production
 - Building temporary control units and provide to suppliers



Neutron Optics & Polarisation

Equipment to support quality & performance and installation



PSI SCHERRER INSTITUT
FAT at PSI LIN/NUM

The purpose of the Factory Acceptance Test is to formally document that the system meets acceptance criteria. The Acceptance Test enables the project management to decide whether to accept the presented system.

PROJECT IDENTIFICATION	Project Number	Date Created
Optical Bench System		

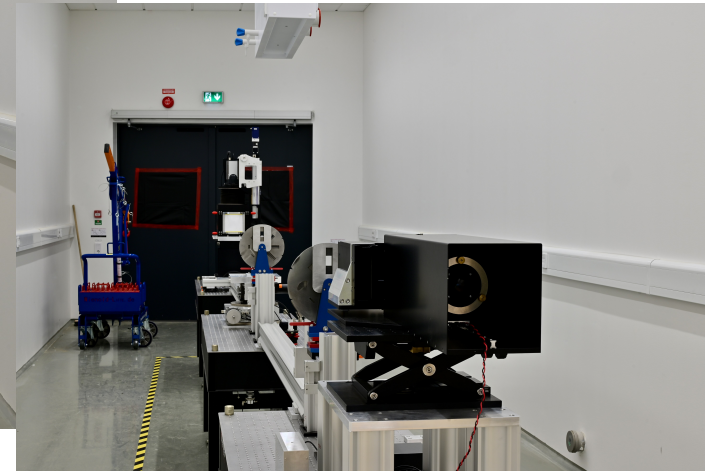
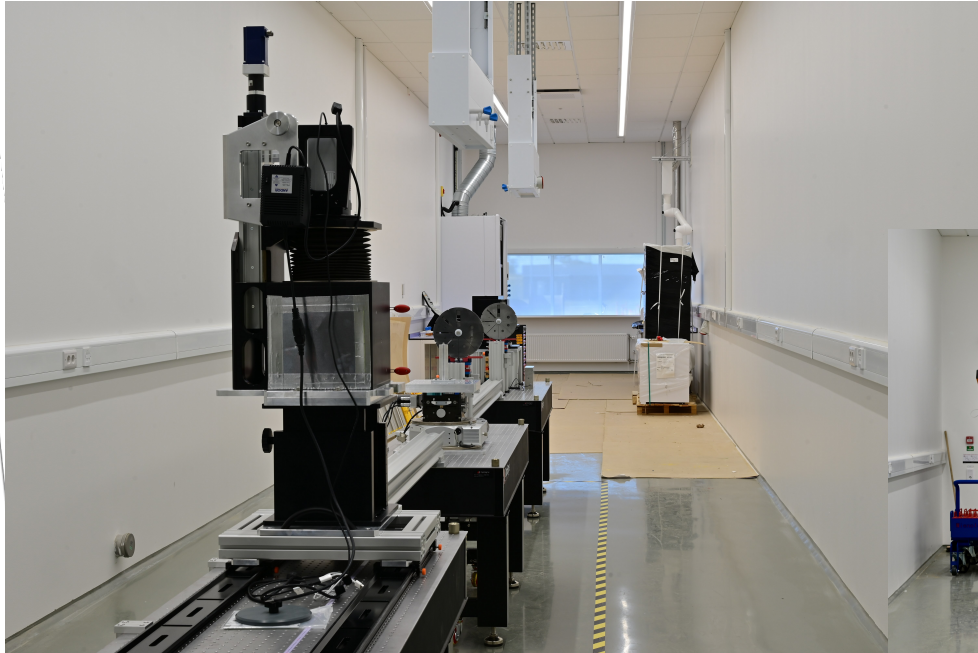
TEST A.1 – SYSTEM LED-SETUP OVERVIEW 3

- Test A.1.1 – Procedure – General Visual Inspection of Setup 4
- Test A.1.2 – Procedure – Functionality Test – Mechanical parts – Labjack* 4
- Test A.1.3 – Procedure – Functionality Test – Mechanical parts – 3-Point Level* 5
- Test A.1.4 – Procedure – Functionality Test – Mechanical parts – Railsystem for LED-Holder* 6
- Test A.1.5 – Procedure – Functionality Test – Mechanical parts – Exchangeability of Mirrorbox & Laserbox* 6
- Test A.1.6 – Procedure – Functionality Test – Mechanical parts – Adjustability Laser in Laserbox* 7
- Test A.1.7 – Procedure – Functionality Test – Mechanical parts – Plug-In Aperture* 8
- Test A.1.8 – Procedure – Visual Inspection – Cables, Connectors, Powersupply and LED 9
- Test A.1.9 – Procedure – Functionality Test – Electronics – LED-Light on/off/dimmable via current* 9

TEST A.2 – SYSTEM APERTURE WHEELS OVERVIEW 10

- Test A.2.1 – Procedure – General Visual Inspection of Setup 10
- Test A.2.2 – Procedure – Functionality Test – Mechanical parts – Vertical Adjustment* 11

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Neutron Optics Test Bench was installed & commissioned by PSI in August (FAT was done remotely before summer break)

- Implementing ESS standard Motion Control System is currently being done
- NOTB will then be ready to support installation and test activities/procedures

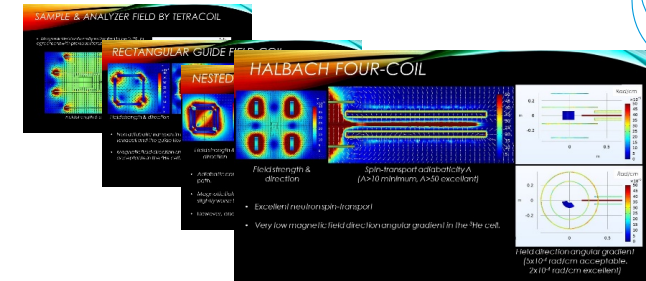


Neutron Optics & Polarisation

At present 8 instrument supported
incl 5 out of first-eight instruments

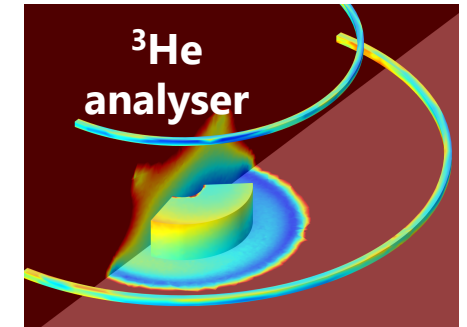
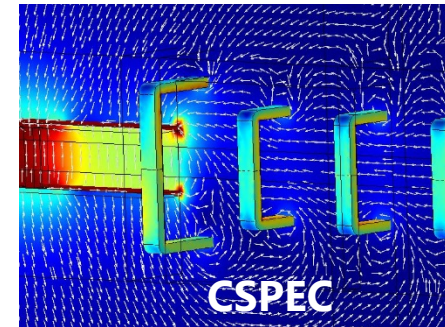
Lund Univ bachelor student (Andrea Monzani) project

- Magnetic field design for **DREAM**.
Delicated balance: spin-transport v.s. polarised ^3He .
Useful results: potential solution for guide field.
- Thesis defence on 27/5. Passed with "excellance" grade.
Student graduated with distinction.
Will continue to joint LU-Purdue Univ. graduate degree.



SREss3 project (LU colleagues, ODIN, LoKI and SKADI instrument scientists)

- Polarised SANS postdoc: **Annika Stellhorn**, Ph.D. this year. Starts in August.
- Polarised Imaging postdoc: **Alexander Backs**, Ph.D. this year. Starts in August.
- Research engineer: **Joel Hagman**, Ph.D. Started on 15/6

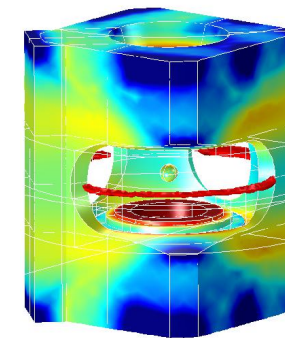


Additional work:

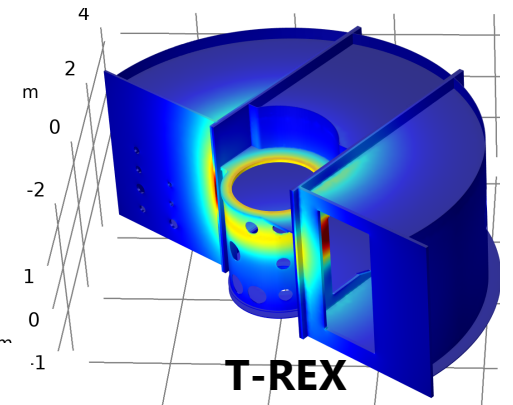
- Proposal to Swedish Research Council "Cooperation with ISIS instrumentation and methods for ESS". Polarisation for **BIFROST**, **CSPEC**.
- Magnetic field for polarisation setup, new high-field magnet, magnetic interference evaluations.
- Outfitting Optics Lab for polarisation support work



Optics Lab B02



H. Field magnet



T-REX

ESS – ILL User Meeting 2022, Lund



- Date: 5-7 October 2022
- Venue: Central Lund, AF Borgen and Palaestra
- Program: Plenary Sessions, Parallel Sessions, Posters, Site Visit

