

# Final General Assembly Meeting

## WP2: A strategy to deliver neutrons for Europe and beyond

### WP Co-Leaders

- **Andreas Schreyer**, ESS
- **Mark Johnson**, ILL
- **Lambert van Eijck**, TU Delft



BrightnESS<sup>2</sup> is funded by the European Union Framework Programme for Research and Innovation Horizon 2020, under grant agreement 823867



# WP 2 Objectives

Specifically, WP 2 aims to define the best way to provide **neutron instrumentation**, associated **characterisation methods** and **analysis tools** in a strategic and coordinated fashion to the European user community and beyond.



Andreas Schreyer, ESS

2.1

Establish a common roadmap and implementation strategy for future neutron capability.



Lambert van Eijck, ENSA  
Andrew Venter, Necs  
Peane Maleka, iThembalabs

2.2

Define the needs of the user communities relative to new neutron-based methods, in alignment with ESS facility capabilities (Europe and South Africa).

Explore and implement more efficient ways to use neutrons, beginning with pilot programmes targeting engineering and soft matter/life sciences.

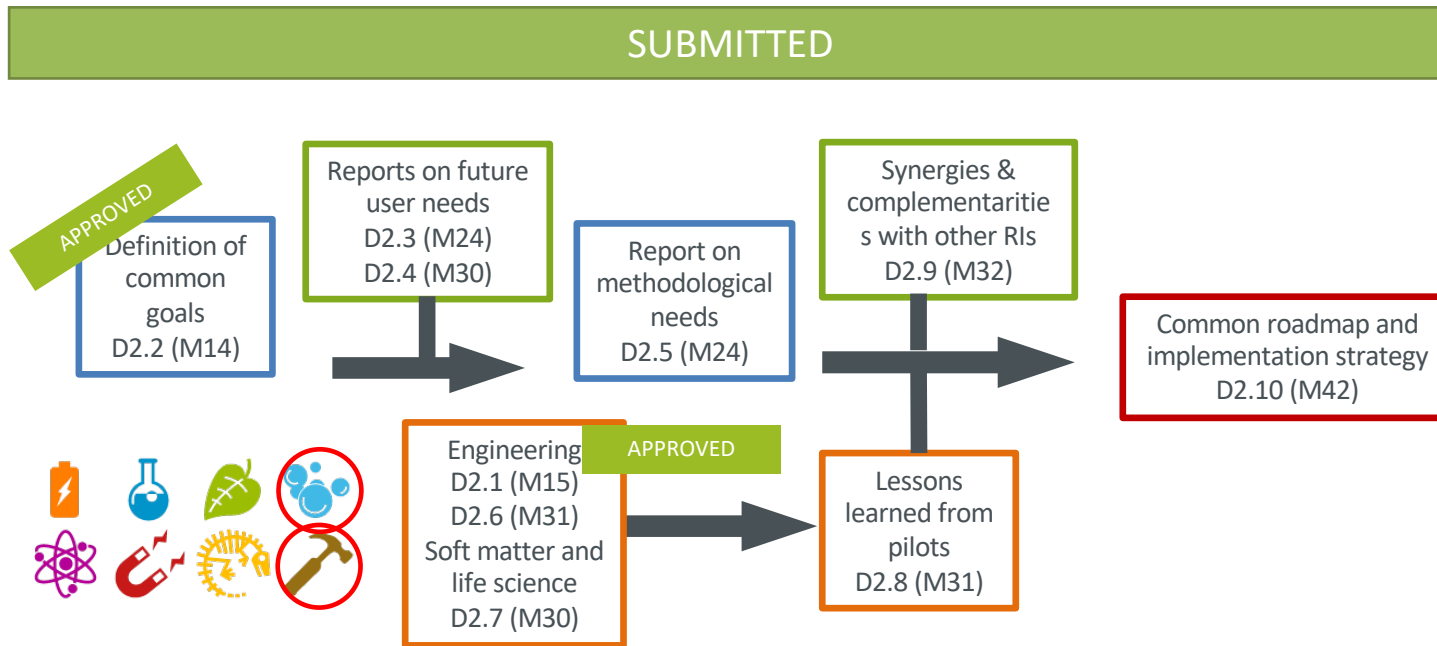
2.3



Sandra Cabeza, ILL  
Anna Leung, ESS



# WP2 Deliverables Timeline



# Task 2.1 Establish a common roadmap and implementation strategy for future neutron capability

**BrightnESS<sup>2</sup> supports LENS activity in the context of sustainability of the neutron community and sources**



## JAN 2021

- **LENS Information Manager** hired following an initiative from BrightnESS<sup>2</sup> & STFC. This establishes the **first paid position within LENS**, and the first **LENS activity jointly financed by LENS facilities**
  - Maximise **impact** of LENS communications. Website, Social media, Webinars, Newsletters. Increasing maturity of LENS Communication strategy

## FEB 2021- NOV 2021

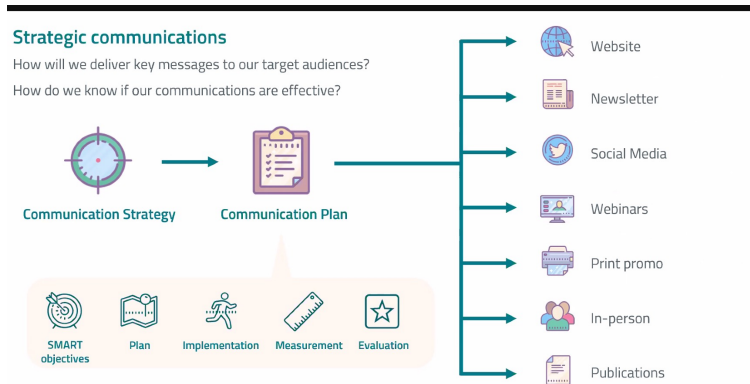
- The successful **Webinar Series** organised by **LENS WG 3** features expert speakers from across the world:
  - **How neutron science contributes to the Fight against Global Health Threats**
  - **New directions in Neutron Instrumentation**

## JAN 2022

- BrightnESS<sup>2</sup> helps to arrange and financially support external maintenance of the LENS website: **www.lens-initiative.org**



BrightnESS<sup>2</sup> is funded by the European Union Framework Programme for Research and Innovation Horizon 2020, under grant agreement 823867

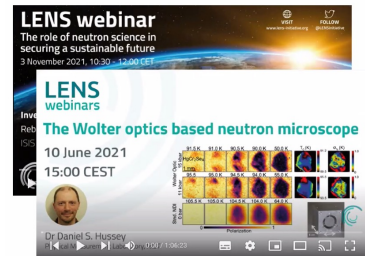


### Social Media

#### YouTube

Webinars

An introduction to the LENS Initiative



## FEB 2021

- LENS Webinar: *Exploring the potential of neutron imaging and diffraction techniques on IMAT instrument at ISIS, UK* with Genoveva Burca of ISIS (UK)

## MAR 2021

- LENS Webinar: *Elucidating amyloid aggregation mechanisms behind neurodegenerative diseases* with Emma Sparr of Lund University (SE) and Pau Bernadó, CBS/CNRS Montpellier (FR)
- LENS Webinar: *Drug development and drug delivery systems* with Andrey Kovalevsky of ORNL (USA) and Marianna Yanez Arteta of AstraZeneca Mölndal (SE)

## MAY 2021

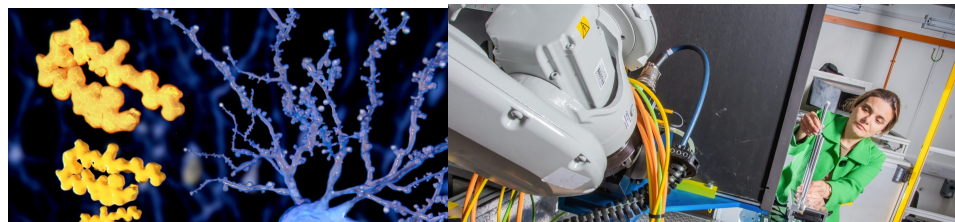
- LENS Webinar: *Ultra-high field magnets for neutron scattering: latest developments and possibilities* with Mark D. Bird of The National High Magnetic Field Laboratory (USA)

## JUN 2021

- LENS Webinar: *The Wolter optics based neutron microscope* with Daniel S. Hussey of NIST (USA)

## NOV 2021

- An extended LENS Webinar: *The role of neutron science in securing a sustainable future* as part of a full-featured online campaign to promote neutron science in conjunction with the 26th United Nations Climate Change conference, COP26



Addressing the climate crisis

The role of neutron science in securing a sustainable future

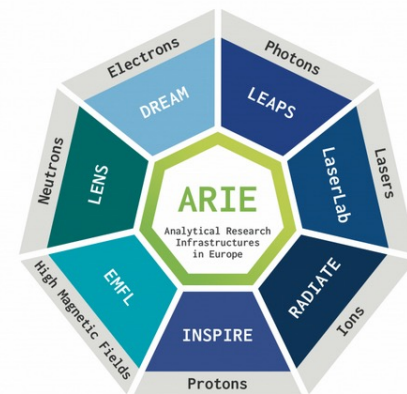




Establishing good working relations with LEAPS and contributing to the development of ARIE position papers



**LENS Science and Policy Colloquium**  
11 February 2020, Brussels



# D2.10: The Common Roadmap

The second period of BrightnESS<sup>2</sup> was dedicated to bringing the consensus-based foundation established during the first period to a finalized deliverable: the common roadmap and implementation strategy for future neutron capability.

- **3rd LENS Vision Document Writing Workshop:** online 12-13 January 2021. Full and active participation with high-level representatives from all LENS member facilities and ENSA
- **4th LENS Vision Document Writing Workshop:** online 15-16 April 2021. First full draft of the LENS roadmap document was produced. The four chapters of the document are critiqued. Sample layout prepared and collective decisions made on style and presentation
- **The LENS Vision Document writing group collectively agreed to establish an editorial board to finalise the text and layout of the LENS Vision document**





# D2.10: The Common Roadmap

The LENS Vision Document Editorial Board comprised eight people included representatives from ESS and ILL, the LENS Chair and people working on the text, layout and project management.

- **5th LENS Vision Document Writing Workshop:** online 18 June 2021. Refinement of the texts identified. Sample images and bespoke graphics were presented to the group
- **6th and final LENS Vision Document Writing Workshop:** online 30<sup>th</sup> to 31<sup>st</sup> of August 2021. The progress made by the editorial board since the last workshop was shared with the wider writing group and a professionally produced draft of the first chapter was also presented.
- Final input was collected from participants and collective **approval given to share the document with the LENS GA**



# D2.10: The Common Roadmap

JAN  
2022

- The editorial board meet in person for the first time, over two days at ESS in Lund for a **editing workshop**

FEB  
2022

- The **LENS General Assembly** and **LENS Council** meetings are held online over two days. The LENS Council endorses the document

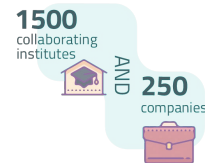
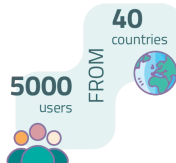
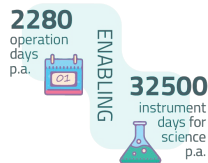
JUN  
2022

- Publication of ***Neutron Science in Europe: Strengthening World-Class Research and Innovation; Delivering Economic and Societal Impact***



# D2.10: The Common Roadmap

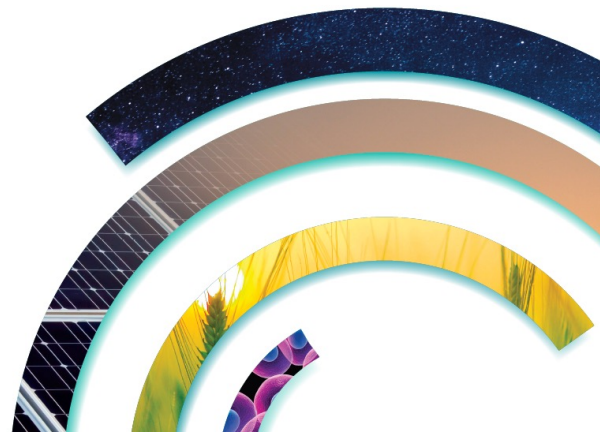
## Neutron Science in Europe: Strengthening World-Class Research and Innovation; Delivering Economic and Societal Impact



STRENGTHENING WORLD-CLASS RESEARCH AND INNOVATION  
 DELIVERING ECONOMIC AND SOCIETAL IMPACT

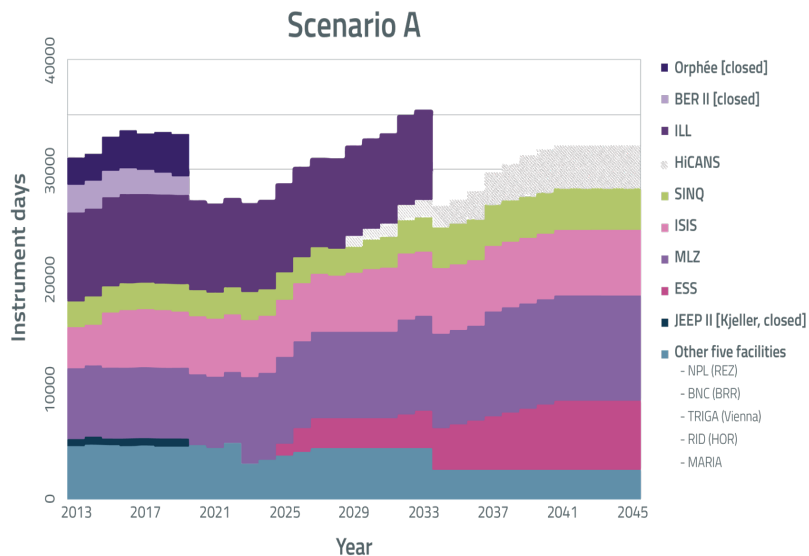
“The world-leading ecosystem of neutron facilities in Europe, supporting a world-leading community of researchers, has been created by decades of investment, but the landscape is now undergoing major changes.”

Neutron Science  
 in Europe

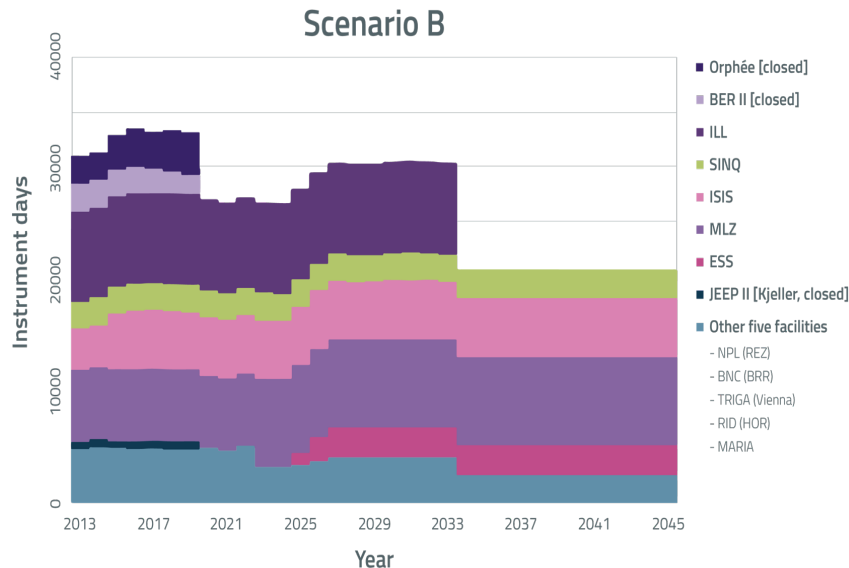


# D2.10: The Common Roadmap

Update of plots in 2016 ESFRI study



A projection of available capacity in Europe based on full implementation of all identified opportunities



A projection of available capacity in Europe based solely on already existing capacity and projects currently under construction.



## Neutron science in Europe – THE WAY FORWARD

### THE NEUTRON ECOSYSTEM

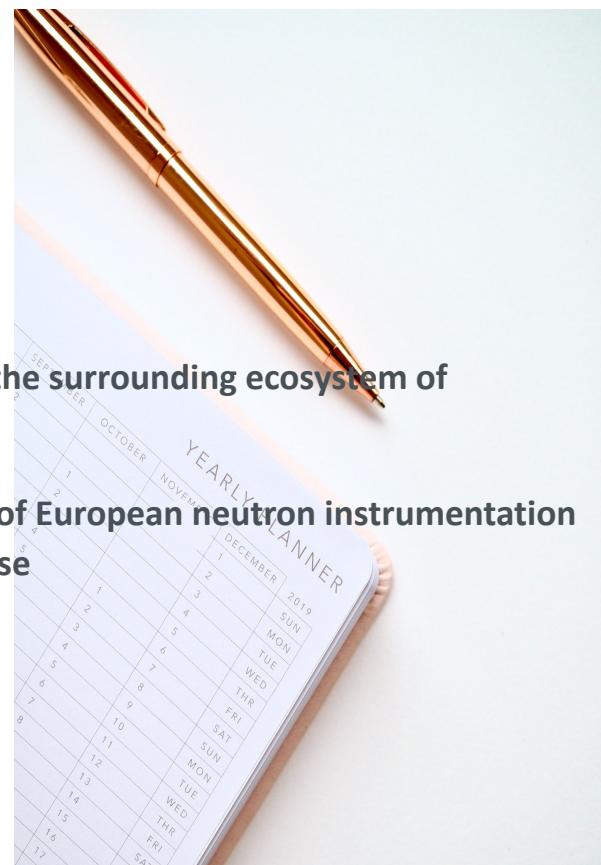
- Operational effectiveness and efficiency
- Environmental sustainability
- Collaborative research and development programmes
- A strong and dynamic European skills base

### FACILITIES AND ACCESS

- International flagship facilities and can only be effectively exploited if the surrounding ecosystem of national facilities has sufficient strength and depth.
- National facilities are a cornerstone of neutron science in Europe
- Cross-border open access allows users to employ the full complement of European neutron instrumentation
- Neutron knowledge centres will contribute to the continuity of expertise

### FUNDING

- New funding instruments
- Coordination of national planning and funding at the European level



# D2.10: The Common Roadmap

## Neutron Science in Europe: Strengthening World-Class Research and Innovation; Delivering Economic and Societal Impact

“Coordination of national planning and funding at the European level, with organisational and funding decisions being taken within the next few years, will be critical to ensure that Europe can maintain its world-leading role in neutron science. Opportunities beyond 2030 have been presented ... .

These include

- Build-up of ESS towards full capacity and specification,
- Build-up of capacity and capability in national facilities, and
- Deploying HiCANS facilities based on the delivery of a first operating facility in the 2020’s. ”

NEUTRON TECHNIQUES MAKE SIGNIFICANT CONTRIBUTIONS TO SCIENTIFIC DISCOVERY, THE CREATION OF NEW TECHNOLOGY AND ADDRESSING SOCIETY’S GREATEST CHALLENGES.



Published on behalf of the League of advanced European Neutron Sources (LENS) by the BrightnESS<sup>2</sup> project.



## D2.10: The Common Roadmap

### The Way Forward:

- The concept of a **'European Laboratory for Neutron Science' (ELNS)** will be developed as a **pan-European consortium** to facilitate the sustainable development and optimal exploitation of a **world-leading neutron ecosystem**, with the capacity and capability to **meet the research needs of a skilled and diverse community** of researchers across academia and industry
- The **finalised deliverable** presents the **shared vision in Europe** of the **contribution of neutrons to major societal challenges, the neutron landscape (facilities and users) in Europe and beyond**, the challenges and opportunities currently facing neutrons in Europe and the way forward for neutron science in Europe

## D2.10: The Common Roadmap

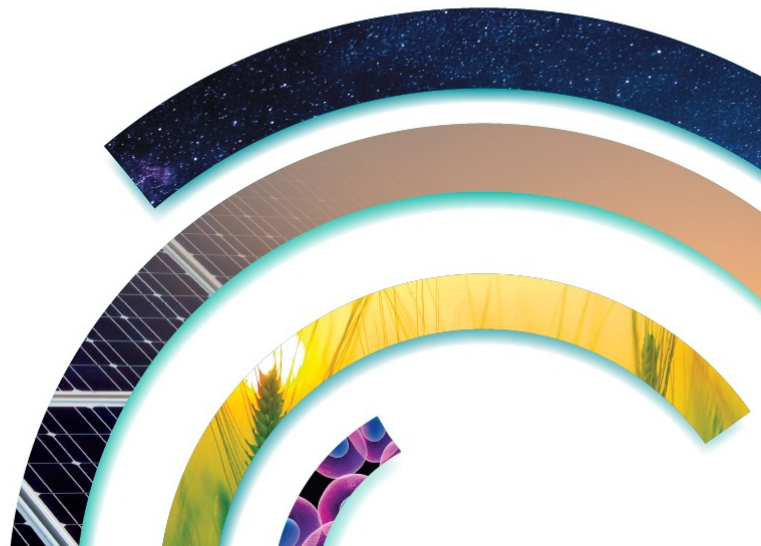
Published today on the LENS website:

<https://lens-initiative.org/2022/06/10/neutron-science-in-europe/>

A printed copy will be sent to all participants of this meeting

STRENGTHENING WORLD-CLASS RESEARCH AND INNOVATION  
DELIVERING ECONOMIC AND SOCIETAL IMPACT

Neutron Science  
in Europe







# Neutron community needs

Lambert van Eijck, Evgenii Velichko,  
ENSA & TU Delft, Netherlands

Henrik Rønnow  
EPFL, Switzerland

Final General Assembly 13/14 June 2022

The European Union flag, featuring a circle of twelve gold stars on a blue background, is positioned at the top of a green circular graphic.

**brightness<sup>2</sup>**

This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 823867



# D2.3

Step 3 of 4

### Future needs (facility related)

In this block of questions, we would like to collect your thought and expectations for the future of the neutron-based experiments and the way they are organized.

#### At which stages of neutron-based research would you like to see improvements?

- Before the experiment
- During the experiment
- After the experiment

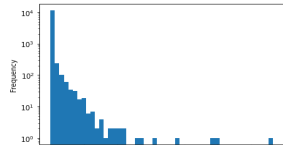
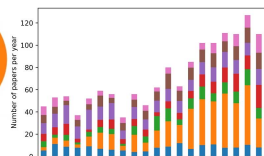
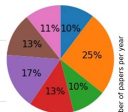
#### What would be your dream scenario in regard to future neutron science?

Text input field for dream scenario.

#### How can the European Spallation Source (ESS) help in realizing this dream?

Text input field for ESS help.

Previous Next



## Survey responses

Step 3 of 4

### Future needs (facility related)

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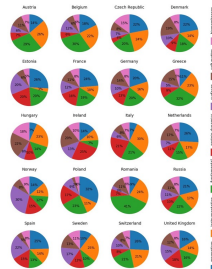
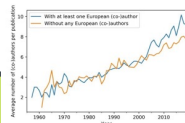
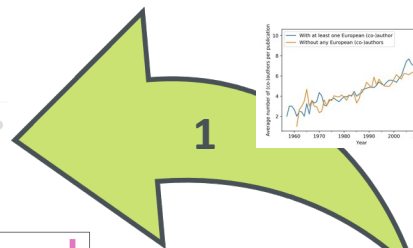
#### Which aspects of the pre-experimental stage should be improved?

- Proposal system
- Contact with the facility staff members
- Access options
- Possibilities for sample transportation to the instrument
- Education in neutron science
- Instrument-related training
- Something else

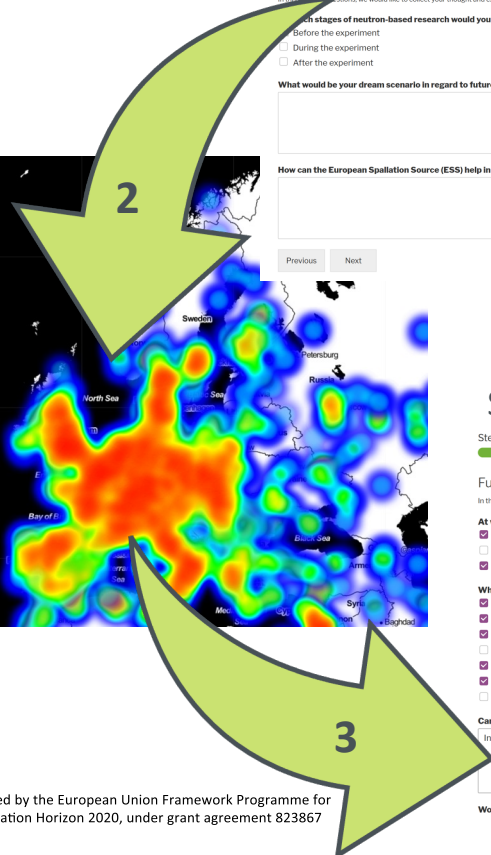
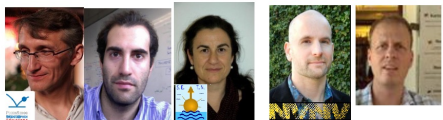
#### Can you elaborate on the proposal system improvements?

In PhD projects, the risk of not getting beam time awarded has a large impact on the progress of the scientific work of the PhD student.

Would you like to have a European single access proposal system (nonspecific to an Instrument, or a neutron source; beamtime can be granted at an Instrument X In



## ENSA delegates



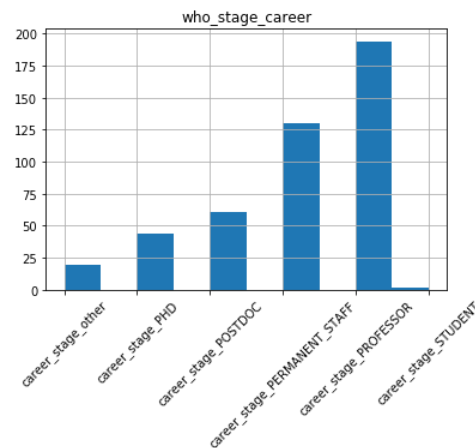
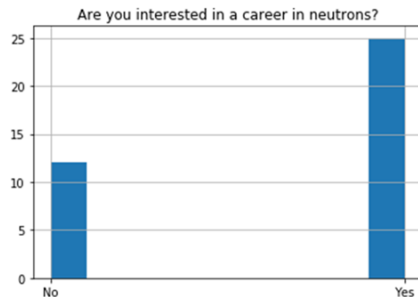


# Outcome of survey

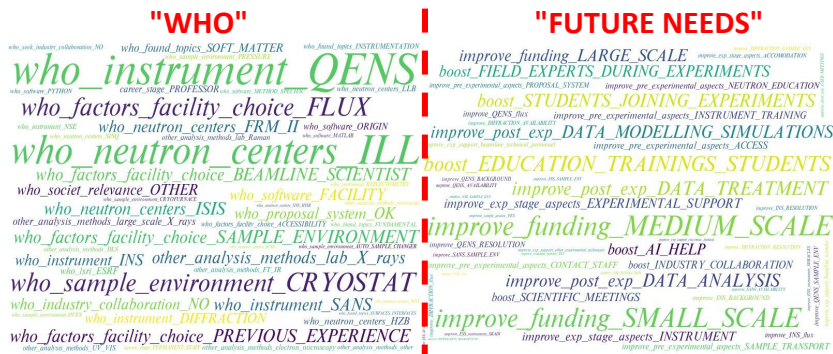
## 13500 inter-related answers + comments

Questions relate to:

Career stage, expertise, methods used, complementary methods used, instruments used, future needs before experiment, future needs after experiment, instrument needs, needs for training/expertise, funding needs, etc.



Inter-relations between questions/answers are depicted in 'wordclouds'



brightness<sup>2</sup>



# Projection on the 'career axis'

who\_societ\_relevance\_OTHER other\_analysis\_methods\_lab\_X\_rays  
career\_stage PROFESSOR  
who\_factors\_facility\_choice\_FLUX  
who\_software\_FACILITY who\_instrument\_SANS  
who\_neutron\_centers\_ILL  
who\_instrument\_DIFFRACTION  
who\_software\_METHOD\_SPECIFIC  
who\_software\_ORIGIN  
who\_neutron\_centers\_ILL  
who\_neutron\_centers\_FRM\_II  
who\_instrument\_DIFFRACTION  
who\_software\_METHOD\_SPECIFIC  
who\_software\_ORIGIN  
who\_neutron\_centers\_ILL  
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who\_software\_METHOD\_SPECIFIC  
who\_software\_ORIGIN  
who\_neutron\_centers\_ILL  
who\_neutron\_centers\_FRM\_II  
who\_instrument\_DIFFRACTION  
who\_software\_METHOD\_SPECIFIC  
who\_software\_ORIGIN

improve\_post\_exp\_DATA\_ANALYSIS  
improve\_DIFFRACTION\_RESOLUTION  
improve\_post\_exp\_DATA\_MODALING\_SIMULATIONS  
improve\_funding\_SMALL\_SCALE  
improve\_exp\_stage\_aspects\_INSTRUMENT  
boost\_STUDENTS\_JOINING\_EXPERIMENTS  
improve\_funding\_MEDIUM\_SCALE  
boost\_FIELD\_EXPERTS\_DURING\_EXPERIMENTS  
boost\_EDUCATION\_TRAININGS\_STUDENTS  
boost\_AI\_HELP  
improve\_post\_exp\_DATA\_TREATMENT  
improve\_SANS\_SAMPLE\_ENV  
improve\_DIFFRACTION\_RESOLUTION  
improve\_SANS\_SAMPLE\_ENV

other\_analysis\_methods\_lab\_X\_rays  
career\_stage other  
who\_factors\_facility\_choice\_FLUX  
who\_software\_OTHER  
who\_neutron\_centers\_FRM\_II  
who\_Isri\_ESRF  
who\_software\_FACILITY  
who\_instrument\_DIFFRACTION  
who\_software\_METHOD\_SPECIFIC  
who\_societ\_relevance\_OTHER  
who\_software\_METHOD\_SPECIFIC  
who\_software\_ORIGIN  
who\_neutron\_centers\_ILL  
who\_neutron\_centers\_FRM\_II  
who\_instrument\_DIFFRACTION  
who\_software\_METHOD\_SPECIFIC  
who\_software\_ORIGIN

improve\_post\_exp\_DATA\_ANALYSIS  
boost\_INDUSTRY\_COLLABORATION  
improve\_exp\_stage\_aspects\_INSTRUMENT  
boost\_AT\_HELP  
boost\_SCIENTIFIC\_MEETINGS  
improve\_funding\_MEDIUM\_SCALE  
improve\_funding\_LARGE\_SCALE  
boost\_FIELD\_EXPERTS\_DURING\_EXPERIMENTS  
boost\_EDUCATION\_TRAININGS\_STUDENTS  
improve\_pre\_experimental\_aspects\_INSTRUMENT\_TRAINING  
improve\_funding\_SMALL\_SCALE  
improve\_exp\_stage\_aspects\_EXPERIMENTAL\_SUPPORT  
improve\_EXP\_INSTRUMENT\_SKADI  
improve\_POST\_EXP\_DATA\_TREATMENT

career\_stage PHD  
other\_analysis\_methods\_lab\_X\_rays  
who\_factors\_facility\_choice\_FLUX  
who\_factors\_facility\_choice\_SAMPLE\_ENVIRONMENT  
who\_industry\_collaboration\_NO  
who\_student\_neutron\_career\_YES  
who\_found\_topics\_FUNDAMENTAL  
who\_proposal\_system\_OK  
who\_neutron\_centers\_ILL  
who\_societ\_relevance\_OTHER  
who\_seek\_industry\_collaboration\_NO  
who\_factors\_facility\_choice\_PREVIOUS\_EXPERIENCE

improve\_post\_exp\_DATA\_TREATMENT  
boost\_STUDENTS\_JOINING\_EXPERIMENTS  
improve\_post\_exp\_DATA\_MODALING\_SIMULATIONS  
improve\_funding\_SMALL\_SCALE  
improve\_pre\_experimental\_aspects\_PROPOSAL\_SYSTEM  
improve\_post\_exp\_DATA\_ANALYSIS  
boost\_INDUSTRY\_COLLABORATION  
boost\_FIELD\_EXPERTS\_DURING\_EXPERIMENTS  
boost\_EDUCATION\_TRAININGS\_STUDENTS  
improve\_pre\_experimental\_aspects\_INSTRUMENT\_TRAINING  
improve\_exp\_stage\_aspects\_INSTRUMENT  
improve\_funding\_MEDIUM\_SCALE

career\_stage POSTDOC  
who\_instrument\_SANS  
who\_industry\_collaboration\_NO  
who\_software\_METHOD\_SPECIFIC  
who\_sample\_environment\_CRYOSTAT  
who\_factors\_facility\_choice\_SAMPLE\_ENVIRONMENT  
who\_factors\_facility\_choice\_PREVIOUS\_EXPERIENCE  
who\_found\_topics\_MAGNETISM  
who\_neutron\_centers\_FRM\_II  
who\_proposal\_system\_OK  
who\_neutron\_centers\_ILL  
who\_instrument\_DIFFRACTION  
who\_software\_FACILITY  
who\_seek\_industry\_collaboration\_NO  
other\_analysis\_methods\_lab\_X\_rays  
who\_factors\_facility\_choice\_FLUX

boost\_STUDENTS\_JOINING\_EXPERIMENTS  
improve\_funding\_MEDIUM\_SCALE  
improve\_funding\_LARGE\_SCALE  
improve\_funding\_SMALL\_SCALE  
boost\_AI\_HELP  
boost\_FIELD\_EXPERTS\_DURING\_EXPERIMENTS  
improve\_pre\_experimental\_aspects\_INSTRUMENT\_TRAINING  
improve\_post\_exp\_DATA\_MODALING\_SIMULATIONS  
boost\_EDUCATION\_TRAININGS\_STUDENTS  
improve\_post\_exp\_DATA\_ANALYSIS  
improve\_post\_exp\_DATA\_MODALING\_SIMULATIONS  
improve\_exp\_stage\_aspects\_INSTRUMENT  
improve\_post\_exp\_DATA\_TREATMENT  
boost\_SCIENTIFIC\_MEETINGS

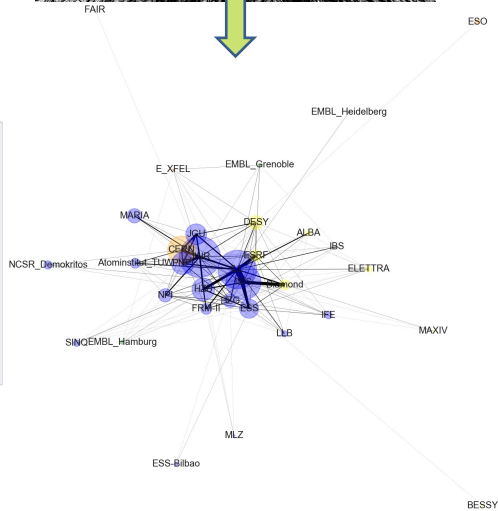
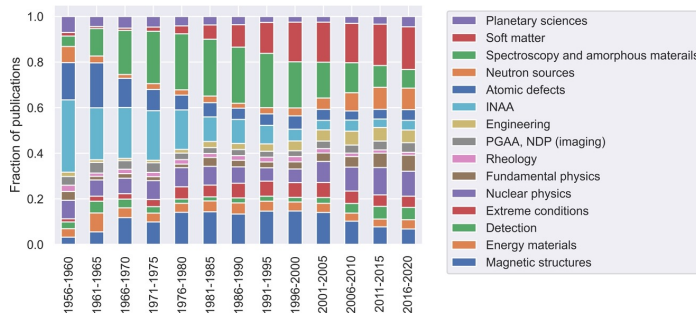
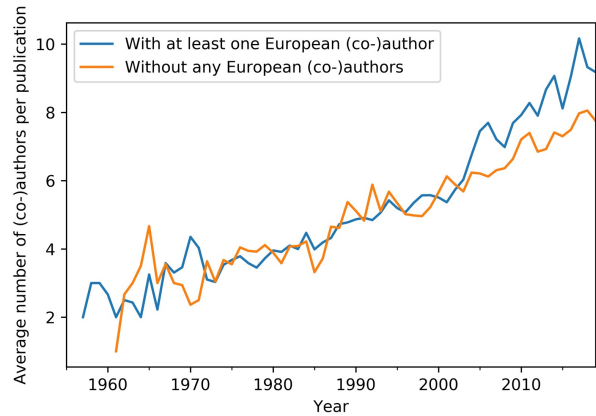
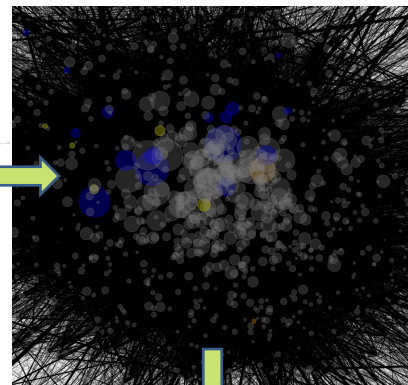
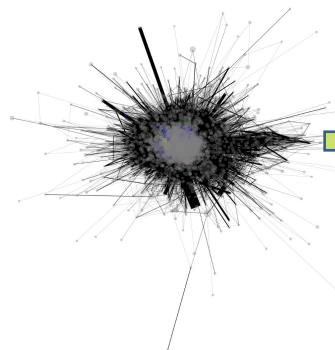
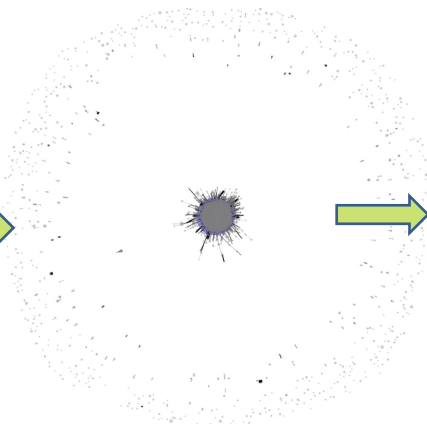
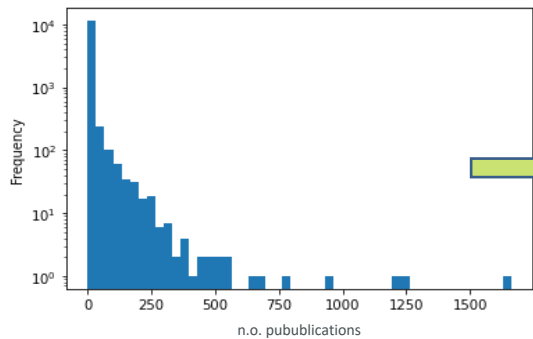


BrightNESS<sup>2</sup> is funded by the European Union Framework Programme for Research and Innovation Horizon 2020, under grant agreement 823867

Survey  
Written  
Responses +  
Comments

Interpreted  
By ENSA  
delegates









## WP2 – Task 2.2: “Assessing the needs of the South African science community for neutron scattering methods”

**Andrew Venter and Robert Nshimirimana**

Necsa SOC Limited, Pretoria, South Africa

**Peane Maleka**

NRF-iThemba LABS, Cape Town, South Africa

13-14 June 2022, ESS Campus, Lund

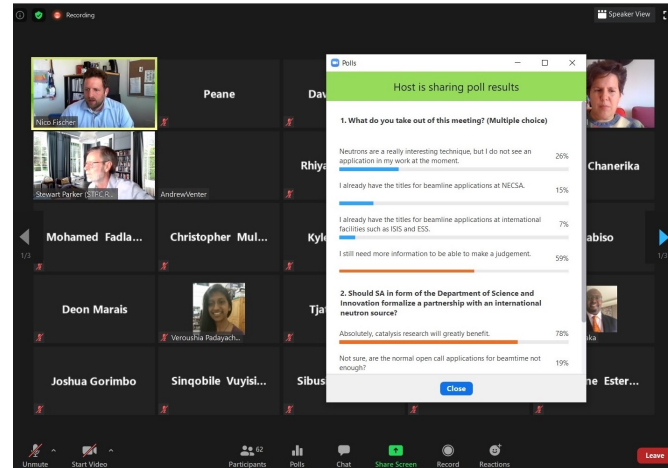
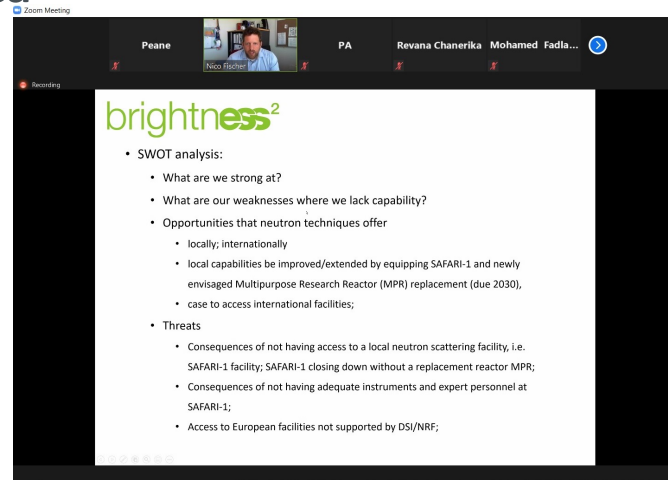


brightness<sup>2</sup>

This project has received funding from  
the European Union's Horizon 2020  
research and innovation programme  
under grant agreement No 823867

## **Task 2.2:** Assessing the needs of the South African science community for neutron scattering methods

- The main goal for the period **M19 – M42** were to:
  - engage the South African research community,
  - identify cohort of experienced local and international neutron facility Users
  - stimulate new interest through an in-person workshop (MS4) followed by ten thematic mini-symposia (supplement of workshop **MS10**) all highlighted by expert international key note contributions,
  - assess short- and long-term User needs to build the neutron community and
  - get inputs from the community on modalities to build local research infrastructure and access to premier international facilities.



- 2<sup>nd</sup> South African Workshop (**MS10**) held as series of ten 2.5 hour thematic virtual mini-symposia;
- Sessions comprised of talks by international and national experts, with involvement of inexperience neutron users, concluded with consultative discussion (refer also to 3<sup>rd</sup> General Assembly contribution for more details)
- The team completed Deliverable **D2.4** ‘Report on user Needs in South Africa’, using information gathered during the two workshops, **MS4 and MS10**. Additional input from consultations with TCs and DSI were included.
- The team completed a **promotional publication** that will be dissemination to relevant stakeholders within the South African science landscape and industry.

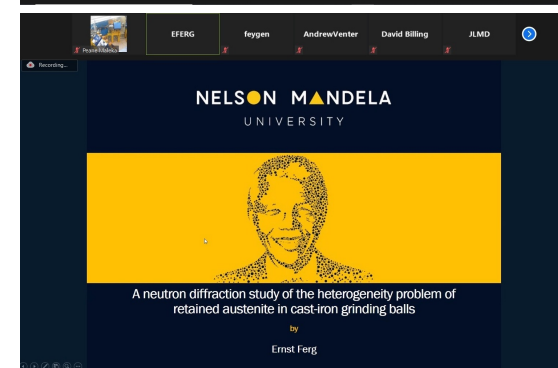
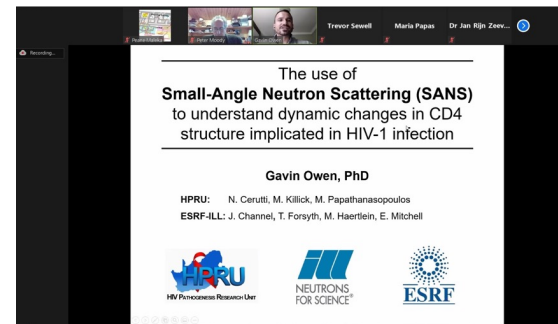
# Results for Impact

1. South Africa has a small, but vibrant, multi-disciplinary neutron science community that performs high-level research utilising neutron techniques at National facilities and leading International facilities.
2. Experienced South African neutron users have established collaborations with prominent practitioners and facility personnel to complement capabilities that do not exist in South Africa.

➤ **The South African research community through Stakeholder Engagement Workshops, the following were recommended:**

- Training the next generation of neutron scientists should be a strategic priority.
- Build on existing national capacity towards full exploitation of the capabilities and potential of the national facilities as a bridge to modern international flagship facilities.

➤ **Necsa will apply to be a Licensee of the NQL Trademark.**



## WP2 - Task 2.3: [A] Engineering Science

Pilot project for a common *Neutron Quality Label* for residual stress analysis



Sandra Cabeza, ILL  
13-14.06.2022, Lund



R. Ramadhan



S. Cabeza



D. Marais



S. Kabra



T. Pirling



J. Rebelo Kornmeier



A. Venter



M. Hofmann

## D2.1 Calibration protocols

### Common Samples

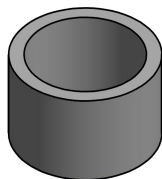
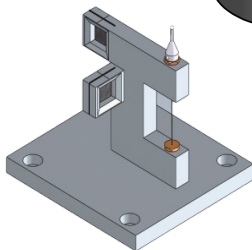
### Accuracy of GV positioning

### Important considerations

### Guidelines

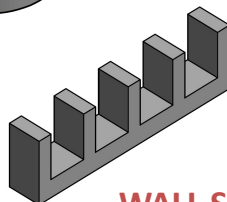
#### CALIBRATION SAMPLE

pin and foils to  
calibrate  
instrument optics  
(i.e centre and  
instrumental GV)



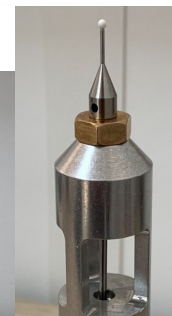
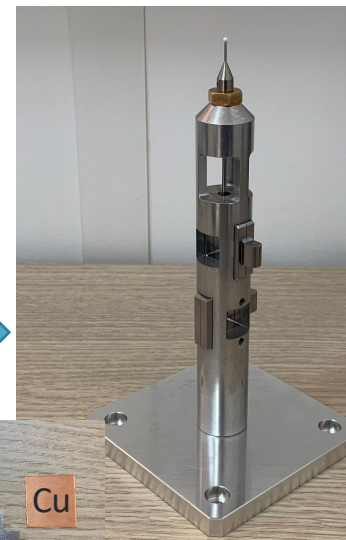
#### HOLLOW CYLINDER SAMPLE

entry scan on a curved  
sample vs wall results



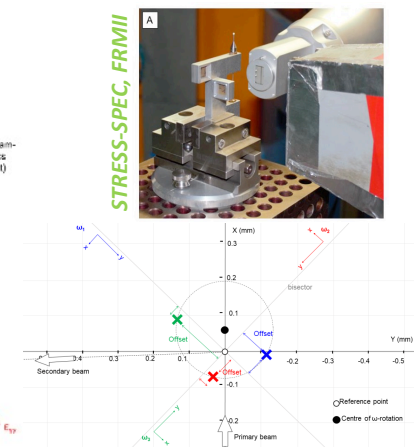
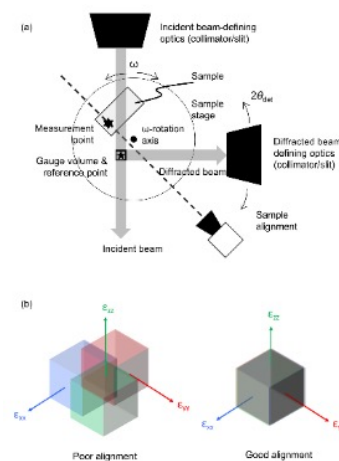
#### WALL SAMPLE

entry scan vs alignment,  
reproducibility, motor/s positioning



## D2.1 Specific Guidelines

- Determination of the centre of  $\omega$ -rotation (PIN)
- Alignment of the beam apertures (PIN)
- Measurement of reference point vs. centre of  $\omega$ -rotation (FOILS)
- Measurement of GV size (FOILS)
- Determination of sample alignment system precision (WALL&CYLINDER)
- RECOMMENDATIONS:
  - ✓ optics shall be re-aligned or report on displacement error when monochromated instruments operate at different 2Theta positions further than 40deg
  - ✓ Surface determination with entry scans in curved surfaces should be revised



R.S. Ramadhan et al. "Quantitative analysis and benchmarking of positional accuracies of neutron strain scanners" Nuclear Inst. and Methods in Physics Research, A 999 (2021) 165230

# D2.1 Common report template

<b>NEUTRON STRAIN CHARACTERIZATION REPORT</b> 22/02/2021	
<b>COMPANY :</b>  <b>TITLE :</b>	
<b>ABSTRACT:</b>	
<b>INSTITUTE:</b> <b>INSTRUMENT:</b> <b>Address:</b> <b>Date:</b> <b>Ref. N :</b> <b>Contact :</b>	<b>COMPANY:</b> <b>Address:</b>
Document Distribution	
Mail distribution	

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### 2. CALIBRATION REPORT

#### 2.1. General Instrument set up

	nominal values	units
<b>Monochromator</b>		
Type:		
cut:		
TM used:		
omega angle:		Deg
take-off angle:		Deg
wavelength:		Å
curvature:		m
distance to ref. point:		m
Other:		
<b>Time of Flight - ToF</b>		
total flight path:		m
wavelength range:		Å
channel width:		s
inc. beam divergence:		Deg
Other:		
<b>Primary optics</b>		
<input type="checkbox"/> slit		
Primary slit width - PSW:		mm
Primary slit height - PSH:		mm
Primary slit distance - PSD:		mm
<input type="checkbox"/> collimator		
horizontal focal distance:		mm
vertical focal distance:		mm
horizontal FWHM:		mm
vertical FWHM:		mm
<b>Secondary optics</b>		
<input type="checkbox"/> slit		
Secondary slit width - SSW:		mm
Secondary slit height - SSH:		mm
Secondary slit distance - SSD:		mm
<input type="checkbox"/> collimator		
horizontal focal distance:		mm
vertical focal distance:		mm
<b>Detector</b>		
Distance to reference point:		m
<input type="checkbox"/> Monochromated		
Beam		
Position Sensitive PSD:		mm
Ref. Det. Distance:		mm
Area:		cm <sup>2</sup>
Pixel size hor./vert.:		Deg
angular range hor./vert.:		Deg
Other:		
<input type="checkbox"/> TOF		
angular acceptance horiz.:		Deg
Angular acceptance vert.:		Deg
Other:		

The NQL trademark is supported by [BRIGHTNESS](#) a European Union project within the European Commission's Horizon 2020 Research and Innovation programme under grant agreement 101019749.

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Sample Stage	nominal values	Units
Type Hexapod / XYZ table		
positioning accuracy		
repeatability		
Other:		
Type omega rotation		
positioning accuracy		
repeatability		
Other: eccentricity vs 2Theta		
Type cradle ±45°		
positioning accuracy		
repeatability		
Other: sphere o. conf.		
Type Rotation stage 360		
positioning accuracy		
repeatability		
Other:		
Type Temperature		
Room temperature test		
Furnace		
accuracy		
repeatability		
Other:		
Type Loading rig		
Load range		
accuracy		
repeatability		
Other:		

#### 2.2. Particular instrument configuration for the measurement

Detector calibration	Measured values	uncertainty	units
channel width			Deg
Ref. Detector distance			mm
Other:			
<b>Beam alignment</b>			
Pin diameter			mm
Primary beam	horizontal		mm
Secondary beam	vertical		mm
error on beam position	horizontal		µm
Other:			
<b>Wavelength spread, shape of gauge volume</b>			
Foreshet (diagonal scan)			mm
delta lambda			Å
Other:			

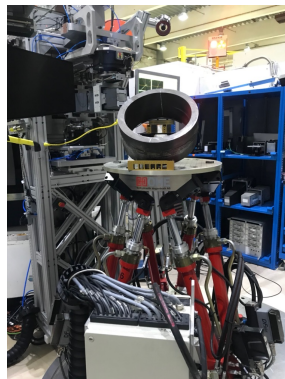
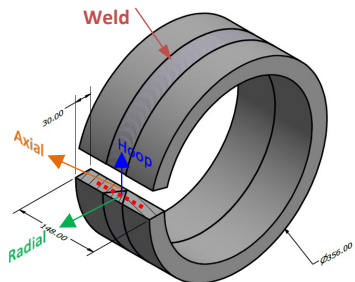
The NQL trademark is supported by [BRIGHTNESS](#) a European Union project within the European Commission's Horizon 2020 Research and Innovation programme under grant agreement 101019749.

- In-house quality certification
- More specific and compliant with ISO 21432:2019
- Traceability
- Multiple beam time campaigns / instruments
- Familiar format (confidence, exchangeability)

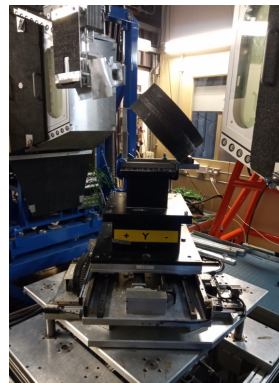


## D2.6 Industrial application of the NQL

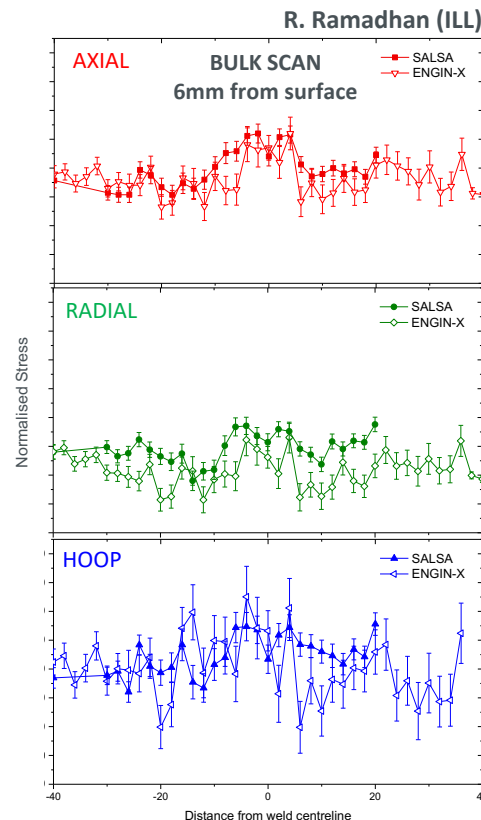
EDF – R&D (Robin Vincent, France) :  
Steel cylindrical weld – a bulk study



SALSAL, ILL (FR), Aug 2020



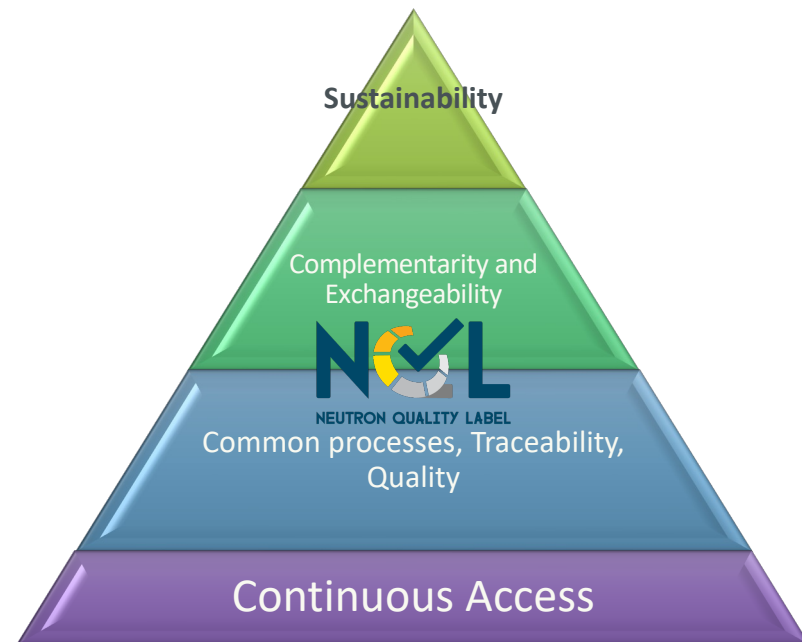
ENGIN-X, ISIS (UK), Sept 2020



## D2.8 Conclusions from Pilots

*Collaborative method development between neutron facilities are beneficial, scientifically and economically:*

- *establish novel or efficient methods or procedures extends the capabilities of neutron facilities, enabling high-impact scientific experiments.*
- *Harmonization increases confidence regardless of which neutron facility (instrument) they are located in.*



# WP2 – Task 2.3: [B] Deuteration Pilot

Anna Leung, ESS

13-14.06.2022, Lund



brightness<sup>2</sup>

This project has received funding from  
the European Union's Horizon 2020  
research and innovation programme  
under grant agreement No 823867

Lipids: naturally-occurring **small molecules** with a **big impact** in soft matter science – from medicinal chemistry and drug mechanism studies to food and pharmaceutical formulation science

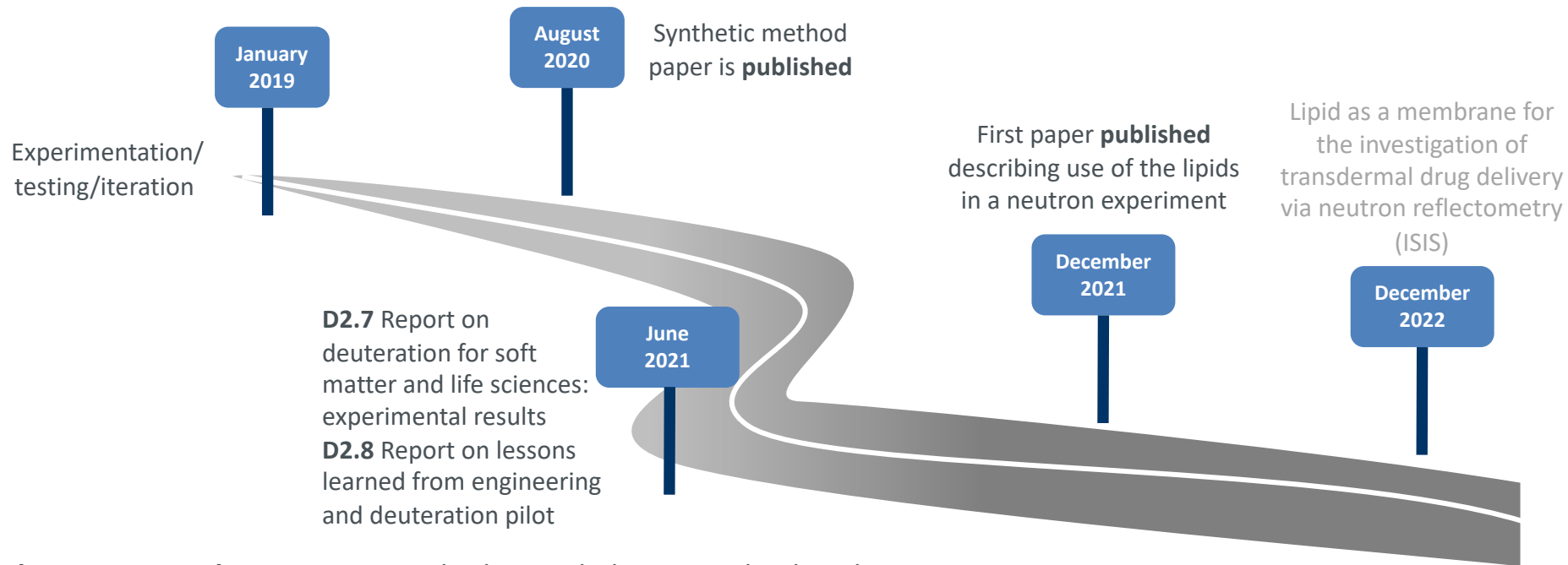
Deuterium-labelled lipids are used in neutron scattering experiments at ISIS and other neutron sources, but some are challenging to make

This pilot established the use of **biological catalysts (enzymes)** to improve their synthesis

specific	mild
non-toxic	efficient



# Progress Update: Subtask 2.3b



**February 2020-February 2022:** method extended to 3 new lipid analogues

**July 2021-May 2022:** 4 lipids supplied to 3 PIs from 3 countries for NR, SANS and NSE experiments at 2 neutron facilities



BrightnESS<sup>2</sup> is funded by the European Union Framework Programme for Research and Innovation Horizon 2020, under grant agreement 823867



Science & Technology Facilities Council

ISIS



NEUTRONS  
FOR SCIENCE

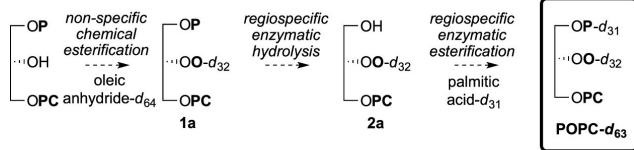


## Enzyme-Assisted Synthesis of High-Purity, Chain-Deuterated 1-Palmitoyl-2-oleoyl-*sn*-glycero-3-phosphocholine

Oliver Bogojevic and Anna E. Leung\*

Cite This: *ACS Omega* 2020, 5, 22395–22401

Read Online

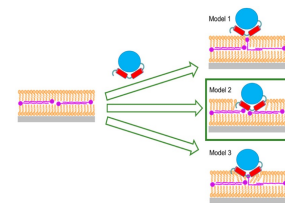


P = palmitoyl; O = oleoyl; PC = phosphocholine.

Article

## New Insights into the Interaction of Class II Dihydroorotate Dehydrogenases with Ubiquinone in Lipid Bilayers as a Function of Lipid Composition

Juan Manuel Orozco Rodriguez <sup>1</sup>, Hanna P. Wacklin-Knecht <sup>2,3,\*</sup>, Luke A. Clifton <sup>4</sup>, Oliver Bogojevic <sup>3,†</sup>, Anna Leung <sup>3</sup>, Giovanna Fragneto <sup>5</sup> and Wolfgang Knecht <sup>1,\*</sup>



- Four neutron experiments facilitated by lipids unavailable elsewhere
- Two scientific articles published (more in preparation)
- Bespoke lipids offered as part of a catalogue that ESS can offer to neutron researchers on-demand

## Deuteration and Macromolecular Crystallisation Platform

### Product List

January 2022

Biological: proteins .....	2
Biological: lipid mixtures .....	2
Chemical: carboxylic acids, alcohols, alkyl halides .....	3
Chemical: surfactants .....	4
Chemical: phospholipids .....	5
Chemical: aromatic molecules .....	6
Chemical: other .....	6
Crystallisation support: .....	7

## Collaboration

Experimentation

Iteration

Inception

Publication



# Acknowledgements

- Oliver Bogojevic, Dr Jia-Fei Poon



- Dr Peixun Li, Dr John Webster



- Dr Wolfgang Knecht (Lund Protein Production Platform), Dr Katherine Thompson (Birkbeck, University of London), Prof Gerhard Gröbner (Umeå University), Dr Michihiro Nagao (NIST/University of Maryland)
- Dr Sandra Cabeza (ILL) and Dr Ranggi S. Ramadhan (ILL) (Subtask 2.3a)





# Sustainability of WP2



## Task 2.1 “Developing a European Neutron Strategy in a Global Context”

- *Baseline set, next step: European Neutron Science Lab (ENSL)*



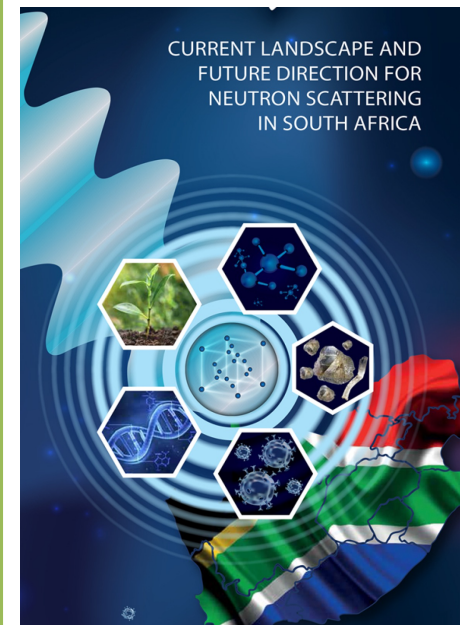
## Task 2.2 “Assessing the needs of the European Science Community for New Neutron-based Methods”

- *Natural language based analysis of neutron science output allowed quantification:
 
  - *the neutron scattering community, and*
  - *evolution of scientific and technological domains to which neutron techniques contribute**
  
- *Established analysis tools will be used for longitudinal analyses of future evolution of the user community and domains of use*
  
- *Implementation of country specific analyses to guide national strategies and roadmaps*
  
- *For ENSA, sustainable enhancement of operations
 
  - *Evolution of LENS through BrightnESS2 support provided ideal facility interface to ENSA as scientist association*
  - *Partnership in BrightnESS2 expanded ENSA sphere of activities**
  
- *ENSA now geared to engage in similar future joint projects to enhance impact ESS, of neutron science capabilities and of the predicted sharp growth of neutron community*



## Task 2.2 “Assessing the needs of the European Science Community for New Neutron-based Methods”

- **Deliverable 2.4** “Report on User Needs - South Africa” is used to advise the Department of Science and Innovation (DSI) on:
  - the level and extent of the South African neutron scientists support that is required,
  - access to international Large Scale Research Infrastructure,
  - how to facilitate and drive neutron science in South Africa as an imperative component and contributor to a knowledge-based economy in the short, medium and long term.
- A **promotional publication** will be disseminated to relevant stakeholders within the South African science communities (e.g. universities, industries, science councils, etc.)



# brightness<sup>2</sup> Task 2.3a Engineering Pilot

## Establishing the NQL

- Registered trademark in EU and UK; awaiting for USA, Canada, China and Switzerland; rejected in Australia
- License free of charge for 10 years (to be signed by all partners in pilot)
- Open to new members: proposals submitted and discussed with ANSTO and PSI
- Dedicated website NEUSS (Neutron Strain Scanning): method, instruments and NQL.

→ <http://neusscan.eu/>

## On-going working group

- Instrumental and Method development, industrial applications and access enhancement:
  - improve entry scan codes
  - common DEC look up table
  - in-situ high T characterization
  - d0 for additive manufacturing
  - Instrument uncertainties translation to stress

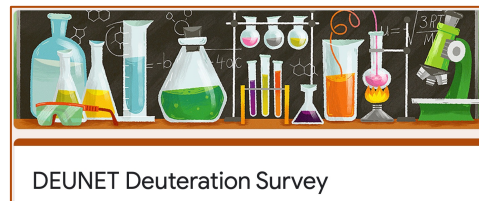


# brightness<sup>2</sup> Task 2.3b Deuteration Pilot

- Published methods have been utilised by new team member in the ESS DEMAX lab
- The sustainability of this programme is ensured by the DEUNET: a consortium of deuteration laboratories who collaborate to share methods, materials and expertise



- Continued scientific collaboration, e.g., sending/hosting PhD students/postdocs for cross-training to share materials and knowledge



DEUNET Deuteration Survey

- Continued collaboration for securing external funding

