BrightnESS²

Bringing Together a Neutron Ecosystem for Sustainable Science with ESS

H2020-INFRADEV-3-2018-1

Grant Agreement Number: 823867

Deliverable Report

D2.2: Intermediate report on definition of common goals

1. Project Deliverable Information Sheet

BrightnESS^2 Project	Project Ref. No. 823867	
	Project Title: BrightnESS^2 – Bringing Together a Neutron Ecosystem for Sustainable Science with ESS	
	Project Website: https://brightness.esss.se	
	Deliverable No.: **D2.2: Intermediate report on definition of common goals**	
	Deliverable Type: **Report**	
	Dissemination Level:	Contractual Delivery Date: 29.02.2020
		Actual Delivery Date:
	EC Project Officer: René Martins	

2. Document Control Sheet

Document	Title: **D2.2: Intermediate report on definition of common goals**	
	Version: V1	
	Available at: TBD	
	Files: 1	
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BrightnESS^2 is funded by the European Union Framework Programme for Research and Innovation Horizon 2020, under grant agreement 823867

3. List of Abbreviations and Acronyms

AI	Artificial Intelligence
AOCNS	Asia-Oceania Conference on Neutron Scattering
AONSA	Asia-Oceania Neutron Scattering Association
BER-II	Berlin Experimental Reactor II
BNC	Budapest Neutron Center
CANS	Compact Accelerator-Based Neutron Source
CATSA	The Catalysis Society of South Africa
CEA	Commissariat à l'Énergie Atomique et aux énergies alternatives
CNR	Consiglio Nazionale delle Ricerche
CNRS	Centre National de la Recherche Scientifique
DSI	Department of Science and Innovation (South Africa)
EB	Executive Board
EC	European Commission
ENCS	European Conference on Neutron Scattering
ENSA	European Neutron Scattering Association
EOI	Expression of Interest
EPFL	École Polytechnique Fédérale de Lausanne
ERIC	European Research Infrastructure Consortium
ESFRI	European Strategy Forum on Research Infrastructures
ESS	European Spallation Source ERIC
EU	European Union
FRM-II	Research Neutron Source Heinz Maier-Leibnitz
FZJ	Forschungszentrum Jülich
GA	General Assembly
H2020	Horizon 2020
HOFs	Heads of Facilities
HPC	High-Performance Computing
ICNS	International Conference on Neutron Scattering
ICRI	International Conference of Research Infrastructures
IFE	Institutt for Energiteknikk

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IK	In-Kind
IKC	In-Kind Contribution
ILL	Institut Laue-Langevin
INFN	Istituto Nazionale di Fisica Nucleare
ISIS	ISIS Neutron and Muon Source
iThemba LABS	iThemba Laboratory for Accelerator-Based Sciences
J-PARC	Japan Proton Accelerator Research Center
LEAPS	League of European Accelerator-based Photon Sources
LENS	League of advanced European Neutron Sources
LLB	Laboratoire Léon Brillouin
MLZ	Heinz Maier-Leibnitz Zentrum
Necsa	South African Nuclear Energy Corporation
NLP	Natural Language Processing
NRF	National Research Foundation (South Africa)
NSSA	Neutron Scattering Association of America
PSI	Paul Scherrer Institute
RI	Research Infrastructure
STFC	Science and Technology Facilities Council
TU Delft	Technical University of Delft
TUM	Technical University of Munich
WG	Working Group
WP	Work Package

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6. Executive Summary: A strategy to deliver neutrons for Europe and beyond

The European neutron science landscape is undergoing significant evolutionary change. This was most comprehensively assessed by the 2016 European Strategy Forum on Research Infrastructures (ESFRI) report, *Neutron scattering facilities in Europe: Present status and future perspectives*, which raised the alarm for both the scientists that use neutrons and the national and trans-national research facilities that provide them.[1] The report emphasised the urgent need for a coherent organisation of neutron facilities to address the anticipated neutron gap with a "strategy-led approach". This action was prescribed to coordinate long-term technical and scientific strategies across facilities, but also to pool the community's collective authority and expertise in order to guide European decision makers toward the funding and policy actions that will best support neutron scientists and the socially significant science and innovation results they produce. At stake, noted the ESFRI report, is the world-leading neutron science ecosystem that Europe has developed over five decades.

Photo 1: Neutron reflectometer REFSANS at FRM-II/TUM

From its conception as an EC INFRADEV-03 project application in 2017, BrightnESS² has kept these objectives in focus. It has long been understood within the science community that the long-term sustainability of the European Spallation Source (ESS) is dependent above all on the long-term sustainability of the existing community of European neutron scientists and facilities. A key emphasis of the ESFRI report was that a successful ESS is simply not possible if its construction should result in a significant reduction of European neutron science capacity as a whole. This essential co-dependency among European facilities large and small is at the heart of BrightnESS² and its support for the League of advanced European Neutron Sources, LENS.

[1] ESFRI Physical Sciences and Engineering Strategy Working Group, Neutron Landscape Group. Neutron scattering facilities in Europe: Present status and future perspectives, **2016**.

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The BrightnESS² project's first year has notched notable progress in the development of a neutron strategy for Europe. The following "Intermediate report on the definition of common goals" for BrightnESS² Work Package 2 (WP 2) will demonstrate how BrightnESS² has worked month over month to establish a solid foundation for an inclusive, consensus-based, reality-based, meaningful and lasting strategy for European neutron science. The WP 2 final deliverable, "a common roadmap and implementation strategy for future neutron capability" (hereafter, "the common roadmap"), is taking shape as a document that will be produced by LENS, with contributions from the European Neutron Scattering Association (ENSA), and will reflect the collective vision of the European neutron science community for its future. The goals to be addressed in the document are:

- to secure the European scientific user base for neutrons;
- to advance synergies in instrument design and other technical developments;
- to define the community's orientation toward socially impactful research outcomes;
- and to ensure the sustainability of Europe's neutron science labs and infrastructures.

This document is now being drafted by decision-makers from all LENS member facilities, and with the participation of ENSA within the context of its co-leading role in WP 2 (Task 2.2), where it is tasked with defining and reporting the needs of the user community in terms of new neutron-based methods. Additionally, the user-level knowledge-sharing with South African scientists that is also a part of WP 2 (Task 2.2 and 2.3) is helping to establish a template to develop Europe's neutron strategy with a global perspective.

The common roadmap will serve as the principle guide for all actors navigating the near-term and long-term challenges anticipated for neutron science in Europe, but it remains only the map. Europe's neutron science stakeholders must also secure the support necessary to implement it. It is here that a mature LENS organisation will be critical. Thanks to support from BrightnESS², the five LENS working groups are now operational, strongly evidenced by the organisation's October 2019 Executive Board Meeting and General Assembly, where several priority actions were identified and advanced.[2]

One of these priority actions, concerning deuteration support for neutron researchers working primarily in soft matter studies and the life sciences, is very closely aligned with one of the two pilot projects launched as part of WP 2. The deuteration pilot (Task 2.3 [B]), together with the engineering materials *Neutron Quality Label* pilot (Task 2.3 [A]), have been designed to define new, more efficient ways of working among neutron science facilities, which is also a major objective of LENS. It will also likely be the role of LENS to facilitate the development of the business model established by the pilots.

The goal here is twofold, and cleanly demonstrates one of the solutions to the paradoxical problem that European neutron science is facing: a need for more users of increasingly scarce beam time. It is a truism for neutron scattering that the fewer scientists using neutrons, be it through a lack of instrument days or services, the smaller the user base becomes now and in the future. A shrinking user base, which is most strongly correlated with decreased access, is the outcome Europe must avoid at

[2] https://www.lens-initiative.org/2019/10/24/european-neutron-facilities-come-together-for-lens-general-assembly/

all costs. This would have negative impacts for a generation of fundamental science, innovation and the ability of European society to meet its ambitions.

Creatively addressing the capacity gap by standardising some user services across facilities—as the pilot programmes serve to demonstrate—also expands the user base for neutrons among, for example, life scientists, soft matter experts and industrial users. Bringing these pilot programmes and similar initiatives up to scale means that facilities will have more resources for their users and that they will in turn be able to accommodate more users through a more efficient use of the available beam time. These are two outcomes essential to securing Europe's future neutron capability.

In one the project's most recent developments, BrightnESS² has played an instrumental role in bringing LENS together with another major umbrella organisation for European large-scale analytic facilities—LEAPS, the League of European Accelerator-Based Photon Sources. Collectively representing 25 facilities used by some 30,000 researchers, cooperation between LENS and LEAPS has the potential to create significant strategic advantages as European research infrastructures begin to align their efforts toward European-wide mission- and challenge-led approaches designed to find solutions for society's grand challenges.

What the present report demonstrates above all is the impact that BrightnESS² is having on the convergence of the European neutron community at the highest possible levels, and to a degree that has never been attempted before. This cohesion is critical to the development of the common roadmap, and consequently to the long-term stability of Europe's world-leading neutron science community.

Photo 2: More than 60 project participants from 11 nations, including South Africa, attended the BrightnESS² kick-off meeting in Rome on 15 January 2019.

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7. Introduction: Present opportunities and challenges for European neutron sources

The fundamental basis for BrightnESS²'s WP 2 lies in the co-dependency between individual European neutron sources and the collective strength of the neutron science community as a whole. The long-term sustainability of ESS urgently needs to be secured, but of equal importance is the necessity to coordinate on the long-term sustainability of the entire ecosystem of neutron science in Europe. ESS will be Europe's next flagship facility, but if it is not able to hold the centre of the broader neutron science landscape, this centre could shift outside of Europe, leaving the future of ESS and European science and innovation compromised.

BrightnESS² WP 2 brings together both the facility side and the user side in order to shape this future and initiate its implementation. It is therefore structured as follows:

- Task 2.1 is dedicated to developing a European neutron strategy in a global context and includes the key user facilities that in the course of 2018-19 have formed LENS.
- Task 2.2 is dedicated to assessing the needs of the European science community for new neutron-based methods, with ENSA in the lead. BrightnESS² has enabled ENSA for the first time in its history to act in the capacity of a fully resourced legal entity.
- Task 2.3 is dedicated to exploring and implementing new ways of working for the most efficient usage of neutrons through two pilot programmes. The first [A] is an engineering initiative led by ILL that aims to establish an experimentally validated *Neutron Quality Label* for residual stress in engineering materials. The second [B] targets the expansion of neutron instrument techniques among soft matter and the life sciences by establishing programmes at ESS and STFC to increase the availability of deuterated samples to researchers.

Tasks 2.2 and 2.3 will feed up into the more fundamental deliverable of Task 2.1, which is to publish the "common roadmap and implementation strategy for future neutron capability" in October 2021, month 34 of the project.

7.1. The European neutron science landscape

The neutron is a unique probe with characteristics that cannot be supplanted by other methods. Neutrons allow scientists to understand the world at the atomic and molecular level in a non-destructive manner. This makes neutron science one of the most useful analytical techniques deployed across numerous science and technology disciplines, and an essential complement to completing characterisations created by other methods. Neutrons are an essential tool used in support of the science addressing the EU's Grand Challenges and have a half-century legacy of significant socio-economic impact in Europe.[3]

Fifty percent of neutron science publications globally are attributed to European researchers from academia and industry, working at European neutron sources.[4] Neutrons can record, for example, the

[3] Technopolis/STFC. ISIS Lifetime Impact Study, Vol. 1, **2016**.

interior dynamics of lithium-ion batteries, reveal obscured minutiae from ancient artefacts or clarify the mechanisms of antibiotic resistance in bacteria. Cancerous tumours are treated with radiopharmaceuticals produced with neutrons. Neutrons are also critical for industrial and engineering researchers developing more efficient fuel cells for electric vehicles or testing stress and strain during the manufacturing of carbon-free steel. They will contribute to more cost-effective health care devices, advances in quantum computing and artificial intelligence, alternative energy technologies, hydrogen storage, food production and fundamental advances in structural biology.

Photo 3: Four of Europe's major neutron sources. Clockwise from top left, ILL, ESS, FRM-II and ISIS.

The European neutron science user community is widely acknowledged as the largest and the most diverse in the world.[4,5] According to the 2018 BrightnESS survey, *Neutron Users in Europe: Facility-Based Insights and Scientific Trends*, it includes roughly 5,800 researchers performing nearly 4,000 experiments with about 25,000 instrument days annually across a network of international and national neutron sources.[6] Europe has been the global leader in scientific output by neutron scientists for four decades, led by ILL in Grenoble and the ISIS Neutron and Muon Source near Oxford. Meanwhile in southern Sweden, the ESS construction project has reached 65% completion and the facility is

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[4] ESFRI Physical Sciences and Engineering Strategy Working Group, Neutron Landscape Group. Neutron scattering facilities in Europe: Present status and future perspectives, **2016**.

[5] A Report by the APS Panel on Public Affairs. Neutrons for the Nation: Discovery and Applications while Minimizing the Risk of Nuclear Proliferation, p. 10, **2018**.

[6] European Spallation Source ERIC. Neutron Users in Europe: Facility-Based Insights and Scientific Trends, **2018.**

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scheduled to begin its scientific user programme in 2024. Once it achieves steady-state operations, expected in 2026, ESS will be the most powerful and scientifically advanced facility of its kind globally.

The challenges and opportunities facing Europe's neutron community in the coming decade have been well-documented in recent years. The above-cited reports make clear that the opportunities inherent in Europe's world-leading status and the construction of ESS are self-evident and must be optimised. LENS was established by Europe's nine leading neutron science facilities in September 2018 to bring new coherence to this mission.

Scarcity of beam time and a drop off in funding, progressing hand-in-hand, are the most immediate challenges facing the neutron community. Europe begins 2020 with what amounts to a 20% drop in capacity from 2018 [Fig. 1]. Two of Europe's major neutron sources ceased operations at the end of last year: the Orphée reactor used by the Laboratoire Léon Brillouin (LLB) near Paris, and the BER-II research reactor at Helmholtz-Zentrum Berlin (HZB), both hosting users and experiments—and in the case of BER-II, the highly productive ESS test beamline V20—up until their final days of operation. A third, smaller research reactor at Norway's Institute for Energy Technology (IFE), JEEP-II, also officially closed down during 2019.

Each of these reactors operated as a national facility primarily serving researchers in France, Germany and Norway, but also hosted scores of international researchers through trans-national access programmes. BER-II and Orphée were highly productive research facilities that were each closed for reasons unique to its national research agenda, but ultimately because funding was rescinded. This means that Germany and France, home to half of the European user base, have entered 2020 with the 50-year-old ILL in Grenoble and the FRM-II research reactor in Garching as the only remaining advanced neutron sources in their respective countries.

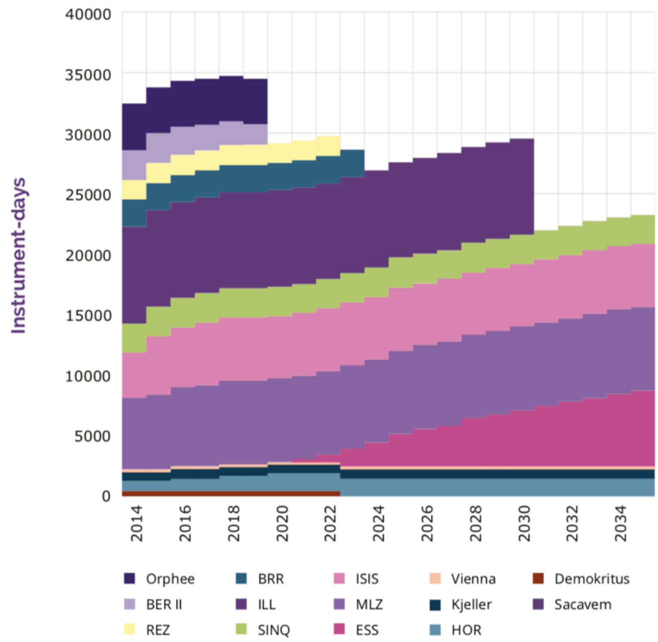

Fig. 1: The ESFRI (2016) best-case, "enhanced baseline" scenario for European neutron capacity shows a 33% drop in instrument days by 2031, with only four neutron sources in operation.

Meanwhile, the user program for ESS is scheduled to begin with three instruments in 2024. Ramping up gradually from this point, it is estimated that the facility's full capacity (with at least 22 instruments) will not be attained for nearly a decade thereafter. This means that even with the addition of ESS to the European landscape capacity will be strained to its limits.

Europe's world-leading position in neutron science has been achieved and is sustained thanks to its rich and storied legacy in the development of neutron research techniques, along with the related expertise of facility staff and supplier companies. The relationship to European industry is a long-

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standing one that is both self-perpetuating and reciprocal, but which must continuously be nurtured and advanced.

The industrial use of neutrons is primarily achieved through collaborations with academia through the peer-review process, and currently accounts for 15% of European beam time.[7] This approach serves to strengthen the knowledge transfer from basic science to applied research, and accelerates the development of novel products and services. Moreover, development of the cutting-edge technology associated with European neutron sources provides their suppliers with a sound reference, allowing them to successfully compete in other high-tech fields.[8]

The leadership of LENS is confident that with the proper level of support the European neutron community will meet the challenges ahead.[9] One way that LENS will do this is by targeting a more efficient use of existing resources through enhanced cross-facility coordination. So while LENS is not a direct beneficiary of BrightnESS², its key member facilities are, and the advancement of LENS's high-level objectives and its development into a strong organisation is therefore at the heart of BrightnESS² WP 2.

ENSA, on the other hand, has recently celebrated its first 25 years at the centre of the European user community. It is a single legal entity that is well-positioned to represent the needs of its 7,000 members across 22 countries. BrightnESS² nonetheless represents the first time that ENSA is fully resourced in this role. As part of the project, ENSA will bring the user perspective to the neutron roadmap by assessing its members' needs relative to new neutron-based methods of research.

CHRONOLOGY

Autumn 2017
INFRADEV-03 call opens with the focus on long-term stability of RIs. ESS sets up BrightnESS² consortium to ensure the LTS of neutron facilities in Europe.

March 2018
BrightnESS² proposal is submitted with 15 partners, including the future key LENS member facilities and ENSA.

June 2018
BrightnESS (2015-2018) Closing Conference is held in Brussels and includes first public presentation of LENS by ILL Director Helmut Schober.

August 2018
BrightnESS² is awarded with ESS as project owner.

September 2018
LENS Charter is signed during ICRI meeting in Vienna. The EC's Jean-David Malo gives the keynote address.

January 2019
The BrightnESS² kick-off meeting is held in Rome, back-to-back with ENSA's annual meeting, including more than 60 project participants from 11 nations.

March 2019
LENS holds first General Assembly in connection with ESFRI meeting in Liblice, where statutes are signed.

Fig. 2: Chronology of the early development of LENS.

[7] European Spallation Source ERIC. Neutron Users in Europe: Facility-Based Insights and Scientific Trends, p. 10, **2018.**
[8] Technopolis/STFC. ISIS Lifetime Impact Study, Vol. 1, **2016**.
[9] Schober, H. 2020, "Let the beams shine bright", *Research* Europe*, 9 January 2020, p. 13.

7.2. Convergence: LENS, ENSA and BrightnESS²

From well before the project began, ESS and BrightnESS² have been working to coordinate the activities of LENS and ENSA, the two organisations that, respectively, represent the alpha and omega of European neutron science, the facilities and their users. The BrightnESS² proposal has served as the lever to facilitate greater cooperation and awareness between them, already in its first year establishing a systematic working relationship between the two [Fig. 2].

In response to the INFRADEV-03 call, ESS gathered together a BrightnESS² consortium with an eye toward shaping a new European neutron strategy. In March 2018, the BrightnESS² proposal was submitted with a consortium of 15 institutions and organisations, including those that would eventually stand as the key LENS facilities, as well as ENSA.

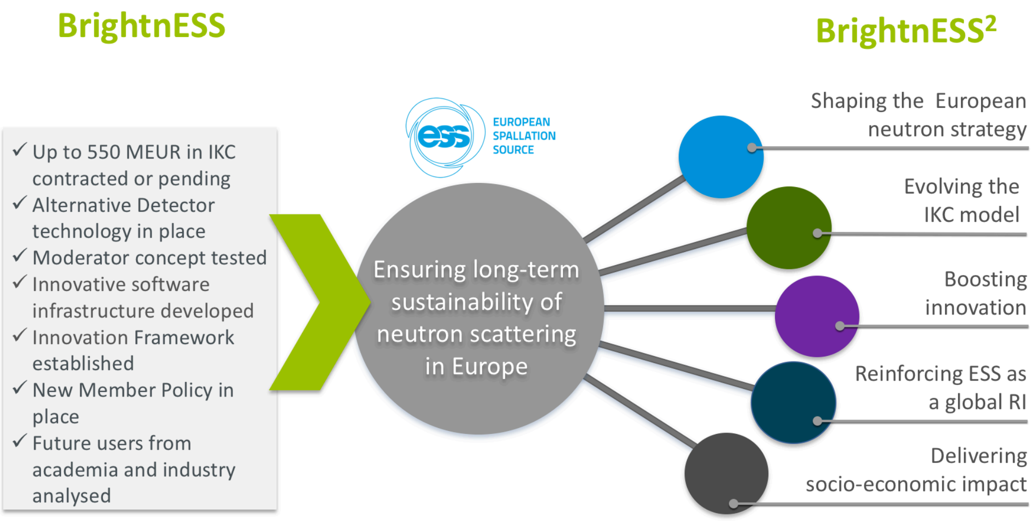

Fig. 3: Results of BrightnESS provide basis for the objectives of BrightnESS².

Meanwhile, the Horizon 2020 BrightnESS (2015-2018) project held its closing conference in the summer of 2018, where ILL Director Helmut Schober publicly presented the LENS concept for the first time. This served to underscore the planned continuity between the two projects, BrightnESS and BrightnESS² [Fig. 3], while reinforcing the broad-based backing BrightnESS²'s goals could expect from the neutron facilities themselves. The success of BrightnESS (2015-2018) in mitigating risk in the completion of the ESS project by advancing both the technical sustainability of ESS, and that of the ESS in-kind model, has established a strong basis for the objectives of BrightnESS².

Shortly after BrightnESS² was awarded, the LENS Charter was signed at the September 2018 meeting of the International Conference of Research Infrastructures (ICRI) in Vienna. DG Research and Innovation's director, Jean-David Malo, served as the event's keynote speaker, signalling the support of the European Commission for this alignment of objectives.

To further underscore the new cohesion at the centre of Europe's neutron science community, BrightnESS² kicked off project activities in Rome in January 2019 alongside ENSA's annual meeting. Ensuring the active participation of the user community in the creation of a neutron strategy for

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Europe is a BrightnESS² priority, and ENSA has actively participated in all BrightnESS² events to-date. To further facilitate ENSA's participation in the project, BrightnESS² brought on its 16th beneficiary in 2019, the Technical University of Delft (TU Delft).

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8. LENS: Toward a new vision for neutron research infrastructures in Europe

Photo 4: The signing of the LENS Statutes in Liblice, 26 March 2019.

8.1. LIBLICE: First Executive Board Meeting and General Assembly March 2019

LENS began its activities with its first Executive Board Meeting and General Assembly in Liblice on 26 March 2019, where it welcomed its ninth member facility, Forschungszentrum Jülich (FZJ).[10] At the invitation of ESFRI, LENS joined its launch event to the 68th ESFRI Forum Meeting, which took place the following day. This enabled the participation in the public part of the meeting of senior science policy officials representing the European national ministries and the European Commission.

Sponsored by BrightnESS², the historic meeting included the signing of the LENS statutes detailing the purpose of LENS, guiding the work of the statutory bodies, and laying the framework for the working groups responsible for the execution of the organisation's operational activities. Director of ILL Helmut Schober was elected LENS Chair and Director of ISIS Robert McGreevy as Vice-Chair.

Fig. 4: The nine LENS member facilities.

The four working groups established at this meeting were:

1. Strategy, promotion and policy
2. Neutron usage and innovation
3. Synergies in technological development and operation
4. Computing and data

A fifth ad-hoc working group to explore possibilities for compact accelerator-based neutron sources (CANS) in Europe would be added later in the day.

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[10] https://europeanspallationsource.se/article/2019/03/26/lens-launches-activities-strengthen-european-neutron-science

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LENS then immediately moved into its first General Assembly and Executive Board meeting with presentations on the first actions to be taken by the four working groups. It was here that LENS took the lead on developing the BrightnESS² common roadmap, initiated its Horizon Europe position paper, took the decision to pursue an association with the European Battery Alliance, and advanced a number of other initiatives that would eventually become priority actions.

Photo 5: LENS launch, Liblice, March 2019.

The internal meeting was followed by a highly visible public event that celebrated the launch of LENS in the presence of some of Europe's major stakeholders for research infrastructures, including ESFRI, ENSA, the EC and LEAPS. The forum had the added value of ensuring that LENS, as a new and untested organisation, would be held accountable to deliver on its ambitious project.

Photo 6: LENS launch, Liblice, March 2019

In addition to the newly elected chair and vice-chair of LENS, keynote speakers included ENSA Chair Christiane Alba-Simionesco, ESFRI Chair Jan Hrušak, and Diamond Light Source CEO Andrew Harrison, representing LEAPS. The panel served to underscore the interconnectedness of these four organisations and the RI community generally. The event went on to address the two pillars of LENS, scientific excellence and the long-term sustainability of RIs, in the form of panel discussions featuring many of Europe's leading lights in neutron science and RI policy.

The significance of this first General Assembly for BrightnESS² is that it established from the get-go that the project's WP 2 objectives would be aligned with those of LENS. Primarily this would happen through LENS WG 1, which is co-led by ESS Director for Science Andreas Schreyer, who also serves as co-chair of BrightnESS² WP 2. With BrightnESS² serving as LENS' primary funding mechanism, through the project's support of LENS member facilities, other synergies have developed as well [Fig. 5].

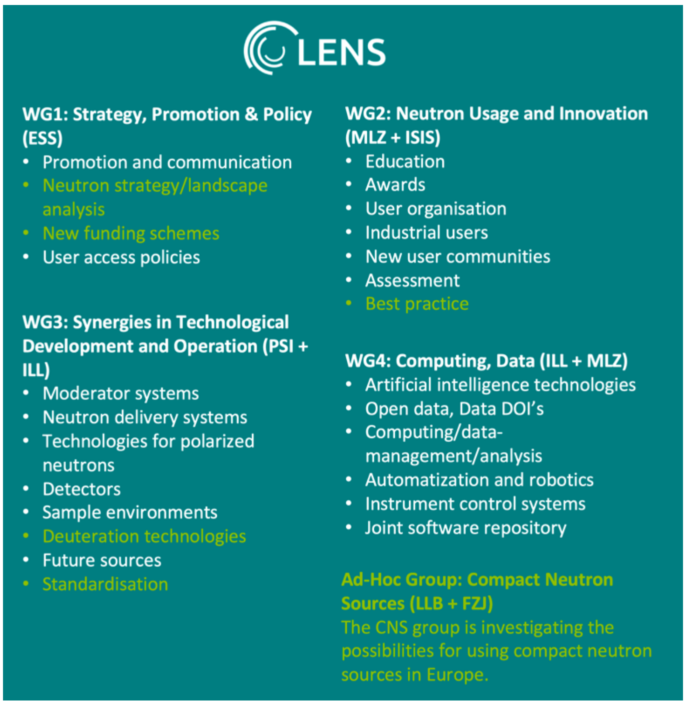

Fig. 5: BrightnESS² deliverables embedded in LENS working groups (highlighted).

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8.2. DÜSSELDORF: LENS WG 1 Meeting June 2019

Chaired by Schreyer and FZJ's Thomas Brückel, LENS working group 1 kicked off its activities in June 2019 by first defining the four subgroups for the WG, their leaders, and their individual goals and objectives. The "Promotion and communication" subgroup would kick things off by establishing LENS' online and social media presence, and by producing a flyer for distribution at that summer's major neutron science event, the European Conference on Neutron Scattering, ECNS 2019. These activities were all ultimately funded through BrightnESS².

The second subgroup, "Neutron strategy/landscape analysis", is led by Schreyer and PSI's Michel Kenzelmann. The subgroup's first action was to adopt BrightnESS² deliverables 2.2 and 2.10—the common roadmap—as its responsibility. A library of existing national and trans-national strategy documents was established on the BrightnESS² website[11], and a large meeting was planned for the sidelines of ECNS 2019 that would establish a first consensus for the document's table of contents. As the first input into this document, it was agreed that LENS would produce a position paper relative to the EU's proposed 9th Framework Programme, Horizon Europe, by the end of the year.

"New funding schemes" is the name given to subgroup 3, which is led by BrightnESS² Project Coordinator Ute Gunsenheimer of ESS, ILL's EU Office Head Miriam Förster and LLB's Alain Menelle. Working closely with subgroup 2, subgroup 3 would be responsible for delivering the LENS Horizon Europe position paper. Together with the fourth and final subgroup for LENS working group 1, "User access policies", subgroup 3 would explore funding options for a common entry point for access to Europe's neutron facilities. It was agreed that all four subgroups would submit working papers to the General Assembly in the fall.

8.3. ST. PETERSBURG: LENS at ECNS 2019 July 2019

Photo 7: LENS Vice-Chair Robert McGreevy giving a keynote address introducing LENS to the nearly 600 participants at ECNS 2019 in St. Petersburg, Russia.

[11] https://brightness.esss.se/partners/library

The LENS-ENSA-BrightnESS² convergence made a big splash in the summer of 2019 at ENSA's quadrennial gathering, the European Conference on Neutron Scattering, ECNS, held on this occasion in St. Petersburg, Russia.[12] By leveraging the major event of the 2019 neutron science calendar, BrightnESS² ensured that a strong delegation of LENS facility leaders were present and that LENS was visible to the nearly 600 neutron users from 33 nations who joined the week-long meeting.

ENSA, which celebrated its 25th anniversary at the event, did its part by giving LENS Vice-Chair and Director of ISIS Robert McGreevy a prime-time speaking slot to introduce the new organisation during the opening plenary. McGreevy used his talk to underscore the long history of collaboration among Europe's neutron community extending back through the EU's early Framework Programmes in the 1980s. These scientific and technical collaborations were a terrific success for European neutron science, noted McGreevy, contributing significantly to Europe's ability to maintain its world-leading position throughout the last four decades. LENS, he said, was a natural outgrowth of this history.

Photo 8: LENS stickers (top left) were included on posters from LENS member facilities during the massive ECNS 2019 poster session.

On the Wednesday of the conference week, 20 representatives from LENS member facilities and ENSA gathered for a BrightnESS² WP 2 meeting to produce the first draft of the table of contents for the common roadmap.[13] This working document was later distributed to the LENS General Assembly, and updated in a July 11 conference call among the LENS heads-of-facilities (HOFs).

[12] https://www.lens-initiative.org/2019/07/15/lens-participates-in-ecns-for-the-first-time/

[13] Christof Niedermayer (PSI), Henrik M Rønnow (ENSA, EPFL), Christiane Alba Simionesco (ENSA, LLB), Carina Lobley (ESS), Robert Mc Greevy (LENS, ISIS), Andrew Venter (Necsa), Peter Müller-Buschbaum (TUM, MLZ), Thomas Gutberlet (FZJ), Mark Johnson (ILL), Sharon Cosgrove (ESS), Andreas Schreyer (ESS), Eric Eliot (LLB), Tamás Belgya (BNC-Wigner), Earl Babcock (FZJ), Gregory Chaboussant (LLB), Arno Hiess (ESS), Evgenii Velichko (ENSA, TU Delft), Lambert Van Eijck (ENSA, TU Delft), Margaret Armstrong (BrightnESS², ESS), Lenka Petková (ESS)

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Meanwhile, LENS and BrightnESS² attendees ensured that various LENS promotional materials were on display and distributed throughout the week-long conference, and for the first time made extensive use of the LENS website and Twitter platforms.[14]

8.4. BRUSSELS: LENS at European Research & Innovation Days September 2019

In late September 2019, LENS Chair Helmut Schober moderated the panel discussion "Let's speak about Europe's scientific excellence" at the EU's sprawling co-creation event for Horizon Europe, Research & Innovation Days.[15] The platform served to highlight the benefits of EU funding to the scientists and facilities that have pushed the boundaries on research and innovation, enabling some of humanity's most significant breakthroughs in science, technology and medicine.

Photo 9: Handover from LENS Chair Helmut Schober to DG-RTD's Adam Tyson of the LENS position paper on Horizon Europe at European Research & Innovation Days, September 2019.

Following the discussion, Schober handed over to the Commission's head of research and industrial infrastructures at DG Research and Innovation, Adam Tyson, the newly released LENS Horizon Europe position paper, which outlines LENS' early stance relative to the proposed €100 billion EU research and innovation framework programme.[16]

Requiring buy-in from all nine member facilities, this position paper was the first joint public statement issued by LENS. The drafting process, heavily supported and facilitated by BrightnESS², served as an early opportunity to test and reinforce the LENS collaboration. Its success has led to the subsequent

[14] https://www.lens-initiative.org/ and @LENSinitiative
[15] https://www.lens-initiative.org/2019/09/26/lens-horizon-europe-position-paper-handed-over-to-european-commission-at-brussels-event/
[16] https://www.lens-initiative.org/wp-content/uploads/2019/09/LENS-Horizon-Europe-position-paper.pdf

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release of two additional position papers referencing the BATTERY 2030+ project and the European Green Deal.[17,18]

8.5. GRENOBLE: LENS General Assembly and Executive Board Meeting October 2019

The October 2019 LENS General Assembly and Executive Board Meeting at ILL was a watershed event for the maturing organisation.[19] The two-day gathering began with individual meetings by the five working groups as well as the Executive Board, which served to reach consensus on the priority actions to be advanced the following day at the General Assembly open and closed sessions.

These actions, together with the positive and productive atmosphere of the meeting, brought LENS and its five working groups wholly into their role as operational collaborations across the nine member facilities. A major outcome of the meeting was the initiation of what promises to be a long but exciting process to define and scope priority actions to exploit technical and scientific synergies across facilities. This included an initiative to enhance the BrightnESS² deuteration pilot activities, among several others that solicited expressions-of-interest from member facilities.

Photo 10: The LENS Executive Board Meeting and General Assembly was held at ILL in October 2019.

Most significant for BrightnESS² was the advancement of ongoing work in LENS working group 1. This included coordinating approaches to national and trans-national funding schemes by identifying where LENS facilities should focus their collective efforts. Among other initiatives, the meeting launched working group 1's actions that would shortly consolidate LENS' support for BATTERY 2030+ in its efforts

[17] https://www.lens-initiative.org/wp-content/uploads/2020/01/LENS-BATTERY-2030-roadmap-position-paper.pdf
[18] https://www.lens-initiative.org/wp-content/uploads/2020/02/LENS-Green-Deal-position-paper.pdf
[19] https://www.lens-initiative.org/2019/10/24/european-neutron-facilities-come-together-for-lens-general-assembly/

to secure Horizon 2020 funding, as well as result in the delivery of a position paper on the project's draft roadmap in January 2020.

The Grenoble meeting also advanced the common roadmap through further discussion on the draft table of contents, and a decision was taken to hold a writing workshop in the spring that would include high-level representatives from all LENS member facilities, ENSA and additional BrightnESS² partners. The intent of the workshop would be to bring a new level of detail to the table of contents that would allow for the production of a first draft of the common roadmap. At the meeting, LENS WG 1 Co-Chair Andreas Schreyer introduced the ESS-based scientific writer and editor recruited in September 2019 through BrightnESS² who would help guide the common roadmap to completion.

Other collaborative firsts resulting from this meeting included a joint press release from LENS and ENSA highlighting the impact of the impending December 2019 closures of the Orphée (used by LLB) and BER-II research reactors in Paris and Berlin; and an agreement to recruit a LENS Information Manager, funded on a subscription basis by all member facilities, that would enable enhanced communication activities as well as sustain the global neutron science website, neutronsources.org.

8.6. BRUSSELS: The LENS Colloquium February 2020

Photo 11: LENS Colloquium panel discussion, from left, Maria Paula M. Marques, Kristina Edström, Allan Larsson, Adam Tyson, Wim Bouwman and Helmut Schober.

The BrightnESS²-sponsored *LENS Colloquium: How neutrons contribute to mission-based research* was held at Brussels' Bibliothèque Solvay on February 11, and marked the LENS consortium's first public forum. Directed at the EU-level policies exemplified by Horizon Europe and the European Green Deal, the standing-room-only colloquium featured keynote speakers addressing neutron science's contributions to mission- and challenge-oriented policies. These followed an opening presentation by DG-RTD's Adam Tyson that set the terms of engagement from the policy side.

The Commission's proposed 9th Framework Programme, Horizon Europe, hopes to dedicate nearly €100 billion toward the achievement of five soon-to-be-defined missions in the areas of cancer, adaptation to climate change, oceans, seas and inland waterways, climate-neutral and smart cities, and soil health and food. This is a significant shift in funding allocations from previous framework programmes, and the underlying motivation for the colloquium was to explore how Europe's research infrastructures can best position themselves to contribute to these missions.

Photo 12: The leadership of LENS and LEAPS met February 11 to discuss a strategic collaboration.

The scientific speakers—who reviewed recent neutron research in areas such as cancer therapy, battery innovation, food production, quantum computing and health care—served to highlight the ways in which this was already being done and those areas where adaptation would be necessary.

Photo 13: A full house at Brussels' Bibliothèque Solvay for the February 2020 LENS Colloquium.

The event took on extra significance with the inclusion of LENS' sister consortium LEAPS, the League of European Accelerator-based Photon Sources. A meeting was held between the leadership of both organisations immediately prior to the colloquium, where a long-term strategic partnership was proposed in order to coordinate the two organisations' approach to national funding agencies and the EU. LEAPS Chair Caterina Biscari was invited to address the colloquium attendees as part of the formal programme. Together, the two umbrella organisations represent 25 European research infrastructures serving 35,000 scientists, and the prospect of collective action is a welcome one to all concerned, as Tyson highlighted in his opening address.

Photo 14: Kristina Edström of Uppsala University, coordinator of BATTERY 2030+.

The colloquium included a panel discussion that featured the addition of Sweden's former finance minister, Allan Larsson. Larsson played an instrumental role in locating ESS in southern Sweden and currently serves on the EU's mission board for Climate-Neutral and Smart Cities. The event concluded

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with LENS Chair Helmut Schober and Vice-Chair Robert McGreevy formally handing over the LENS Green Deal Position Paper to Tyson.

Like the two position papers before it, the LENS Green Deal paper will additionally serve as a critical, consensus-based input for the common roadmap and implementation strategy taking shape under BrightnESS² WP 2.

9. ENSA and the European neutron user community

9.1. ENSA and BrightnESS²

The scientists visiting large-scale neutron research infrastructures are organized in user communities on a national level, which in turn are gathered in the European Neutron Scattering Association (ENSA) through their respective national delegate. ENSA recently celebrated its 25th anniversary and represents some 7,000 neutron scientists who investigate topics ranging from the fundamental interactions of matter and the universe, to materials science, biology, engineering and industrial processes.

Fig. 6: ENSA logo

Every four years ENSA organizes an international conference, the European Conference on Neutron Scattering (ECNS), and awards three prizes to scientists in the field of neutron scattering. It represents the user community and its scientific wishes to the facilities, to society and to sister organisations in Africa, USA and Asia.

The core competences of ENSA and its community are:

- Addressing the societal grand challenges through basic or applied research, in the fields of physics, chemistry, biology, metallurgy, archaeology, geology, etc.
- Interfacing with other scientists directly linked to European universities and industries.
- Academic education of next-generation scientists at the BSc, MSc and PhD levels.
- Since January 2019, partnering in the European-wide programmes of Brightness² and LENS.

ENSA's role in BrightnESS² is tied primarily to Task 2.2 of WP 2: *defining and reporting the needs of the user communities in terms of new neutron-based methods in alignment with the ESS facility capabilities*. ENSA proposes to accomplish this through, first, a process of data mining tens of thousands of neutron user publications, and second, by using these results to conduct a bespoke, targeted survey of its 7,000 members.

9.2. ROME: ENSA annual meeting and BrightnESS² General Assembly/Kick-off January 2019

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The ENSA meeting of January 2019 was held in Rome, back-to-back with the Brightess² GA, inaugurating the participation of ENSA in the Brightness² project. This would be the first time ENSA formally participates in an EU project, so the organisation of ENSA in this framework was addressed at the kick-off meeting. The scope of ENSA's participation within Brightness² was also clarified with all ENSA delegates, and the most effective modes of collaboration between ENSA and Brightness² were explored.

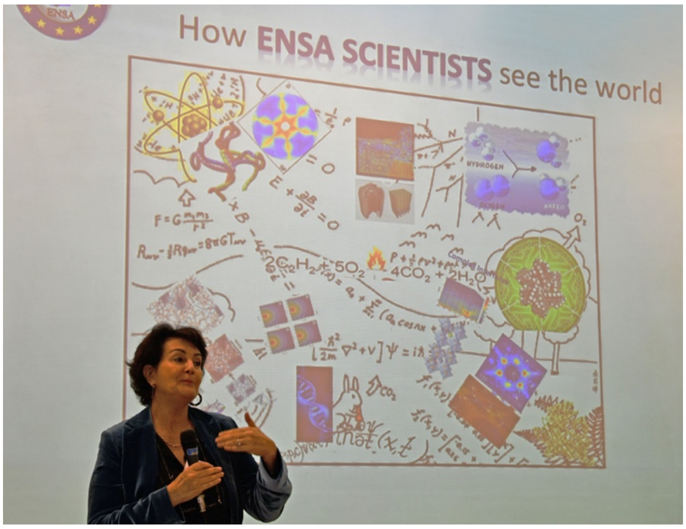

Photo 15: ENSA Chair (2019) Christiane Alba-Simionesco at the BrightnESS² kick-off in Rome.

ENSA is a not-for-profit organisation with no employees, based in Switzerland. ENSA holds no office in any single country, and therefore the choice was made to arrange its participation in Brightness² through TU Delft in the Netherlands, through the affiliation of ENSA Vice-Chair Lambert van Eijck. As such, administration, recruitment, office and employment were ensured, as well as the project management according to Horizon 2020 requirements. For this purpose, the Brightness² consortium was eventually extended with TU Delft as a beneficiary.

In August 2019, Evgenii Velichko was recruited by TU Delft as a postdoctoral scientist to execute BrightnESS² WP 2.2 on behalf of, and in collaboration with, ENSA and its scientific community. He also serves as ENSA's executive officer. Velichko is a data scientist selected, in part, based on prior experience in applying Natural Language Processing for the purposes of data mining, pattern matching and modelling, which are critical skills necessary for ENSA's concept for modelling and surveying the user community for Task 2.2.

Photo 16: ENSA leadership and BrightnESS² delegates at ECNS 2019 in St. Petersburg, Russia.

Key points of contact for Brightness² in 2019 were ENSA Chair Christiane Alba-Simionesco and Lambert van Eijck; since December 2019, Henrik Rønnow (EPFL, Switzerland) is the new chair of ENSA.

9.3. ST. PETERSBURG: ECNS 2019
July 2019

The ENSA VIIth European Conference on Neutron Scattering was an important and highly visible opportunity for BrightnESS², ENSA and LENS to consolidate activities and objectives in support of the

European neutron community's long-term sustainability. Please refer to sections 8.3 and 10.2 for more details on the BrightnESS² activities at this meeting.[20]

9.4. BEIJING, HONG KONG, TAIWAN: ENSA in China November 2019

Chair of ENSA Christiane Alba-Simionesco was invited to present the European neutron user community at the Asia-Oceania Conference for Neutron Scattering AOCNS), held in Beijing November 12-21, and did so with the support of BrightnESS². At the conference, ENSA's sister organisations, the Asia-Oceania Neutron Scattering Association (AONSA) and the Neutron Scattering Society of America (NSSA) presented their communities, and the first outlines were sketched for a future world-wide neutron scattering association of scientists from the different communities, a sort of United Nations for neutron users.

Photo 17: ENSA Chair Christiane Alba-Simionesco at the Chinese Neutron Scattering Society meeting in Beijing, November 2019.

The meetings were combined with visits to the Chinese Institute of Atomic Energy, the CARR and CMMR research reactors, the Chinese Spallation Source in Dongguan, as well as a presentation by ENSA at a meeting of the Chinese Neutron Scattering Society. In each of Alba-Simionesco's presentations she brought news of BrightnESS² and LENS to the Asia-Oceania neutron community.

9.5. Assessing the needs of the neutron user community using NLP: A case study

As part of its work in WP 2, ENSA is applying Natural Language Processing (NLP) to the scientific output of its community. Through this AI inspection of manuscripts, books and other text media, the societal and scientific contributions of its community will be visualized, allowing mapping of underlying scientific networks, trends and topics.

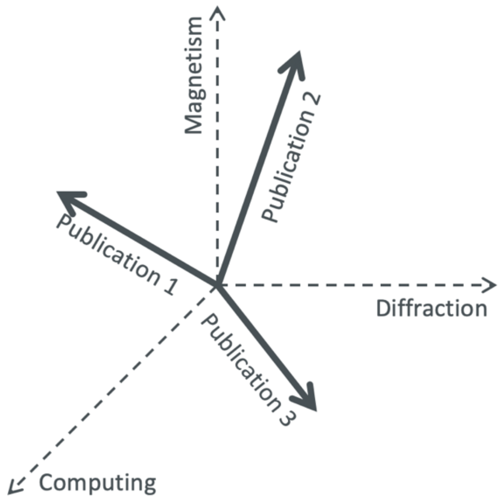

Fig. 7: Natural Language Processing: analysing scientific publications as vectors in n-dimensional token space.

The analysis itself will serve the scientific community to render their contributions to European society visible for policy makers, stakeholders and the public. For the ENSA delegates, the analysis will be used to address their

[20] https://brightness.esss.se/news-and-press/brightness²-activities-during-ecns

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respective communities in a personalized survey, with the analysis serving as the basis on which the community will evaluate its performance and future needs.

While this analysis is ongoing, some preliminary concepts are given here to show its potential.

As a case study, the publications of the 21 ENSA national delegates have been taken for analysis, as registered in *Scopus*, Elsevier publishing's abstract and citation database containing nearly 70 million records. Based on the metadata of *Scopus* publications, a network of scientific collaborations was retrieved, consisting of about 6,000 scientists around the world connected to the 21 delegates. Figure 8 shows the network graph automatically rendered based on the amount of connections between co-authors.

Fig. 8: Graph of (co-)authors of ENSA-delegates. The results shown here are preliminary and for demonstration purposes only.

Each node on the graph corresponds to either an ENSA delegate, or one of their co-authors. Each edge is a publication in common, while the edge's thickness corresponds to the number of common publications. The colour of the node corresponds to the (co-)author's affiliation country, and the size of the node corresponds to the total number of publications published by the (co-)author.

As can be seen from the graph, there is a clear formation of several "clusters" of co-authors, which can be an indication of a specific research topic investigated by such a "cluster". As a first observation, the relatively homogeneous distribution of the colours across the graph and in individual "clusters" indicates strong international collaborations between the scientists across the neutron scattering field and within the specific topics.

In order to gain understanding of the origin of these "clusters", an unsupervised machine-learning algorithm was applied to classify the publications based on their metadata (title, keywords and abstracts). The classification algorithm involved calculation of the similarity matrix for the articles published by each individual delegate. Such results typically show some 5-10 individual classes of publications for each of the national delegates.

These preliminary AI outcomes of the text analysis of the person-specific scientific publication were disseminated to the specific national delegates, who provided feedback for further development of the supervised machine-learning algorithm for the topic modelling. Meanwhile, the work has continued to extend the analysis from metadata to the entire text of each publication, which will allow for more comprehensive understanding of the relations between different research topics as well as between various research techniques complementary to neutrons.

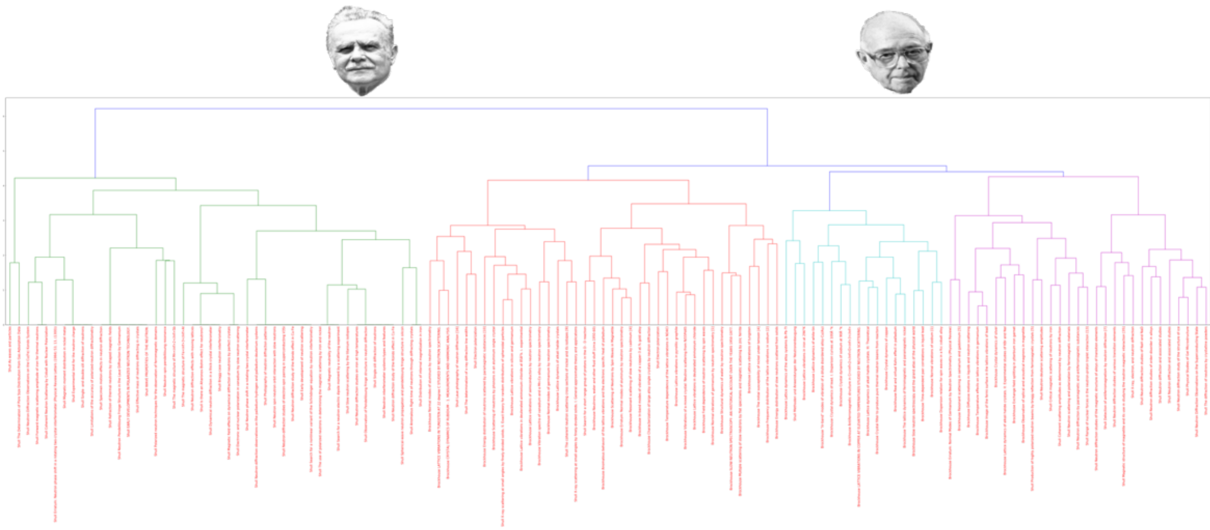

Fig. 9: An example of a NLP-based publications dendrogram using neutron science pioneers Clifford Shull and Bertram Brockhouse based on a machine-based analysis of publication title and abstract (for demonstration purposes only).

The ultimate goal of the analysis is to be able to see the evolution of research topics studied with neutrons over time, as well as to make suggestions for new research topics that could benefit from neutrons. Proceeding with cautious optimism, the model could potentially make predictions on the future development of research involving neutrons.

9.6. ENSA and LENS: To be continued

To capitalise on the synergies between Brightness² and LENS, ENSA has attended both 2019 LENS General Assembly meetings in Liblice and Grenoble as an observer member. The ENSA chair and vice-chair will also both attend the March 2020 writing workshop for the BrightnESS² WP 2 “common roadmap and implementation strategy” document, deliverable 2.10, which is being developed under LENS working group 1. ENSA also intends to participate as an observer in the May 2020 LENS General Assembly in the UK and to remain an active observer of LENS activities.

South Africa has a long history of research using neutrons. Engagement between ESS and South Africa has progressed steadily since 2015, when ESS began working through the European Commission’s Group of Senior Officials (GSO) on Global Research Infrastructures to guide its expansion beyond

Europe. As a part of BrightnESS (2015-2018), a high-level scientific delegation from South Africa visited ESS in July 2018 to explore areas of mutual interest, including material science, technology development and Big Data. The visit laid down a strong foundation for collaboration between ESS and South Africa.[21] Two of the institutes participating in the visit, iThemba Laboratory for Accelerator-Based Sciences (iThemba LABS) and the South African Nuclear Energy Corporation (Necsa), are now involved in BrightnESS² and contribute to the implementation of the project with their expertise. In 2019, BrightnESS² played an instrumental role in facilitating contact between European and South African scientists by organising an interactive workshop and supporting participation in scientific conferences.

[21] https://europeanspallationsource.se/article/2018/07/06/shared-vision-south-african-scientists-explore-common-ground-ess

10. Collaboration with the South African user community

South Africa's neutron user community is participating in BrightnESS² WP 2 through the activities of neutron scientists based at the South African national facility, iThemba LABS, and the state-owned company Necsa. As part of Task 2.2, BrightnESS² is coordinating two South African workshops on capacity building, that will feed into the reporting on the needs of the global neutron community relative to the scientific capacity of ESS.

Moreover, South African research scientist Andrew Venter of Necsa is working directly on Task 2.3 [A], the pilot programme for a cross-facility *Neutron Quality Label* for residual stress in engineering materials. Venter has used beam time at Necsa's MPISI instrument and FRM-II's STRESS-SPEC to perform measurements for the pilot.

The major deliverable for South Africa is D2.4, their report on user needs, that will also include a position paper on neutron scattering in the country. A strategy of deploying designated "Thrust Coordinators" dedicated to certain fields of neutron research has been developed in order to mobilise the local research communities.

10.1. CAPE TOWN: First South African Workshop on Capacity Building August 2019

Photo 18: Participants of the First South African Workshop at iThemba LABS in Cape Town, August 2019.

The *First South African Workshop on Capacity Building: Neutron Research* was held at iThemba LABS on 13-14 August 2019. The workshop brought South African research scientists, engineers and technologists together with their counterparts from ESS. The meeting was hosted by a South African consortium led by the country's Department of Science and Innovation (DSI) and the National Research Foundation (NRF), and included 14 participating universities, institutions and industrial partners.

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The main focus for the workshop was an exchange of ideas on collaboration opportunities presented by the two national facilities, iThemba LABS in Cape Town and Necsa in Pretoria, in connection with the construction of ESS. Additionally, the workshop served to supplement the neutron-based research and innovations at iThemba LABS and Necsa, and explored the need for South Africans to consider an expansion in these fields. Given the focus areas at the South African facilities, there is always a need for their researchers to have access to global neutron sources that can provide complementary research opportunities.

The second BrightnESS² capacity-building workshop will be hosted and organised by Necsa on behalf of the consortium in June 2020 and will be organised around sessions on nine different fields of neutron science, including magnetism, crystallography, the life sciences, catalysis, nanomaterials, engineering, paleo-sciences, geoscience, biology and chemistry.

10.2. ST. PETERSBURG: South African Participation in ECNS July 2019

BrightnESS² supported the participation of Andrew Venter, a research scientist and section leader from Necsa, in the ENSA European Conference on Neutron Scattering (ECNS), which took place in St. Petersburg, Russia, between 30 June and 5 July 2019. The 2019 meeting marked the first truly global participation at ECNS. Neutron scientists from four different regions—Europe, Asia-Oceania, Africa, and America—met in St. Petersburg to present their research results and engage in informative discussions on the current trends and future possibilities in neutron science. During his plenary talk on July 1, Andrew Venter presented a vision of neutron scattering in Africa and the related activities that are planned within the framework of BrightnESS².

Photo 19: Andrew Venter from Necsa presents the vision of neutron scattering in South Africa at ECNS 2019 in St. Petersburg, Russia.

10.3. LANGEBAAN: CATSA 2019 November 2019

ESS instrument scientist Monika Hartl gave a keynote presentation at the Catalysis Society of South Africa's annual conference (CATSA 2019), which took place in Langebaan, South Africa between 11-13 November 2019. As part of ESS enlargement efforts, Hartl outlined the advantages of using neutron scattering in catalysis research for science and industry. The high neutron flux of ESS will enable a new level of in situ observation of catalytic reactions, signalling a breakthrough in this exciting research that has implications for major challenges in the energy and health sectors.

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Currently, the UK's ISIS Neutron & Muon Source and the adjacent Diamond Light Source together serve as the most active European hub for catalysis research, used by academic and industrial researchers alike. Hartl is instrument scientist for the ESS vibrational spectrometer VESPA, which will enable *in situ* analysis of catalytic reactions at the molecular level, which is widely seen as the necessary next step in catalysis research.

Photo 20: Monika Hartl from ESS presenting her keynote presentation on Exploring Catalytic Reactions In-Situ *Using Neutron Scattering at CATSA2019.*

CATSA 2019 was hosted by the University of Cape Town and sponsored by a number of South Africa-based companies. The programme featured a strong cohort of students both on the speaking agenda and in the poster sessions, which highlighted the latest research in "green chemistry" and science-based strategies for the reuse and recycling of materials for catalysis, including 3D printing of catalysts. There was a strong industry presence at the conference, which also included international participation by scientists from Italy, Cyprus, the Netherlands and Sweden.

11. Pilot A: A common *Neutron Quality Label* for residual stress analysis

11.1. Summary

The BrightnESS² pilot project for a common *Neutron Quality Label* for residual stress analysis, the “engineering” pilot, is designed to advance the integration of support laboratories across neutron sources in Europe and beyond. This is a critical element in the ongoing effort to use neutron and non-neutron research infrastructures more efficiently, while also expanding their user base. Research results can be obtained more reliably, faster and cost efficiently by linking sample preparation, experiment validation and analysis tools, and recognizing that methodological specialisation is required to cater adequately for various user communities.

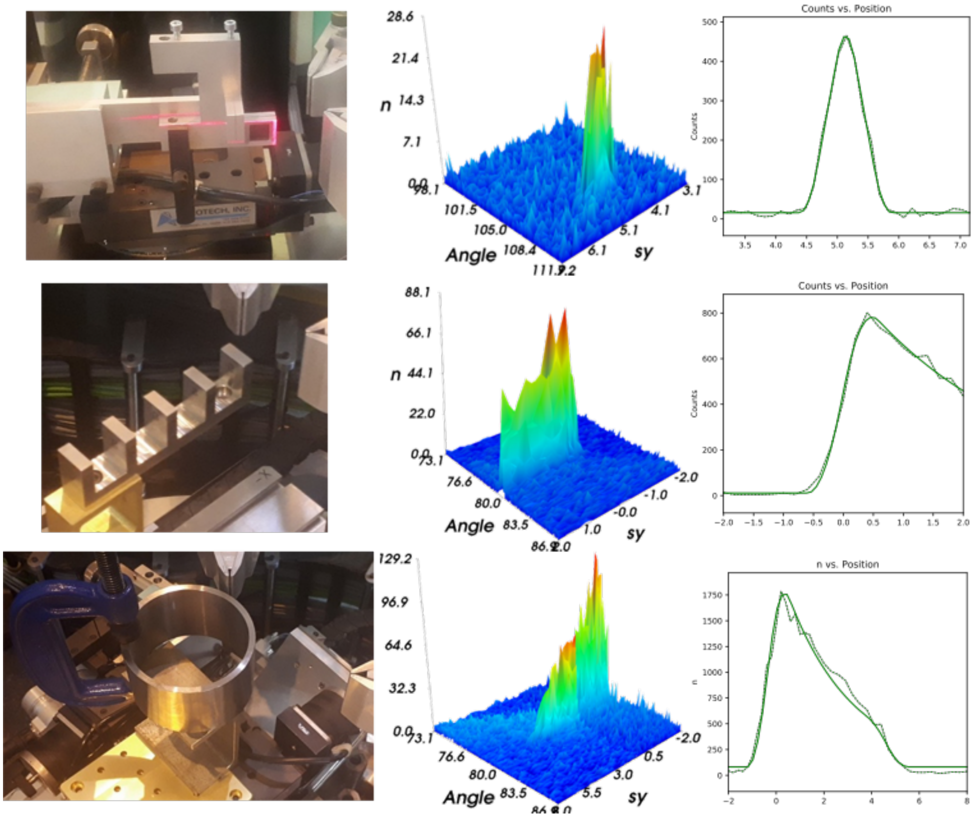

Fig. 10: Images of the three calibration samples, Foil & Pin (top), 5-wall (center), and Tube, and measurement data from MPISI.

The engineering pilot has been set up in the following manner. Calibration samples and measurement procedures have been prepared to perform measurement campaigns at the participating neutron strain scanning instruments: SALSA at ILL, ENGIN-X at ISIS, and STRESS-SPEC at FRM-II, with in-kind contributions from South Africa’s MPISI instrument at Necsa.

This first instrument calibration round aims to assess the accuracy of each instrument’s alignment, sample positioning and movements during real measurements. Measurements have now been performed at all four of the instruments, with the MPISI and STRESS-SPEC results still pending.

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From the first two measuring campaigns, we have observed that the instruments are in good agreement with one another and perform as expected. Lessons learned from the first two experiments were taken on board to produce more efficient calibration procedures for the following two campaigns. With all results together, alignment and positioning accuracy will be reported and its effects on final strain gradients characterization will be assessed. Ultimately, these results will enhance a depurated common calibration protocol and help to define a *Neutron Quality Label* as a standard for reporting the performance of a typical setup in a neutron strain scanner.

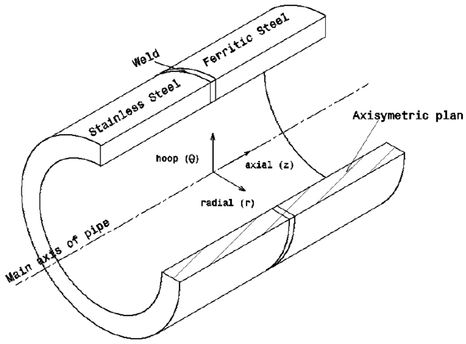

Fig. 11: Potential sample for industrial measurement (WP2 D2.6), AREVA's dissimilar metal welds mock-up.

11.2. Progress

- Meetings about the common calibration protocol and *Neutron Quality Label* have been organized in March and November 2019, joined by the instrument-responsible from each neutron strain scanner. The discussions focused on the background of the problem, possible source of position error in neutron strain scanners, and a strategy for the calibration measurement campaigns. The meetings also included discussions on the option for the measurement to be conducted with an industrial partner for deliverable 2.6, the final report on engineering.
- From the meeting, it is agreed that the main contribution of the work will be on the characterization of positioning errors on a typical setup of a neutron strain scanner, how to obtain them through a common calibration protocol, and how to report the findings in the *Neutron Quality Label*.
- Three sets of calibration samples were obtained, each set comprised of three samples, i.e., Foil & Pin, 5-wall, and Tube sample [Fig. 10] made of ferritic and austenitic steel. The geometry and the material of the sample are optimized for calibration measurements at the four different instruments. The samples have been distributed to each neutron strain scanner.
- Coordinate-measuring machine (CMM) measurements were made on the samples at ILL to establish the geometrical reference for the neutron measurements.
- Measurement on ENGIN-X at ISIS were carried out in July 2019. The data analysis has been performed and the main findings are indicated in Table 1.
- Measurement on SALSA have been carried out in September 2019 and January 2020. The data analysis have been performed and the main findings are indicated in Table 1.
- Measurement on MPISI were carried out in December 2019 and January 2020, while those at STRESS-SPEC were made in February 2020. The data analysis is currently in progress.
- The drafting of the report for the calibration measurement campaigns, calibration protocol and *Neutron Quality Label* is currently in progress.
- Contact has been made with an industrial partner, France's AREVA, to discuss a potential sample for the industrial measurement (WP2 D2.6). AREVA's dissimilar metal welds mock-up [Fig. 11] has been identified as a sample candidate.

11.3. Outlook

- All the experiments and the data analysis will be carried out with a target of completion in March 2020, with the submission date of the final report on the calibration protocol, deliverable 2.1, scheduled for June 2020.
- Meetings and discussions will be carried out in order to summarize and present the results of the calibration measurements and produce the common calibration protocol and the *Neutron Quality Label*. Next meeting of the working group is foreseen in April at FRM-II in Munich.
- Further communication will be made to the industrial partner to finalize the sample for industrial measurement. The date for industrial measurements at the participating neutron strain scanners is currently being discussed, with all four measurements to be completed by October 2020.

Table 1. Main findings of the calibration measurements at SALSA (ILL, FR) and ENGIN-X (ISIS, UK)

SALSA	ENGIN-X
Instruments positioning and alignment accuracy	
For GV = 0.6 mm × 0.6 mm × 2 mm Error of ω-rotation = 170 µm Offset between the centre of ω- and 2θ-rotation = 90 µm Accuracy of sample alignment system (camera) = 70 µm	**For GV = 2 mm × 2 mm × 2 mm** Error of ω-rotation = 20 µm Maximum shift between north and south bank = 0.194 µm Accuracy of sample alignment system (camera) = 84 µm
Edge finding software performance	
Entry scan codes (MathCAD) Accuracy for flat surface (w/o tilt) < 100 µm Accuracy for flat surface (max tilt=10º) = ? Accuracy for curved surface (R=50 mm) < 100 µm	EC Align Accuracy for flat surface (w/o tilt) < 100 µm Accuracy for flat surface (max tilt=10º) = ? Accuracy for curved surface (R=50 mm) < 500 µm

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12. Pilot B: Deuteration for soft matter and life sciences

12.1. Summary

The Deuteration Network (DEUNET), established as part of Horizon 2020's SINE2020 project, facilitates collaboration and knowledge-sharing between deuteration laboratories at Europe's ESS, STFC, ILL, FZJ, as well as ANSTO in Australia and J-PARC in Japan, resulting in the availability of a broad range of deuterated samples for the user community.[22]

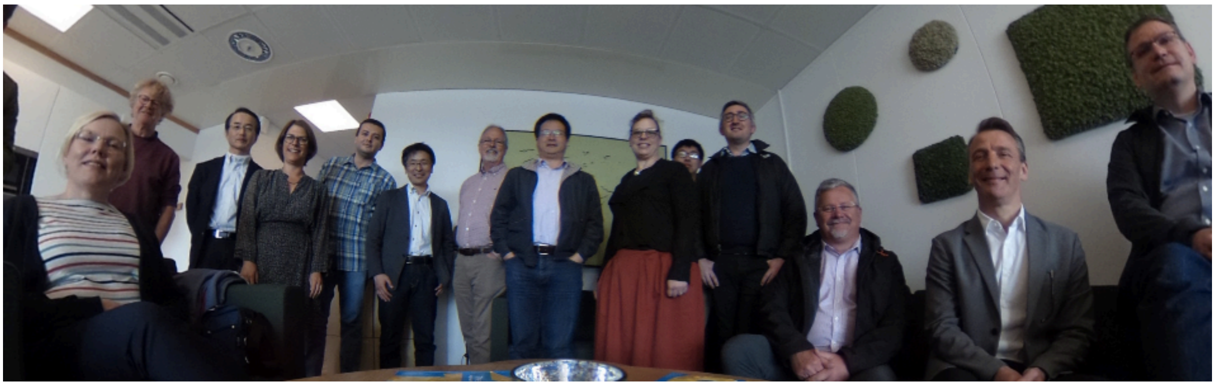

Photo 21: DEUNET.

One of the objectives of BrightnESS² WP 2 is to explore and implement new ways of working for the most efficient usage of neutrons. In the soft matter community, a key requirement for performing meaningful neutron experiments is the availability of relevant samples, which are often deuterium-labelled and produced at specialised biology or chemistry laboratories at neutron facilities. The suite of deuterium-labelled molecules of interest to the community is huge, and the range of skills required to fulfil this is equally far-reaching.

Acknowledging this, the various deuteration laboratories around Europe, in Australia and in Japan, have begun working together in order to reduce the need for duplication of specialised skills such as those in the areas of polymer chemistry (well established at FZJ) and biocatalysis (a new area of research at ESS). Reducing the need for duplication of skills across laboratories allows each group to focus on their area of expertise and push the boundaries of what is possible in these areas. Furthermore, collaborative projects between deuteration laboratories facilitate the production of materials for neutron experiments that a single laboratory could not produce alone and thus facilitate neutron experiments that are otherwise not possible.

Lipids and lipid-based materials are in high demand within the neutron scattering community. The ISIS deuteration laboratory has a wealth of experience synthesising a range of deuterated lipids but the user community is requesting more complex and challenging molecules. A key focus of the recently-

[22] https://deuteration.net

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established chemical deuteration laboratory at ESS is the use of enzymes as biological catalysts for synthesis as a way of improving efficiency and reducing the effort required to produce complex deuterated molecules.

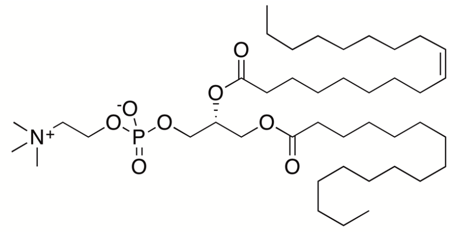

Fig. 12: POPC, a key biological lipid and the target of the deuteration pilot.

Enzymes are known to show high specificity, operate under mild conditions, to be amenable to recycling and for their lack of toxicity. Lipids have recently been identified as potential targets of this work and thus this pilot project is a collaborative effort between the chemical deuteration laboratories at ESS and STFC to improve the efficiency and accessibility of complex deuterated lipid synthesis with enzymatic synthesis.

The target lipid of this project was POPC (1-palmitoyl-2-oleoyl-*sn*-3-glycero-phosphocholine) [Fig. 12], a key component of cellular membranes and of interest for a broad range of research fields.

Ready access to a deuterium-labelled analogue of POPC would enable more realistic neutron experiments to be performed, where currently simpler but less relevant lipid analogues are used due to their availability. In addition to establishing a novel route to deuterated POPC, this pilot will demonstrate its use as a model skin lipid to investigate the possibility of improving transdermal drug delivery with surfactants via neutron reflectometry using the SURF instrument at ISIS.

12.2. Status

Photo 22: ESS scientists Hanna Wacklin-Knecht, Oliver Bogojevic and Anna Leung in the ESS deuteration and crystallography lab, DEMAX.

The deuteration pilot is well underway with the synthesis of required deuterated fatty acids required to produce the deuterated lipid completed in 2019. Significant progress was also made during 2019 on the enzymatic synthesis of POPC-d_{63} using the deuterated fatty acids. The delivery of one of the enzyme catalysts for this work was delayed by 12 months from January 2019 to January 2020 which has so far prevented the completion of the synthesis as planned. However, a modified synthesis of the target molecule was completed in January 2020 wherein the delayed enzyme catalyst was replaced by chemical reagents. With the delivery of the delayed enzyme catalyst, the work to establish the enzymatic synthesis will continue in 2020.

12.3. Activities

The synthesis of palmitic acid-d_{31} and oleic acid-d_{32} has been completed throughout 2019 [Fig. 13, scheme 1].

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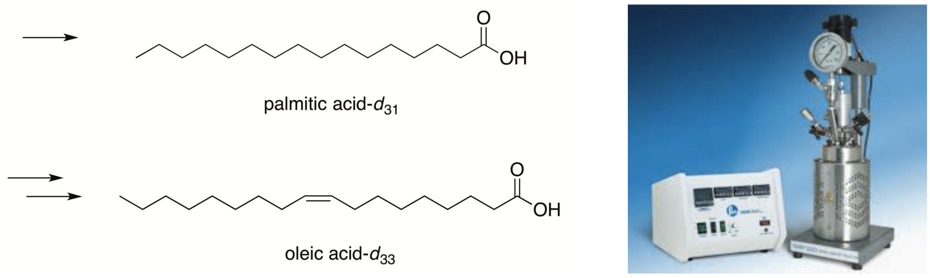

Fig. 13, Scheme 1: Synthesis of palmitic acid-d31 and oleic acid-d32 have been completed at ESS, using a Parr pressure vessel for some key steps.

Work on enzymatic synthesis using *Rhizomucor miehei* lipase (provided by Novozymes) allowed the modification of phospholipids at the 1-position to be established [Fig. 14, scheme 2].

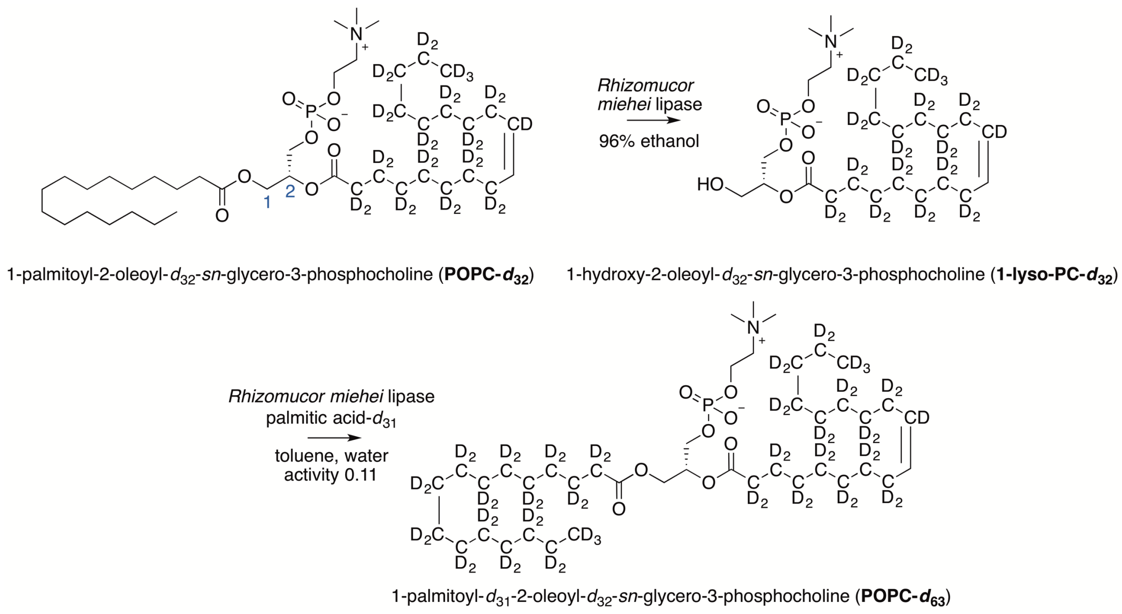

Fig. 14, Scheme 2: Modification of phospholipids using an enzyme catalyst, Rhizumucor miehei lipase.

Delayed delivery of the enzyme catalyst required to modify phospholipids at the 2-position meant that work could not be carried out to establish a method for this. Modification of the route to facilitate synthesis (and to mitigate the risk that the molecule would not be ready prior to the ISIS long shutdown scheduled to begin in September 2020) resulted in the hybrid scheme shown below [Fig. 15, scheme 3]. A disadvantage of the use of chemical reagents here is that the POPC-d_{63} is contaminated by a by-product which so far has proven inseparable.

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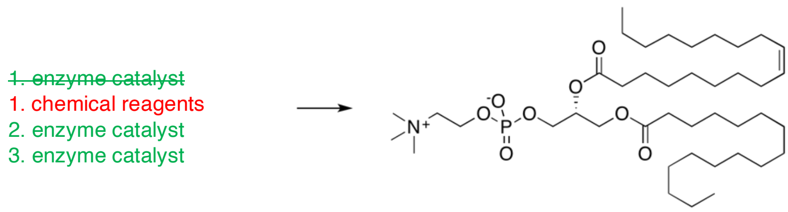

target lipid, POPC-d_{63}

Fig. 15, Scheme 3: Synthesis of POPC-d_{63} *using a combined chemical/enzymatic route.*

12.4. Results

The synthesis of deuterated fatty acids has been completed at ESS, and the target lipid, POPC-d_{63}, has been produced using a mixed chemical/enzymatic approach.

12.5. Outlook

A neutron reflectometry experiment is planned using the SURF instrument at ISIS using the POPC-d_{63} prepared at ESS. In this experiment POPC-d_{63} will serve as a model skin lipid, providing a biologically-relevant model to investigate interactions between skin lipids and surfactants/detergents used to improve transdermal drug delivery.

Concurrently, at ESS, work will commence with the delayed enzyme catalyst in order to improve the synthesis of deuterium-labelled phospholipids further. The partners will also consider how to ensure these methods are robust and can be easily implemented in laboratories within the DEUNET to improve the accessibility of in-demand, deuterium-labelled small molecules to the neutron scattering community.

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13. Conclusion: Deliverable 2.10, The common roadmap and implementation strategy for future neutron capability (December 2021)

This report has outlined the approach that BrightnESS² is taking to establish the strategy to deliver neutrons for Europe and beyond. This approach is anchored by the activities of LENS, which through its Working Group 1 is tasked with delivering the common roadmap.

The path to the common roadmap runs through what this report repeatedly refers to as “the European neutron science community”. The first 14 months of BrightnESS² has led this community to a more structured understanding of both what that is and how it can organise itself to work coherently:

- Cooperation among European and national research infrastructures has entered a new era of accelerated change. BrightnESS² WP 2 has ensured that neutron sources have so far kept up with the pace, and the project is helping them prepare for the future.
- BrightnESS² WP 2 has been instrumental in bringing LENS from a concept to an operational organisation through a structured alignment of goals and deliverables.
- BrightnESS² WP 2 has established a systematic working relationship between LENS and ENSA, ensuring that strategic actions will be coordinated between the two organisations.
- BrightnESS² WP 2 is opening up European neutron science to South Africa (and other non-European nations), enabling it to become an active member of the community.
- BrightnESS² WP 2 has initiated the process of defining new ways of working across facilities to increase efficiencies both technical and scientific.

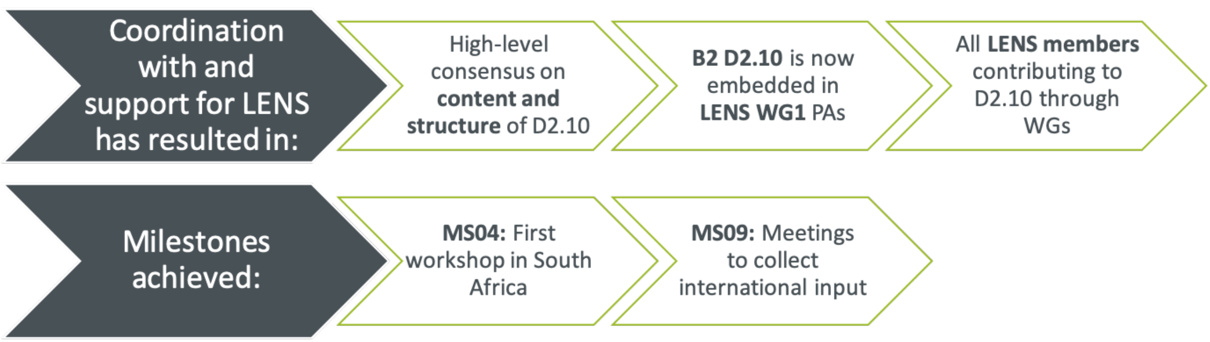

Fig. 16: Deliverable 2.10 progress.

The progress outlined in this intermediate report is the foundation for delivering the common roadmap. In discussions among LENS members an important distinction has been made between the roadmap and its implementation strategy. A “strategy”, it has been said, requires funding, while a roadmap, or vision, is something distinct from this more practical matter of implementation. What LENS intends to produce, therefore, is a “vision” document that also provides an update to the landscape analyses conducted by ESFRI (2016) and BrightnESS (2018). That vision will necessarily include the organisation’s and the community’s proposed approach to securing the funding needed to proceed to a realistic and fully resourced implementation strategy.

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The next steps toward this foundational document and BrightnESS² WP 2 ultimate deliverable are focused on producing the first written draft. The process will continue on the basis that the material contents of the roadmap must be produced through an inclusive, consensus-based approach involving the leadership of all LENS member facilities, BrightnESS² partners and ENSA. Each document that LENS produces, including its three current position papers and, for instance, a forthcoming white paper on European compact neutron sources, will feed up into the common roadmap.

The next step is a writing workshop organised for March 25-27. This will bring together high-level representatives from all stakeholder organisations for a three-day intensive meeting designed to bring a new level of detail to the ideas that are the basis of the document's current table of contents.

The outcomes of this workshop will be high on the agenda of the LENS working group 1 meeting scheduled for May 4, which will take place in advance of the May 5 General Assembly and Executive Board Meeting to be hosted by ISIS. Together, these meetings and discussions should provide the basis for a first draft of the document, which it is expected will be distributed by the end of the year.

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14. APPENDIX 1: European Neutron Vision/Landscape Outline

brightness²
LENS LEAGUE OF ADVANCED EUROPEAN NEUTRON SOURCES

1

Working Group 1.2
Neutron Vision/Landscape analysis

European Neutron Vision/Landscape Document

Description from BrightnESS²: "This document is intended to establish a common roadmap and implementation strategy for future neutron capability in terms of the instrumentation available at neutron facilities and their partners, while taking into consideration global perspectives."

It has, however, been decided in the process of developing the Vision/Landscape document that it is not a strategy document.

- This document is branded under and authored by BrightnESS²/LENS. It is being developed via LENS WG 1.2, and is produced within the BrightnESS² project as a deliverable of WP 2.
- The group is working toward an October 2021 deliverable, with a BrightnESS² WP 2 milestone in December 2019 ("Definition of common goals").
- Estimated length of document is less than 100 pages, including appendices.
- A library of existing related and complementary strategy/vision documents is hosted on the BrightnESS² website (see Annex 2).

The draft outline presented in this working paper was developed over three stages.

- The first draft outline was proposed at the 3 July 2019 meeting during ECNS (Annex 2).[1]
- The ECNS draft was discussed in a teleconference with the Heads of Facilities the following week, resulting in a revised draft (Annex 3). This teleconference was summarised as follows:

  The meeting mainly focused on how LENS could present a better coordination between members than before to convince the EU to provide funding for such LENS coordinated activities.

  The agreement was, that in response to the dramatic change in landscape with fewer remaining major neutron sources, EU research goals/missions should be supported by making better use of the remaining facilities by targeted investments in instruments or other scientific infrastructure. For example, whereas so far there has been no coordination between facilities on which instruments should be built where, there should now be a qualitatively new approach by LENS by coordinating the instrument building on a European scale based on the EU research missions. This coordinated effort should justify EU funding.

  Just to preclude any worries, such an improved cooperation of the major neutron sources should of course go in parallel with an effort on new compact sources. It is envisioned that a white paper on the positioning of compact neutron sources will be written by the LENS Ad-hoc group "Compact Neutron Sources", which will be important input to the Landscape/Vision document.

- The third stage of development has been to take the rough outline and give it an overall structure and increased definition, as well as to sketch out the broad, initial concepts for the LENS vision in line with the LENS position paper developed by WG 1.2 and 1.3. (see

[1] Christof Niedermayer, Henrik M Rønnow, Christiane Alba Simionesco, Carina Lobley, Robert Mc Greevy, Andrew Venter, Peter Müller-Buschbaum, Thomas Gutberlet, Mark Johnson, Sharon Cosgrove, Andreas Schreyer, Eric Eliot, Tamas Belgya, Earl Babcock, Gregory Chaboussant, Arno Hiess, Evgenii Velichko, Lambert Van Eijck, Margaret Armstrong, Lenka Petkova

11-10-2019
www.lens-initiative.org

https://www.lens-initiative.org/2019/09/26/lens-horizon-europe-position-paper-handed-over-to-european-commission-at-brussels-event/)

Next steps to develop this document are proposed as follows:

- Develop a detailed plan for "who does what". This will include exploiting all available synergies with the ongoing work in the five working groups.
- A two-day Writing Camp workshop is proposed as a way to assemble the principle contributors in order to arrive at a first draft of the document. This is tentatively proposed for February 2020.

FRONT MATTER :: 6 pages

- Title pages, foreword, table of contents, etc.
- The mandate for the ESFRI report was characterised as follows: "In the domain of neutron science and analytical facilities, the strategy-led approach must be urgently formulated as no individual ministerial authority or owner-consortium of the current infrastructures is in the position to address it."[2] The LENS/BrightnESS² report adds increased detail to this document and rebaselines it from the position of a coherent umbrella organisation.

EXECUTIVE SUMMARY :: 4-5 pages

- Vision statement for the next decade
- Key findings
- Key recommendations

§1 : NEUTRONS and NEUTRON SOURCES :: 13-14 pages

1. Why neutrons? (4 pages)
    - The case for new materials as the basis of global solutions
    - Advanced neutron sources are a unique analytical method, an essential complement in the discovery and application of new materials
    - Highlights of areas where neutrons excel
    - Key historical applications of neutron science
2. Neutron sources overview (4 pages)

[2] ESFRI Physical Sciences and Engineering Strategy Working Group, Neutron Landscape Group. *Neutron scattering facilities in Europe: Present status and future perspectives*, p. 1, **2016**.

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- Different types of sources offer key complementarity to other types of sources
- Reactors offer unique capabilities, but face challenges related to local anti-reactor sentiment and a guaranteed fuel supply
  - HEU reactors suited for x, y and z
  - LEU reactors suited for x, y and z
- Spallation sources offer unique capabilities
  - continuous sources suited for x, y and z
  - pulsed sources suited for x, y and z
- Compact Neutron Sources are a potential opportunity for narrowing the neutron gap
  - CNS's are suited for x, y and z

3. Overview of existing neutron strategy / roadmap / vision documents (5-6 pages)

- European strategies and visions
  - this document serves as an update of the 2016 ESFRI report, which concluded…
  - this document differs from and complements the ESFRI report how?
  - this document is supported by the conclusions of the 2018 BrightnESS survey
- brief roundup of national strategy publications, including ILL Associates document
- key commonalities across all
- key areas of divergence that serve the vision articulated here
- impact/impotence of previous reviews and strategies

§2 :: LANDSCAPE :: 20 pages

1. Current status in Europe and worldwide (5-10 pages, depending on tables and visuals)

- Intro: clear statement of the case for Europe as world leader in scientific output (and collateral technology development?)
- Visuals: overview of facilities, existing and planned (figures with timescale, tables with parameters and available instruments, e.g. from BrightnESS survey, etc.)
- Visuals: neutron research in Europe (publication output, structure of the user community, network of neutron sources)
- Challenges for the future
  - losses: shutdown of reactors, fewer high-flux sources, stretched capacity of national facilities serving beyond their borders, users migrating to PIK? (instrument class breakout)
  - gains: ramp up of ESS, continuous need for ILL and long-term transition between the two; FILL2030; ISIS II (instrument class breakout)

2. Scenarios for the future of neutron research in Europe (5-10 pages, depending on tables and visuals)

- update ESFRI Scenarios, add level of detail by adding scenarios on research capacity/capability
- instrument class breakdown organised according to EU research missions
- filling the gaps: CNS's, role of PIK, regional distribution, more instruments

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3. View beyond Europe: US, China, Japan, Australia, Africa, Canada, Russia: likely developments outside Europe and their potential impact (1-2 pages)

§3 :: VISION :: 8 pages

1. Vision 1: Europe will see the scientific and societal fruits of a new collaborative approach among neutron sources (and analytical facilities generally) that will ensure capacity and respond to the needs of users (LENS, ENSA, LEAPS)

2. Vision 2: To embrace and ensure delivery of ESS but maintain complementarity, collaboration, regional/national accessibility, and unique range of technical/scientific capacity

3. Vision 3: Europe represents the largest and most coherent neutron science network worldwide and has the science to prove it; this document articulates what comes next:

    - strengthening of coordination through LENS working groups
        - strategy, promotion and policy
        - neutron usage and innovation
        - synergies in technological development and operation
        - computing and data
    - coordination of instrument construction tied to EU policies and its Sustainable Development Goals, specifically the Horizon Europe missions

4. Recommendations on how national funding agencies can help

5. Recommendations on how the European Commission can help

    - complement the activities of the EU member countries on European and national sources
    - help to establish a cross-actors network that leads from basic research at analytical facilities to industry to market, and back again from industry to analytical facilities

SUMMARY / CONCLUSION :: 4-6 pages

BACK MATTER

- Documentation
- Appendices
- Imprint

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ANNEX 1: LENS member commitments

- Engaging in the common promotion of neutron science, with the objective of establishing neutron science as a brand recognized by all the stakeholders, and highlighting the scientific, societal or socio-economic impact of neutron science;
- Coordinating their exchanges with national and European organizations and stakeholders (including users and funders), with the objective of contributing to the shaping of future policies;
- Coordinating technical development strategies in order to profit best from collective expertise and avoid duplication of efforts, with a view to addressing the scientific and societal challenges of the future in the most efficient manner;
- Joining efforts in expanding existing and supporting new user communities both by topic and geographical origin, with the objective of strengthening Europe's neutron expertise;
- Concerting on access, based on the principles of the *European Charter for Access to Research Infrastructures* with an emphasis on standardization for improved user experience;
- Achieving greater coherence in the development of data policy, data-handling, -storage, -analysis, -access along FAIR principles, and promoting Open Science while protecting intellectual property rights, with the objective of facilitating the exchange and use of neutron research data over a broad range of scientific areas;
- Coordinating training activities and enhancing staff qualifications by facilitating staff mobility, with the objective of facilitating international career paths and developing skills in neutron science and neutron technologies;
- Facilitating industrial access and collaboration, with the objective of fostering innovation within the European Research Area.

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ANNEX 2: ECNS first draft

Notes from BrightnESS² WP2 and LENS WG1 meeting
3 July 2019, ECNS – St. Petersburg

List of Attendees
Christof Niedermayer, Henrik M Rønnow, Christiane Alba Simionesco, Carina Lobley, Robert Mc Greevy, Andrew Venter, Peter Müller-Buschbaum, Thomas Gutberlet, Mark Johnson, Sharon Cosgrove, Andreas Schreyer, Eric Eliot, Tamas Belgya, Earl Babcock, Gregory Chaboussant, Arno Hiess, Evgenii Velichko, Lambert Van Eijck, Margaret Armstrong, Lenka Petkova
Library on neutron "strategy" related papers

- Library exists: https://brightness.esss.se/partners/library *(User name: your e-mail address*
- *Password: wp2pass (password can be changed upon login)*
- Some papers are in languages other than English – abstracts in English would be helpful
- Many of them are not national strategy documents even though published in a specific country – important to point this out in the executive summary

Vision/Landscape Document
Draft Table of Content

1. Executive Summary
   a. Key Findings, Vision
   b. Key Recommendations
2. Why Neutrons, Vision
3. Neutron Sources *(Reactors (HEU Challenge?, etc), Spallation Sources, Compact Sources, which source suited for what, continuous versus pulsed)*
4. Overview of Existing Neutron Strategy/Roadmap/Vision Documents
   a. Global *(OECD) ?*
   b. European *(ESFRI, ENSA, BrightnESS)*
   c. National *(DE, FR, UK, IT, SE, DK, …)*
   d. Multipartner *(ILL?)*
   e. Other Continents *(USA, Africa …)*
   f. Summary *(Commonalities, Challenges, Current world leader (quote e.g. US report) Network of Neutron Sources in Europe Basis for World Leadership in Neutron Research…)*
5. Current Status in Europe and worldwide
   a. Overview of Existing and planned Facilities *(Figures with timescale, Tables with parameters, …)*
   b. Neutron Research in Europe *(Publication Output, Structure of the user community, Network of Neutron Sources…, …)*
   c. Challenges for the future *(change of landscape due to shutdown of reactors, less high flux sources, many of them national fulfilling an European task, ramp up of ESS, continuous need of ILL, transition ILL-ESS, ISIS II, two source strategy?? (See Oak Ridge), complement remaining reactor sources by new compact sources, role of PIK, regional distribution…)*
6. Scenarios for the future of Neutron Research in Europe *(update ESFRI Scenarios, include Compact sources, PIK?)*
7. View Beyond Europe *(US, China, Japan, Australia, Africa, …likely developments outside Europe, potential impact,…)*
8. Vision/Recommendations *(Why and how could EC help, complementing the activities of the EU member countries on European and national sources)*

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ANNEX 3: Second draft following HoF telco

Vision/Landscape Document
Draft Table of Content **with additions after the Heads of Facility phone meeting in red**

1. Executive Summary
   a. Key Findings, Vision
   b. Key Recommendations
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   c. Challenges for the future *(change of landscape due to shutdown of reactors, less high flux sources, many of them national fulfilling an European task, ramp up of ESS, continuous need of ILL, transition ILL-ESS, ISIS II, two source strategy?? (See Oak Ridge), highlight gaps and new opportunities in research capability and capacity (e.g.by instrument class) due to changing landscape, complement remaining reactor sources by new compact sources, role of PIK, regional distribution…)*
6. Scenarios for the future of Neutron Research in Europe *(update ESFRI Scenarios, add level of detail by adding scenarios on research capacity/capability (e.g. by instrument class) serving EU research missions, include Compact sources, PIK?)*
7. View Beyond Europe *(US, China, Japan, Australia, Africa, …likely developments outside Europe, potential impact,…)*
8. Vision/Recommendations *(Why and how could EC help, complementing the activities of the EU member countries on European and national sources)*

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15. APPENDIX 2: LENS Horizon Europe Position Paper (September 2019)

LENS LEAGUE OF ADVANCED EUROPEAN NEUTRON SOURCES

LENS in the context of Horizon Europe

Ensuring the success of research and innovation missions through the coordinated contribution of Europe's advanced neutron sources

The innovation that gives rise to new and improved materials—from tissue scaffolds that support surgical reconstructions to wire cables that support suspension bridges—underpins many of the Pillar II clusters of the Horizon Europe programme, including health, industry, energy and food.[1,2] This materials development is itself underpinned by the network of technical capabilities and human skills in the universities and research institutions that comprise the European Research Area. A particular strength of this network lies in the major national and European research infrastructures, which through their multi-actor, bottom-up approach enable a broad range of world-leading materials research by the expert communities that use them.

Neutron sources are one component of this innovation ecosystem, each year enabling top-level materials research by more than 5,000 scientists and engineers across many domains of the life, earth and engineering sciences.

The European network of neutron sources is comprised of a diverse user base that is intrinsically cross-disciplinary and cross-sector, and as such has benefited from decades of continuous European Commission funding within previous and current framework programmes. We have in turn leveraged this support into considerably larger pools of national funding available to the facilities.

Furthermore, the collaboration fostered by the Commission's programmes has time and again allowed for the optimisation of facility resources to target societal impact. These collaborations have contributed to the strong cross-facility relationships that have served as the basis for the 2018 establishment of the League of advanced European Neutron Sources, or LENS.

With this position paper LENS aims to make a proactive contribution to the Strategic Plan for the implementation of Horizon Europe. Success here will significantly enhance the natural alignment between the dynamic research carried out at neutron facilities and Horizon Europe's mission-oriented research and innovation actions.

Established under the guidance of the European Commission, LENS was formed to ensure the strategic coordination of the national and international facilities that comprise its membership.[3] Enhanced coordination will include areas such as technical development strategy, data policy, user access, the increasing use of neutrons by industry, and the promotion and stakeholder engagement required to close the circle on the public's awareness of the socio-economic impact of European neutron science.

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[1] See https://ec.europa.eu/info/sites/info/files/mazzucato_report_2018.pdf , p.15
[2] Mission-oriented Research & Innovation in the European Union, Mazzucato, 2018
[3] LENS Goals & Objectives, https://www.lens-initiative.org/goals-and-objectives , 2019

2019-09-20
www.lens-initiative.org

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LENS will act to reinforce the commitment of European neutron sources to serve society across all science domains. Only through boldly exploring new approaches can Europe maintain its place at the top of the world's science pyramid, and thereby find solutions to the Grand Challenges. Horizon Europe's vision of horizontally integrating research infrastructures with the innovation process is not only one that we share, but one that we have been practicing for several decades.

LENS maintains that European large-scale analytic facilities are a foundational pillar of Europe's highly developed academic and industrial innovation network. We therefore take this opportunity to underscore the fact that the scientific research performed at Europe's neutron facilities enables some of the most sophisticated and otherwise impossible characterisations of many materials and manufacturing processes at the core of technological innovation. As a means by which to probe materials across a staggering range of length-scales, neutron scattering is an irreplaceable tool in the advancement of science and engineering research. Moreover, LENS facilities serve as a critical actor in the education and training of the scientists, academics and technical staff that use, operate and build them. It has been recognised for many years that efforts targeted at fully unlocking the potential of the discipline pay very high dividends.

The landscape of neutron facilities in Europe has, coincidentally, reached a crossroads. We call attention to Annex 1 of this paper, which outlines the challenges and opportunities faced by European neutron sources over the next decade. In this transition period the community requires enhanced support to maintain its momentum and quickly capitalise on the unique opportunities.

In addition, we have included Annex 2 and Annex 3 to highlight the contributions neutron science is currently making to the health and energy clusters included in Pillar II of Horizon Europe's mission-oriented research and innovation plan. These serve as examples of the synergies identified between LENS facilities and Horizon Europe that will support the achievement of the European Union's key policy goals addressing global challenges.

LENS stands ready to work within Horizon Europe to increase efficiencies across our nationally and internationally funded neutron research infrastructures. LENS believes that Horizon Europe will play a key role in securing the materials research programmes of the European neutron scattering user base, the facilities they rely on and the technological knowledge base that underpins the whole enterprise. To this end, LENS aims to strategically align facility-based technological development and exploitation with the clusters and their missions as defined by Horizon Europe. The general target LENS considers of utmost importance is detailed below.

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Developing technological solutions to urgent societal problems is a complex multi-stage process:

- Horizon Europe intends to boost research and innovation impact through a mission-oriented research and innovation approach. It is important for European competitiveness that whenever neutron facilities are able to accelerate the research required by the clusters, their potential is fully exploited by including appropriate research and development activities in the respective calls.
- This demands that the researchers working on the respective scientific or technological developments in the clusters are aware of the capability of the tools and techniques offered by the facilities. They need to have appropriate access to the corresponding services and these services must be adapted to the needs of their development projects.

From its earliest days, research with neutrons has played a role in finding scientific and technical solutions to societal challenges. It is self-evident to the members of LENS that neutron facilities will increasingly fill this need going forward. It is therefore the first priority of the Consortium to capitalise on the opportunity presented by Horizon Europe to advance and improve on this contribution. **LENS will outline clearly and in a timely manner how it can best contribute to Horizon Europe in parallel with the Commission's own process of defining how its missions will be accomplished.** European neutron facilities will thus be enabled to make the measurable and direct impact required for the collective success of Horizon Europe's mission-based goals.

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ANNEX 1: THE EUROPEAN NEUTRON LANDSCAPE

Challenges and opportunities

The European neutron science user community is widely acknowledged as the largest and the most diverse in the world.[4,5] It includes more than 5,000 researchers with over 32,000 instrument days annually across a network of international and national neutron sources.[6] It has been the global leader in scientific output for four decades, led by Institut Laue Langevin (ILL) in Grenoble and the ISIS Neutron and Muon Source near Oxford. The world's newest and most powerful accelerator-based source is under construction in Lund, Sweden, where the European Spallation Source (ESS) is scheduled to begin operations in 2023.

The challenges and opportunities facing Europe's neutron community in the coming decade have been well-documented in recent years. The reports make clear that the opportunities inherent in Europe's world-leading status and the construction of ESS are self-evident and must be optimised. The League of advanced European Neutron Sources (LENS), a consortium of national and international large-scale European neutron facilities, was established in September 2018 to bring new coherence to this mission.

Scarcity of beam time and a drop off in funding are the most immediate challenges facing the neutron community. Two of Europe's major neutron sources will cease operations by the end of the year, but the user program for ESS will only be ramping up between 2024-2028. The growing number of scientists requiring neutrons to advance their research means that even with the addition of ESS to the European landscape, capacity will be strained to its limits. LENS will target a more efficient use of existing resources through enhanced cross-facility coordination in order to address both the impending neutron gap and to ensure sufficient capacity going forward.[7]

Neutrons are special and must be made increasingly available to science and industry

The neutron is a unique probe with characteristics that cannot be supplanted by other methods. Neutrons allow scientists to understand the world at the atomic and molecular level in a non-destructive manner. This makes neutron science one of the most useful analytical techniques deployed across numerous science and technology disciplines.

Due to the characteristics of neutrons—well suited to investigate magnetic properties, light elements, thin films or large samples—they are an essential tool used in support of the science addressing society's Grand Challenges and have a legacy of significant socio-economic impact.

Europe's world-leading position in neutron science has been achieved and is sustained thanks to its rich and storied legacy in the development of neutron research techniques, along with the related expertise of facility staff and supplier companies. The relationship to European industry is a long-standing one that is both self-perpetuating and reciprocal.

The use of neutrons by industry, which currently accounts for 15% of European beam time, serves to strengthen the knowledge transfer from basic science to applied research, and accelerates the development of novel products and services.[8] Moreover, development of the cutting-edge technology associated with European neutron sources provides their suppliers with a sound reference, allowing them to successfully compete in other high-tech fields[9].

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[4] ESFRI Physical Sciences and Engineering Strategy Working Group, Neutron Landscape Group. *Neutron scattering facilities in Europe: Present status and future perspectives*, **2016**.
[5] A Report by the APS Panel on Public Affairs. *Neutrons for the Nation: Discovery and Applications while Minimizing the Risk of Nuclear Proliferation*, p. 10, **2018**.
[6] European Spallation Source ERIC. Neutron Users in Europe: Facility-Based Insights and Scientific Trends, **2018.**
[7] LENS website, *Goals and Objectives*, **2019**.
[8] European Spallation Source ERIC. Neutron Users in Europe: Facility-Based Insights and Scientific Trends, p. 10, **2018.**
[9] https://stfc.ukri.org/files/impact-publications/isis-neutron-and-muon-source-lifetime-impact-report/

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ANNEX 2: HEALTH science case

Fundamental science solves fundamental problems

At the core of medical research related to drug development, healthy living and the ageing process is the need to understand the extremely complex mechanisms of biological systems at the molecular level. Some promising advances in this area of fundamental science are coming from advances in neutron scattering methods and instrumentation. Additionally, neutron scattering is responsible for recent innovations in targeted drug delivery, next-generation biomedical devices and strategies to combat the viruses and diseases that threaten large-scale public health.

The successful structural characterisation of proteins, for example, is at the forefront of diagnostic and pharmaceutical research, and has applications in the treatment of Alzheimer's, diabetes and other intractable public health epidemics. More concretely, recent neutron studies have directly contributed to improvements in breast cancer therapies, anti-fungal drugs, anaesthetics, transplant recovery and our understanding of the elusive hepatitis C virus.

Innovation and device development

Apart from the many ongoing studies on drug delivery and metabolic processes, neutron scattering research on quantum phenomena, polymers and 3D printing technologies promises to contribute to some of the most important breakthroughs in the evolution of everyday medical devices.

The staggering financial burden of health care can be traced clear through the supply chain. The use of neutrons in health science can reduce these costs through improved outcomes generally, but can also accelerate the time it takes medical R&D to reach the market. This can lead to substantial societal cost savings.

The use of medical implants and prosthetics, for example, has become increasingly routine, but there remain several limitations. Neutron reflectometry studies of polymer coatings for metal implants have led to functionalised coatings that promote bone regeneration, granting the devices a longer life span. Neutron imaging studies into advanced 3D printing techniques is another area of research that can deliver on the promise of stronger, more durable and less expensive implants used to treat degenerative diseases.

One albatross hanging from the neck of the world's public health system is the extraordinary cost of the 80 million MRI scans performed annually. Research into the complex interplay of superconductivity and magnetism is one of the most promising areas of neutron spectroscopy research, and one that has the potential to scale down the cost per scan and the complexity of MRI technology.

The increasingly sophisticated use of neutrons in biology and medical research, including in the development of pharmaceutical and device technology, is an important component in securing the well-being and productivity of the world's ageing population.

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ANNEX 3: ENERGY science case

Neutrons are highly suited to energy research
The unique character of neutrons makes them an important probe for energy materials, and neutron scattering is leading the way to ground-breaking technologies aimed at reducing the global reliance on fossil fuels. This is an objective that will only be achieved through the discovery and development of new materials.

Aside from the direct impact of research on alternative energy technologies that would be impossible without neutrons, neutron scattering is used across the complementary disciplines of materials science, engineering, quantum and classical information technology, nuclear science and chemistry. Research with neutrons in each of these disciplines will make critical contributions to the multi-faceted approach essential to solving such a broad-based societal challenge.

Ongoing and proposed research with neutrons promises progress in frontier energy areas, including scalable hydrogen power (fuel cells and storage methods); alternative energy vectors such as ammonia; more powerful and longer lasting batteries; next-generation solar cells (organic and self-assembling); and the development of superconducting and magnetic materials that could revolutionise energy transportation and distribution. Neutron scattering research impacts decarbonisation throughout the production chain, the supply chain and across all sectors through direct contributions on research into new materials for carbon capture and storage, how to reduce energy use through improved catalysis, and the continual development of lightweight materials for transport applications.

Together, this matrix of renewable, high-performing and sustainable energy innovations will underpin the coming transformation of the global energy sector.

Research and innovation, neutrons and industry
The industrial development of new materials and novel applications is a knowledge-based design process predicated on the understanding of the structure and dynamics of matter at the molecular and even atomic scale. While neutron scattering is widely used to provide this information complementary to other techniques, it is frequently the only method able to deliver this critical knowledge.

Because neutrons have no electrical charge and are non-destructive, they are in several cases the only probe available to scientific and industrial researchers to investigate delicate processes without interfering in those processes. This means they can characterise materials *in situ*—materials installed, for example, in their operational context and integrated with real components—and/or *in operando*—detailing a material's behaviour while it or its component parts are in operation. Such studies can answer questions like why a promising energy storage solution fails under some conditions and not others; or which molecular processes determine the efficiency of a particular battery technology, and how these can be manipulated for better performance.

Altogether, neutron research contributes in a unique and indispensable way to the knowledge and technology required to move the energy sector toward responsible resource management, as well as to transform it in ways society has not yet dared to imagine.

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16. APPENDIX 3: LENS BATTERY 2030+ Position Paper (January 2020)

LENS LEAGUE OF ADVANCED EUROPEAN NEUTRON SOURCES

LENS Position Paper on "BATTERY 2030+ Roadmap (Second Draft)"

As the BATTERY 2030+ Roadmap makes abundantly clear, the strategic use of large-scale European analytical facilities will play a critical role in realising the roadmap and especially the Battery Interface/Interphase Genome and Materials Acceleration Platform (BIG-MAP) research area. The neutron and photon facilities represented by the pan-European LENS and LEAPS initiatives are specifically singled out in this respect. With this paper, LENS wishes to clearly support the proposed strategy in a manner that is consistent with and builds upon a complementary paper to be submitted by the light source initiative, LEAPS.

LENS feels that the references made to neutron-based experimental techniques in the BATTERY 2030+ Roadmap could usefully be made even stronger by isolating three areas of contribution that neutron sources will make to this mission-based project. Once these areas are clearly identified as foundational, the specific actions, time scales and funding mechanisms necessary to enable facility contributions will begin to emerge as essential Roadmap milestones.

LENS facilities are important contributors to the BATTERY 2030+ Roadmap early on, where BATTERY 2030+'s success in implementing BIG-MAP will determine the pace for the European Battery Alliance, Batteries Europe and BATTERY 2030+ project as a whole. We feel the fundamental role of Europe's large-scale photon and neutron sources could helpfully be made more explicit in the Roadmap, as the efficient use of these facilities requires careful advance planning.

The 10-year plan for BATTERY 2030+ must rely heavily on infrastructures either already in operation or coming into operation during the next decade. Success relies on identifying from the start how the development and use of specific capabilities, instruments and access protocols needs to be coordinated to support the BATTERY 2030+ mission. This sort of coordination is precisely the role of the LENS initiative, and thus these activities are very much already in motion. But their specific interface with BATTERY 2030+ must be more clearly defined.

LENS therefore recommends that the Roadmap highlight the following three areas of mission-oriented contributions to be made by LENS facilities to the BATTERY 2030+ roadmap:

- Investment in the development of new or upgraded **instrumentation** that will enable the *in situ* and *in operando*, multi-length-scale X-ray and neutron experimental techniques and methodologies necessary for rapid development of better batteries;
- The accelerated development and standardisation of open-source neutron **data management protocols and data analysis software**, along with that of the **shared infrastructure** necessary to extract rapidly the unique information content from the data sets produced at Europe's large-scale facilities;
- The establishment of access channels on those European large-scale facilities that can provide neutron instrumentation best suited to BATTERY 2030+'s research needs during each stage of the project.

Development of advanced instrumentation

The viability of the BATTERY 2030+ project relies on early-stage efforts to establish workflows for both in-depth and high-throughput testing of materials and chemistries, research methodologies that, among other needs, will require the most advanced neutron instrumentation and technologies. These systems will necessarily need to be designed, constructed and operated at high-flux large-scale facilities. The

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current state-of-the-art is not sufficient for what is envisioned during the full operational mode of the BATTERY 2030+ Roadmap, as it will require orders of magnitude increases in the speed of measurement, measurement across length scales from the atomic scale to the micron scale, and an accompanying advancement of methodologies. This can only be achieved through additional investment in close coordination with the facilities and researchers represented by LENS. Given the long lead-times associated with developing instruments and instrument technologies, the actions related to advanced instrumentation must be defined at a very early stage of the roadmap.

Data management, analysis and infrastructure

The other side of the accelerated development of inversely engineered battery designs is BATTERY 2030+'s exploitation of large curated data sets and the e-infrastructures that can support them. Europe's large-scale neutron sources are uniquely positioned not only to generate such data sets but also to provide the competencies required to expand and exploit them. Among LENS (and LEAPS) facilities, several initiatives are already in progress that aim to standardise the management and accessibility of scientific data and data analysis software, as well as to establish shared infrastructures. These include PaNOSC, ExPaNDs and many other activities feeding into the realisation of FAIR data principles for photon and neutron scattering data within the framework of the European Open Science Cloud. Furthermore, on account of the large curated data sets managed by neutron and photon sources, LENS facilities are active in other initiatives targeting the advancement of machine learning and the application of AI to scientific investigations.

Access to beam time

Serving a community of more than 5,000 users, beam time at Europe's neutron sources is severely oversubscribed by a factor of more than two, and demand is increasing. In the case of neutron sources, capacity (as measured in instrument-days) dropped by 17% with the closures of three reactor sources in 2019. The European Spallation Source will come online with three neutron instruments in 2023, but will require nearly a decade more to reach full capacity. It is therefore of utmost importance to the BATTERY 2030+ Roadmap that it develops access channels for beam time at both existing and emerging facilities required during different stages of the project. This will require careful advance planning that will naturally go hand-in-hand with the development of the advanced instrumentation described above.

Europe is extremely well positioned in this respect. It provides a world-leading suite of highly complementary facilities, where the fastest measurements can be made. All of these facilities have strong existing links to the scientific community working on the various aspects of battery development. This has allowed scientists working at Europe's neutron sources to gather tremendous prior competence in the field. Upgrades at all major sources are underway and the world's most powerful neutron source, ESS, will begin user operations in 2023.

This is an ideal moment to realize the specific requirements of the BATTERY 2030+ initiative in a timely manner. LENS very much looks forward to working closely with BATTERY 2030+ to further develop specific actions to achieve the ambitious and highly valuable potential of this pan-European research and innovation effort.

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17. APPENDIX 4: LENS European Green Deal Position Paper (February 2020)

LENS LEAGUE OF ADVANCED EUROPEAN NEUTRON SOURCES

Making it happen

Placing Analytical Research Infrastructures at the heart of the Green Deal

Decoupling economic growth from (non-renewable) resource use and negative environmental impact, in order to guarantee the long-term viability of a fair and prosperous society, is a goal that should be universally welcomed. For this reason, the scientific community enthusiastically supports the *European Green Deal for the European Union and its citizens*[1], which puts Europe in a leading position in the design of tomorrow's society.

European scientists have been successfully working for decades on technologies that lead to higher resource efficiency and lower environmental impact. It is technological breakthroughs such as efficient renewable energy production and mobile storage that make the policy actions underlying the Green Deal possible in the first place. European scientists are keen to continue and strengthen these contributions towards tomorrow's society as an integral part of the Green Deal.

The development of new or improved green materials and processes is a central challenge for the Green Deal. The network of large-scale analytical facilities which allows European scientists to conduct sophisticated and innovative investigations into new materials and processes is undoubtedly one of Europe's outstanding assets in meeting this challenge. Within this network, neutron facilities serve a broad scientific community working on a vast range of societal topics from the quantum world for tomorrow's computing to the concrete and steel of tomorrow's buildings. These facilities provide scientists with access to state-of-the art instruments as well as all the services they need - from sample preparation to data interpretation - to gain an in-depth understanding of the properties of new materials. These facilities have now formed an alliance, LENS, the League of advanced European Neutron Sources. One of the principal goals of this alliance is the coordination of impact strategies. Active involvement in the Green Deal has been identified as central to this strategy.

The Green Deal is not a one-off effort but a clear indication of Europe's determination to become a frontrunner in the ecological transition of the coming decades. One of the main targets is to achieve a carbon neutral economy by 2050. This means that European research will have to act at every level of the technology readiness scale, from the fundamental research of today that will determine the technology of 2050 to the highly targeted investigations needed to overcome the final barriers separating us from the innovative products of tomorrow.

European governments currently spend about half a billion euros every year on the operation of existing neutron facilities and on the construction of future facilities. The business model employed ensures that access is granted to study the most relevant questions. Under the impetus of national and European research policies these questions have, in recent decades, become more focussed on the topics of societal relevance that make up the Green Deal. Consequently, European neutron facilities, already have well-established links to appropriate research teams. These collaborations are a strong foundation on which to build. Dedicated funding would make it possible to strengthen and extend these links.

The LENS facilities and their user communities have greatly benefitted from the funding tools of past and present framework programmes. As outlined in the Green Deal, "All EU actions and policies will have to contribute to the European Green Deal objectives. The challenges are complex and interlinked. The policy response must be bold and comprehensive and seek to maximise benefits for

[1] COMMUNICATION FROM THE COMMISSION TO THE EUROPEAN PARLIAMENT, THE EUROPEAN COUNCIL, THE COUNCIL, THE EUROPEAN ECONOMIC AND SOCIAL COMMITTEE AND THE COMMITTEE OF THE REGIONS of 11 December 2019

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health, quality of life, resilience and competitiveness." LENS proposes to actively respond to these obligations by steering part of future funding into a direction that further enhances the significant contribution neutron science already makes to innovation in relevant areas. This will also favourably contribute to the proposed 25% EU budget target for climate mainstreaming across all EU programmes.

There is a broad overlap between the innovation areas referred to in the Green Deal and the portfolio of science using neutrons. Among others, areas of connection include:

- Energy storage
- Photo-energy conversion
- Alternative transport fuels e.g. hydrogen
- Circular economy
- Energy reduction for intensive industries, such as steel, chemicals and cement

Access to neutron facilities is governed by scientific excellence. This strict selection criterion has, over many decades, guaranteed the quality and impact of the science produced and must also be maintained for the future. Nevertheless, this does not prevent us from taking active steps to further strengthen research activities in relevant areas. The above-mentioned fields certainly belong to this category. This further strengthening of such research activities must be tackled from both sides: (i) the large-scale analytical facilities will have to offer even more sophisticated, specifically tailored services and (ii) the users will have to deploy dedicated resources within their research programmes in order to fully benefit from the results obtained at the large-scale analytical facilities.

LENS proposes to achieve this targeted programme through concerted action. For this purpose, consortia of facilities will be formed to support fields relevant to the Green Deal. These consortia will undertake to:

- collectively and coherently develop infrastructure, such as instrumentation and sample environment, to specifically support fields relevant to the Green Deal in close interaction with expert researchers
- collectively provide software facilitating the exploitation of the corpus of data, including in particular the possibilities offered by the most recent developments in computer science, such as pattern recognition and artificial intelligence
- align as far as possible their operation to guarantee continuous reliable access
- collectively develop programmes for training a new generation of scientists capable of bridging the gap between the analytical techniques in use and the respective research fields in which they are used. These scientists would ideally work with the research teams.

The European Commission could make a significant contribution to boosting the development of these concerted activities by supporting this initiative. LENS would be more than happy to discuss with the Commission the practical aspects of how this might be implemented and funded.

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