Welcome and presentation of the ILL

Jacques Jestin – French Associate Director and Science Director

Summer School 2023 – 04/09/2023

NEUTRONS FOR SOCIETY

Grenoble: High concentration of scientific infrastructure

EPN Campus in Grenoble hosting EMBL, ESRF, IBS and ILL

NEUTRONS FOR SOCIETY

A bit of History

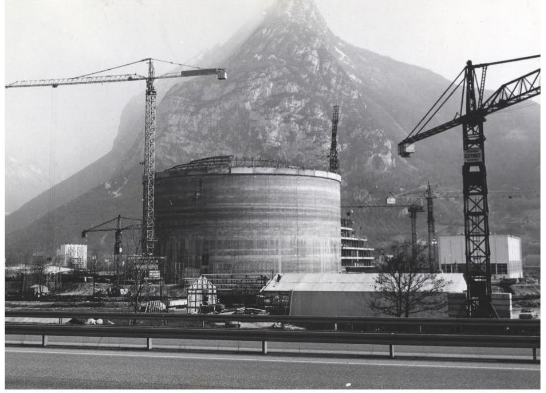
HISTORY

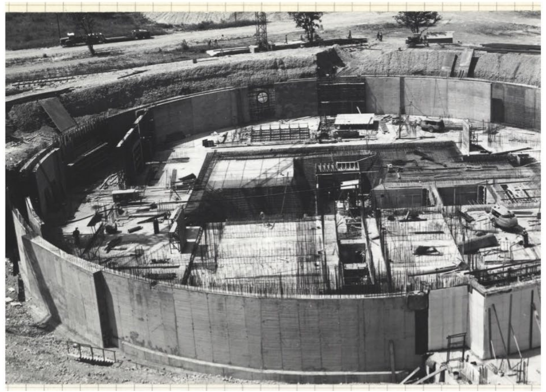
NEUTRONS FOR SOCIETY

More then 55 Years of history of peaceful collaboration

- 18 January 1967 founded with signature between French and German government
- 31 August 1971 reactor critical, full power 21 December 1971
- 1972 first user experiments
- 1973 joined by the United Kingdom as third associate
- Scientific member countries
  - 1987 Spain
  - 1988 Switzerland
  - 1990 Austria
  - 1997 Italy
  - 1999 Czech Republic
  - 2005 Sweden
  - 2005 – 2013 Hungary
  - 2006 Belgium & Poland
  - 2009 Denmark and Slovakia
  - 2011 – 2014 India
  - 2020 Slovenia
- 1991- 1995 Change of the reactor vessel
- No major operation before 2055

The founders:
Louis Néel and Heinz Maier-Leibnitz





INSTITUT LAUE-LANGEVIN

NEUTRONS FOR SOCIETY

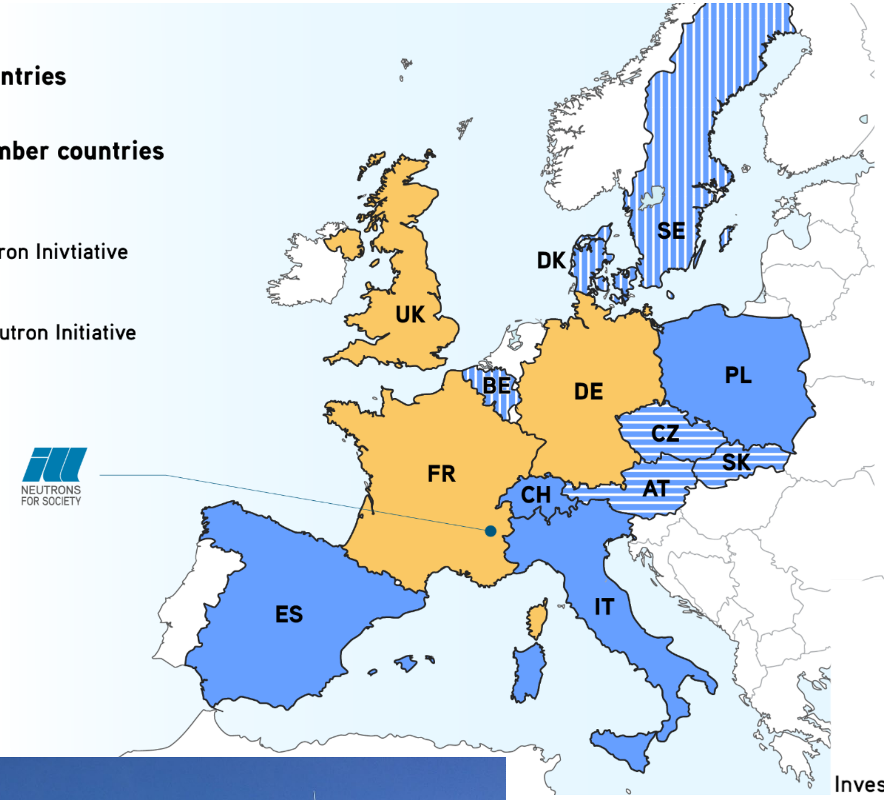
An international center operating worlds leading neutron source for research

ILL Associate countries

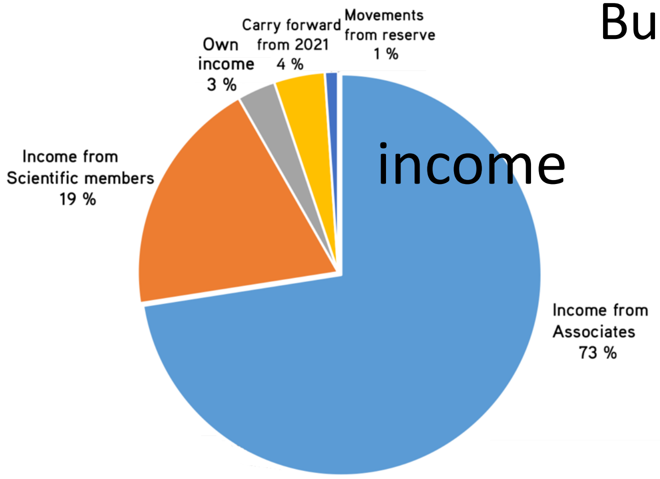
ILL Scientific Member countries

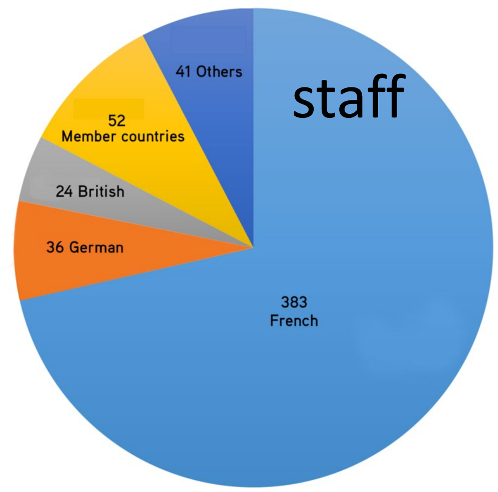
TRANSNI:
TRANSnational Neutron Inivtiative

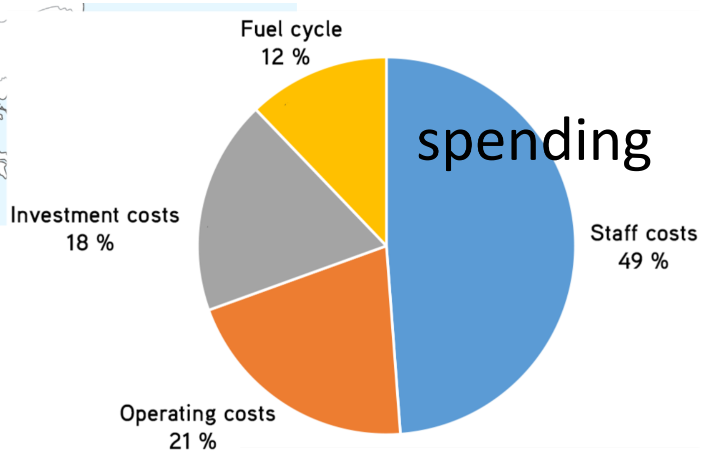
CENI:
Central European Neutron Initiative



Budget 2022: 107,76 M€







NEUTRONS FOR SOCIETY

Why Neutrons?

- Like X-rays they possess ideal wavelengths for revealing where the atoms are
- They in addition possess ideal energies for observing how they move
- The spin interacts with unpaired electrons

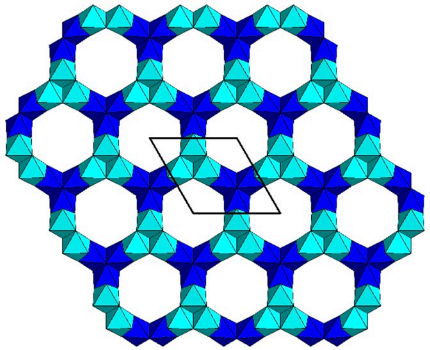
from 100 nm with cold neutrons

to 0.01 nm with hot neutrons

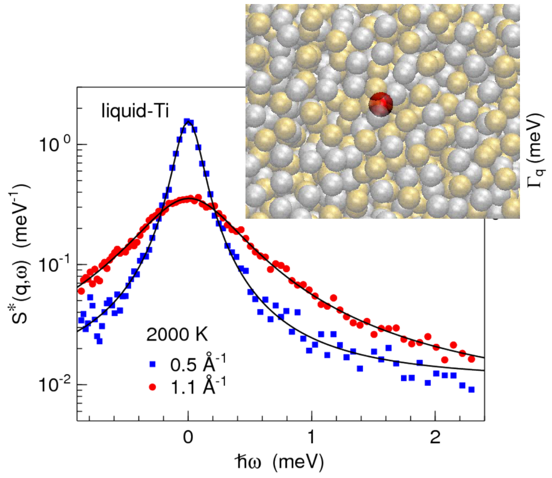
from vibrations to long/range diffusion

Determination of magnetic scattering

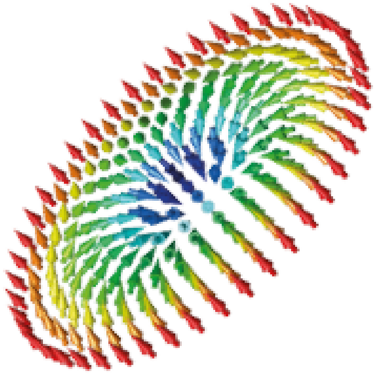
Myosin protein



Oxygen positioning in $Ag_7Pt_2O_7$



Atomic diffusion in liquid metals

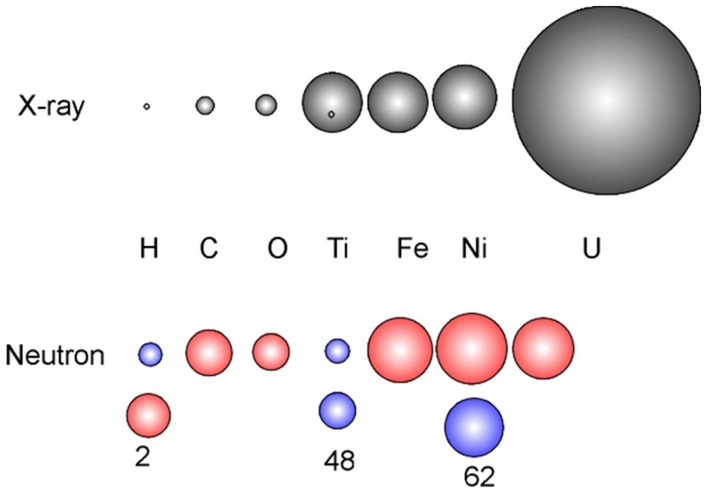


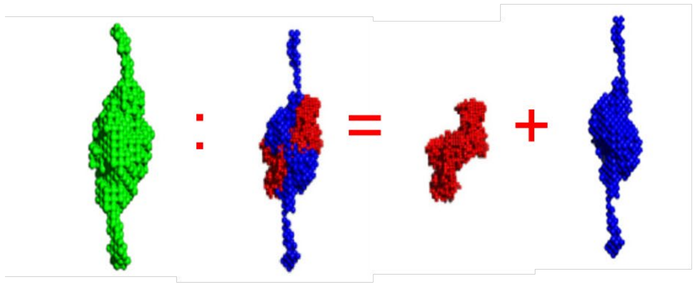
Arrangement of spins in skyrmions

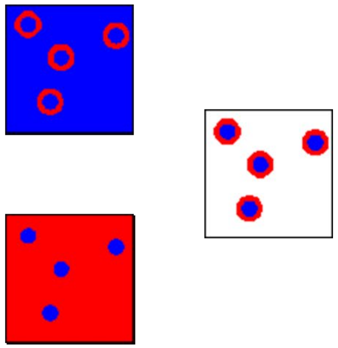
ADVANTAGES OF NEUTRONS

NEUTRONS FOR SOCIETY

- ILL's research reactor is producing the most intense beams of neutrons in the world
- Being electrically neutral, neutron can travel deep into materials and are non-destructive
- A unique feature of neutrons is that they are scattered differently by different isotopes of the same element: by isotopic substitution (H/D), we can increase the contrast of the scattering species in the solvent and make invisible a part of a multicomponent system (mixtures)





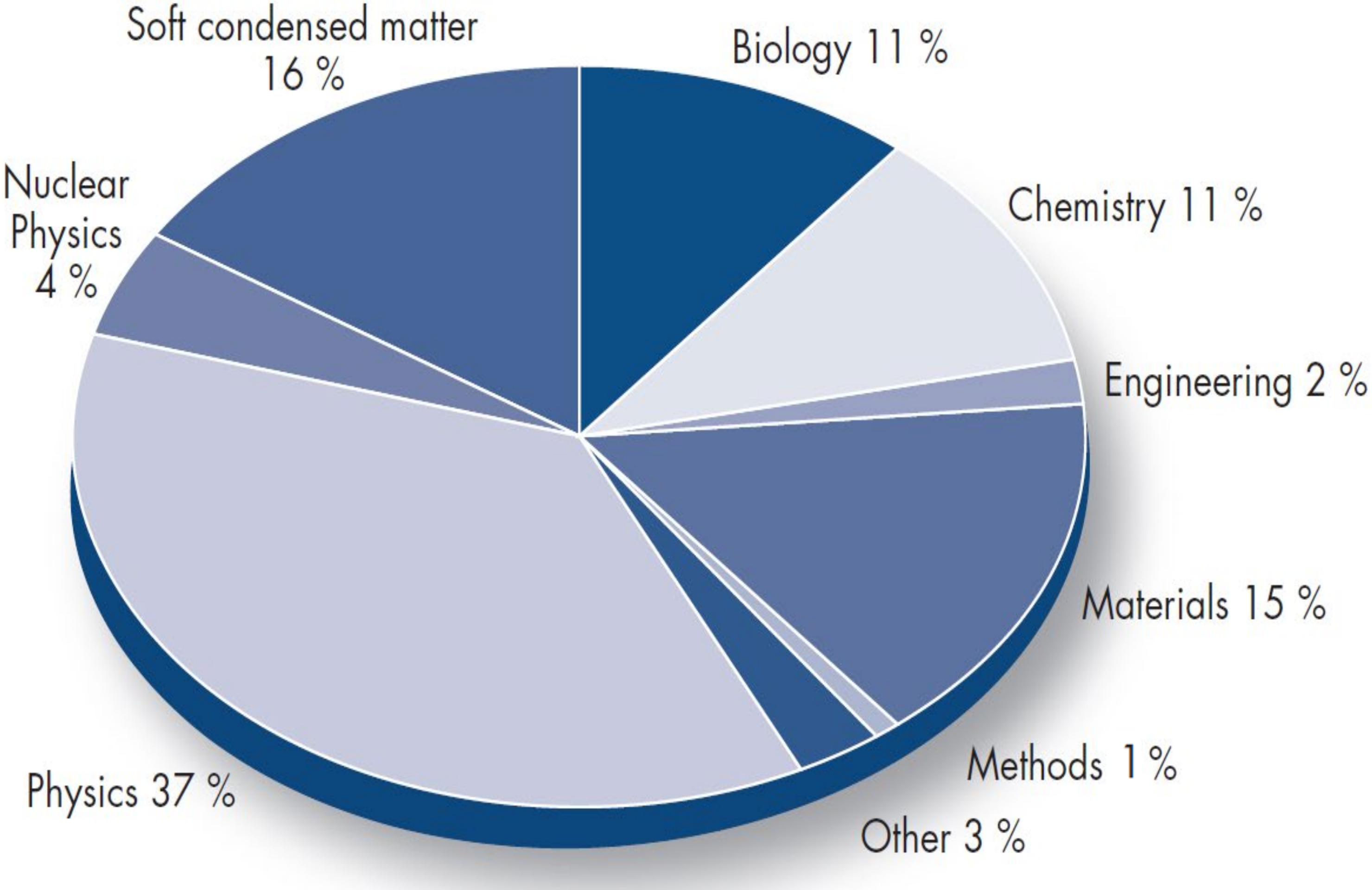


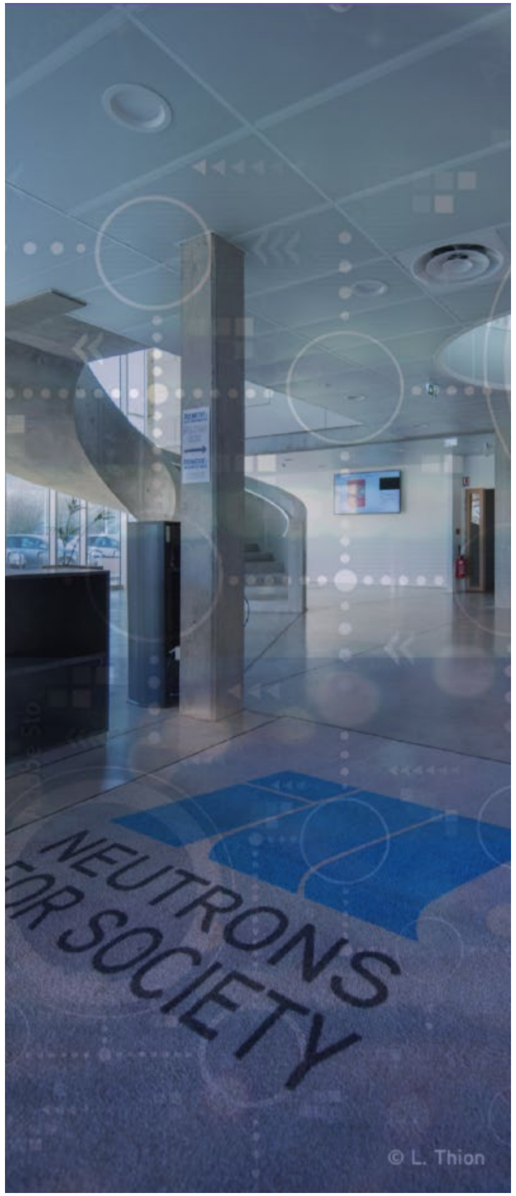
- Strong interaction with hydrogen nuclei that allow the precise determination of location and orientations of hydrogens, protonation, hydration and hydrogen bonding in a macromolecule, crucial for understanding the biological behaviors

Scientific Research Topics

"three thirds"

- Physics
- Chemistry and materials
- Soft matter and biology





SCIENTIFIC OUTPUT

NEUTRONS FOR SOCIETY

- ILL is producing around 600 publication per year with a constant increase of the scientific output

- Science at ILL meets the point between societal challenges and fundamental research

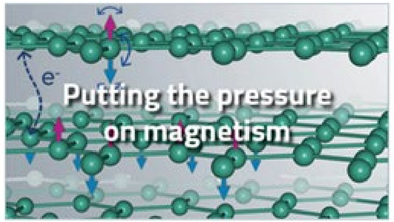
- Health
- Energy materials
- Climate change
- Quantum physics

Scientific Report

Cement and Concrete Research

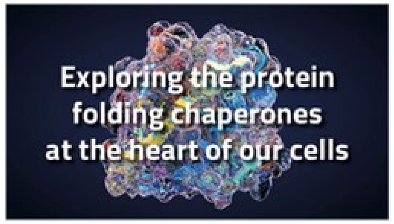
Chem. Mater.

J. Nucl. Med.



Phys. Rev. X

Nature



Nature Communications

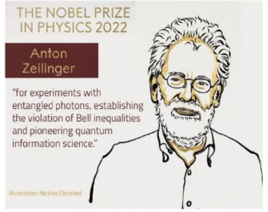
Structure

Phys. Rev. Lett.

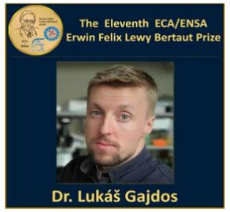
ILL RESEARCHERS RECOGNIZED FOR ACHIEVEMENTS

NEUTRONS FOR SOCIETY

- **Anton Zeilinger**
  - *Nobel prize* in Physics for experiments with entangled photons. Anton worked ('74 to '89) at ILL, performing various experiments to test predictions of quantum mechanics, succeeding in a direct observation of fermion spin superposition on S18.



- **Lukáš Gajdos**
  - *Erwin Félix Lewy Bertaut Prize* of the European Crystallographic Association in recognition of exceptional research on the characterization of the interaction of lectins with sugars by neutron diffraction.



- **Navid Qureshi**
  - Laureate of the *Wolfram Prandl Prize* for young scientists (KFN) for the enormous progress achieved in the use of polarized neutrons in gaining new insights into complex magnetic phenomena.

- **Alessandro Tengattini**
  - Laureate of the *ENSA Neutron Instrumentation and Innovation Award* at ECNS Garching for development of Neutron Imaging.

Neutron scattering covers many orders of magnitude

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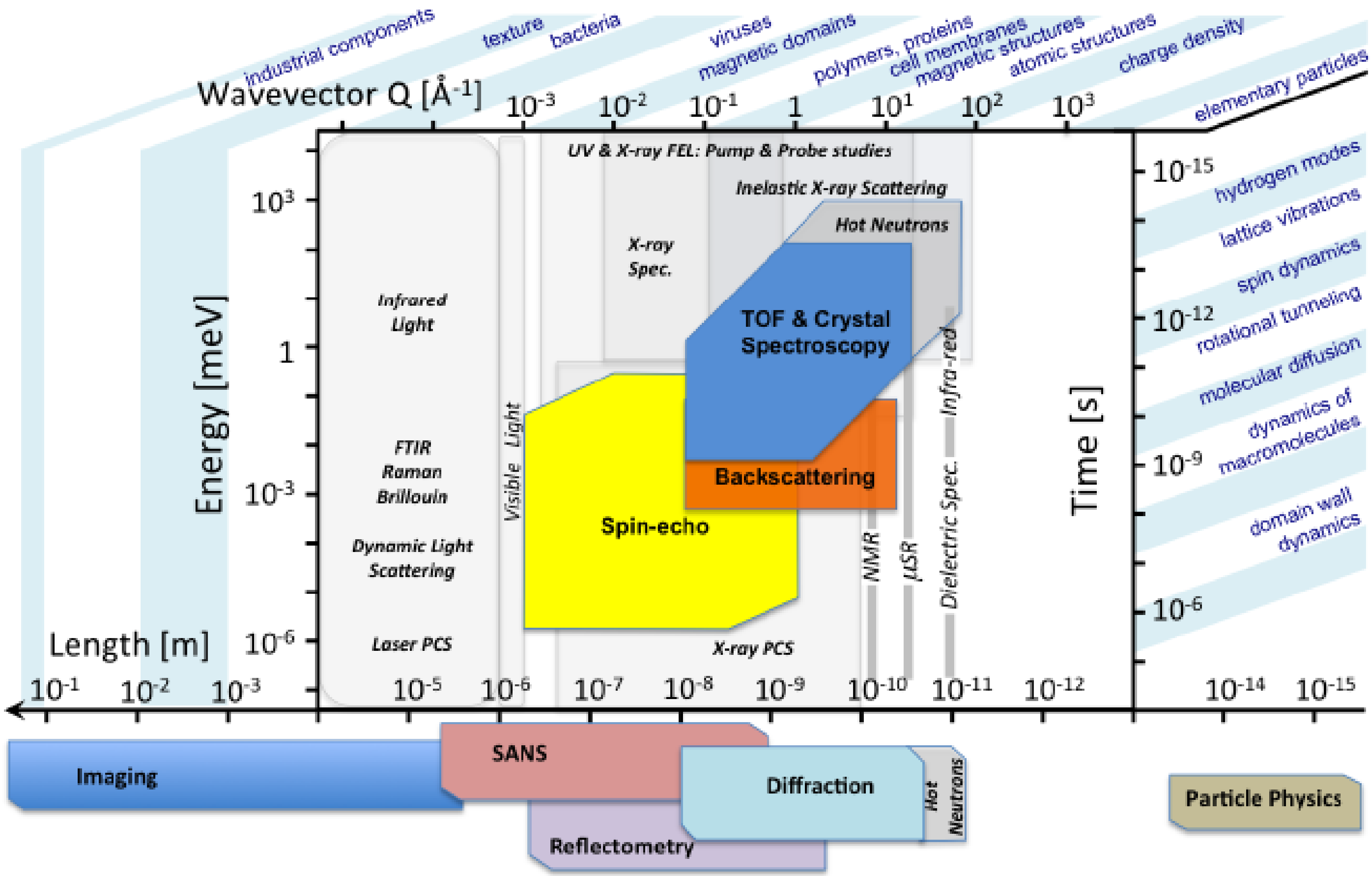
15 ORDERS OF MAGNITUDE IN LENGTH

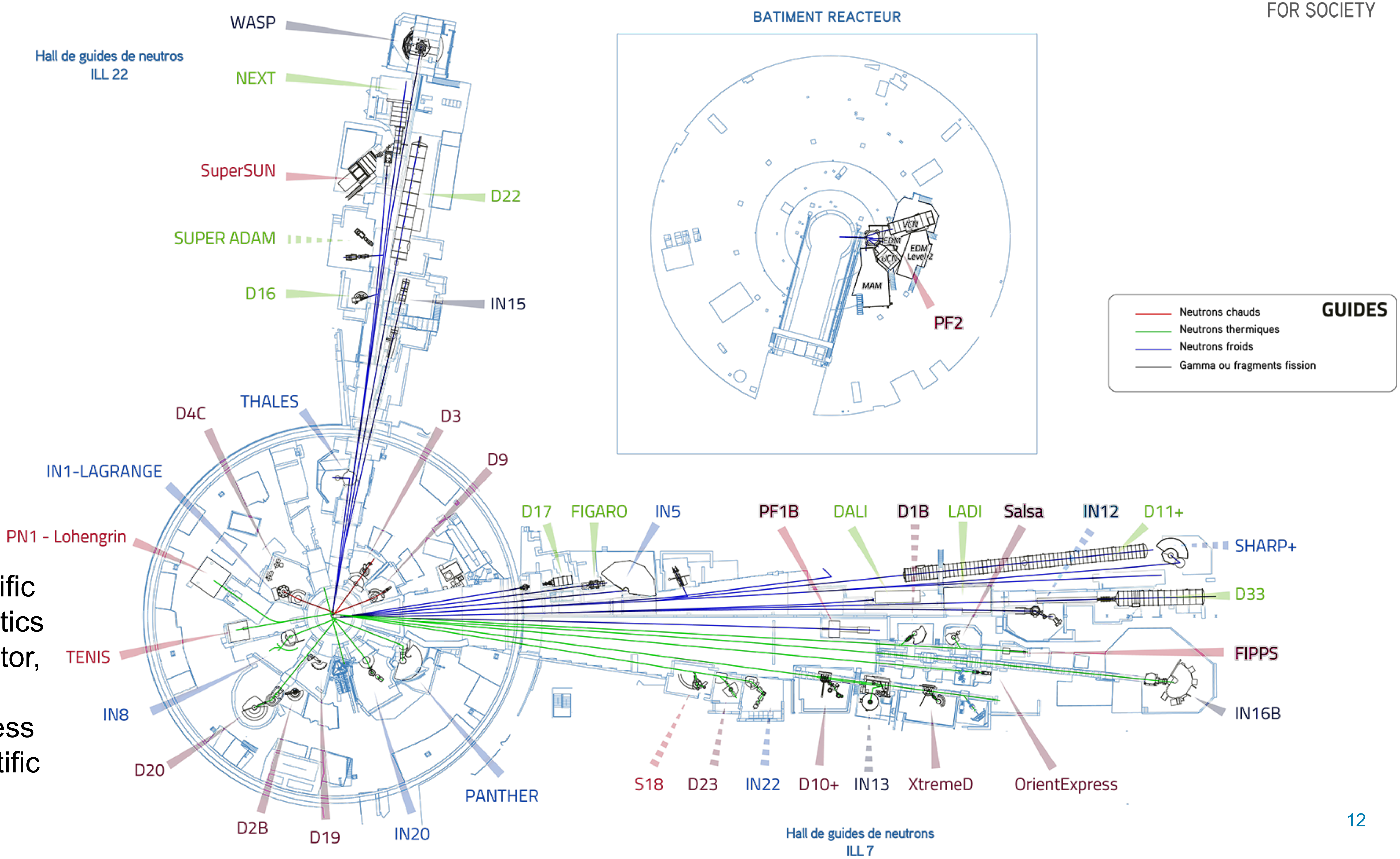
10 ORDERS OF MAGNITUDE IN TIME



NEUTRONS FOR SOCIETY

ILL'S INSTRUMENT SUITE

<u>43 instruments</u>:
35 from ILL
8 from CRG



Instruments have specific and unique characteristics (Flux, resolution, detector, energy range, sample environments) to address a broad range of scientific questions

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Instrument and User support

- Sample environments, high Pressure, high Magnetic field, low Temp, levitation
- Software & MD simulations
- Deuteration Lab & Partnership for Structural Biology PSB
- Chemistry Lab & Partnership for Soft condensed Matter PSCM
- Theory group

PARTNERSHIP FOR STRUCTURAL BIOLOGY PSB

NEUTRONS FOR SOCIETY

2002: MoU creating PSB
2006: CIBB Inauguration
2007: Creation of the UVHCI
2013: IBS integrates the EPN Campus
2017: launch of CM01 operated by the 4 Partners
2021-2025: Ongoing PSB Collaboration Agreement

4 Partners
~ 350 staff involved
~ 75 PhD students
~ 45 Postdocs
~ 13.5% multi-Partner publications

Broad & Diverse Biological Science

- Host-Pathogen Interactions
- DNA/RNA & Gene Regulation
- Stress Response in Prokaryotes
- Cell Division
- Metalloproteins/Enzymology
- Drug design and discovery
- Methodology & instrumentation developments for SB

Technical Platforms

Protein Expression
Cell Free
ESPRIT
Eukaryotic Expression Facility
Deuteration Lab

Sample Characterization
Analytical Ultra Centrifugation
Biophysics
Cell imaging
Mass Spectrometry
Surface Plasmon Resonance

High Resolution Studies
icOS
FIP Beamline
High Field Nuclear Magnetic Resonance
HT Crystallisation
Neutron Diffraction Beamlines
ESRF Structural Biology Beamlines

Supramolecular Structures
Electron microscopy
SANS/ SAXS
Cryo-EM Titan Krios

P S B
THE PARTNERSHIP FOR STRUCTURAL BIOLOGY

EMBL

ESRF

ibs Institut de Biologie Structurale

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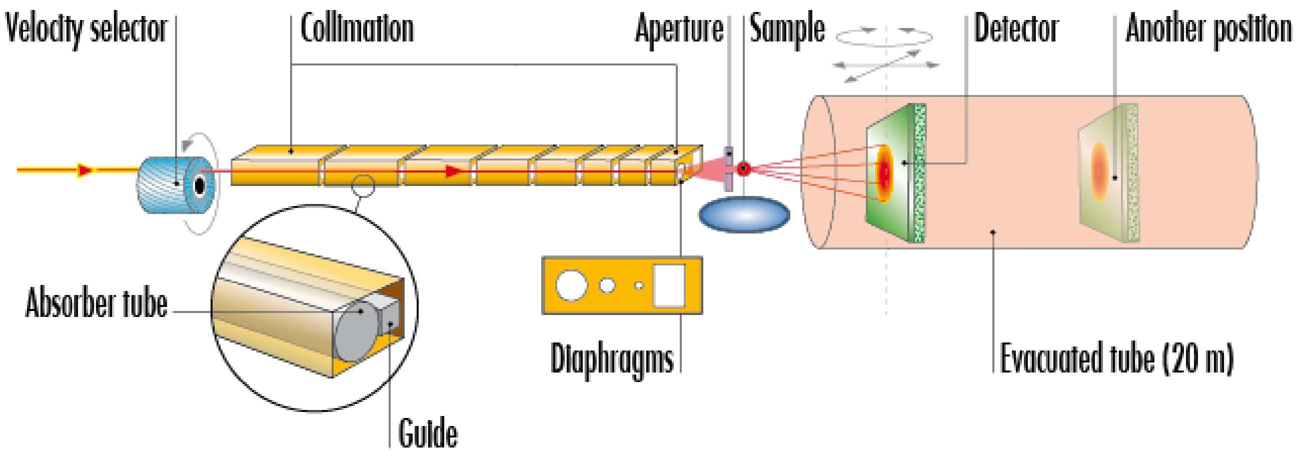
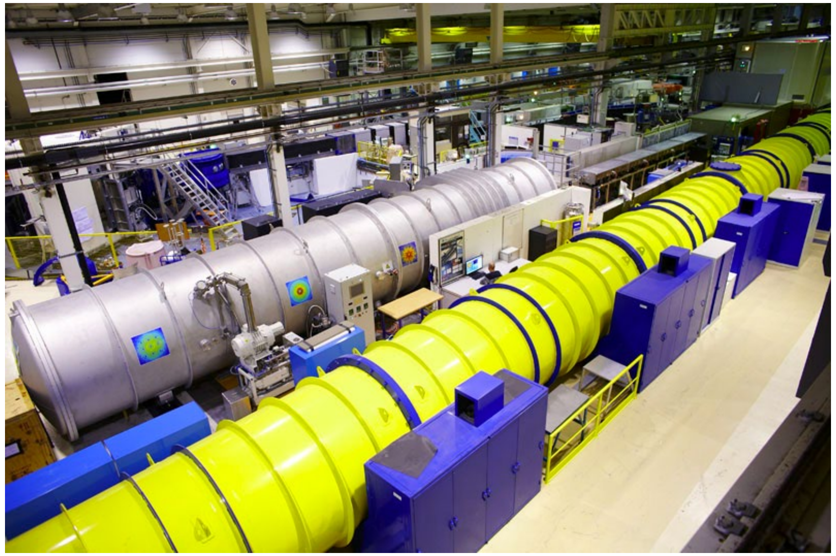
NEUTRONS FOR SOCIETY

One Example: Small Angle Neutron Scattering





- Determine the structure of disordered materials on a length scale of 1 to 100 nm
- Applications in Soft matter, biology, materials science, magnetism
- 4 SANS at ILL: D11, D22, D33 and SAM

Small Angle Neutron Scattering

Soft Matter

ROYAL SOCIETY OF CHEMISTRY

PAPER

View Article Online
View Journal

Cite this: DOI: 10.1039/d2sm01252a

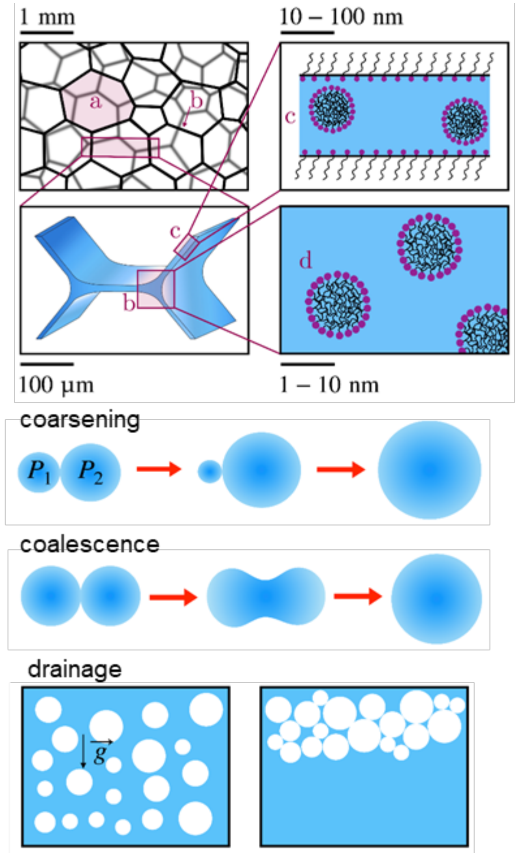
Probing foams from the nanometer to the millimeter scale by coupling small-angle neutron scattering, imaging, and electrical conductivity measurements†

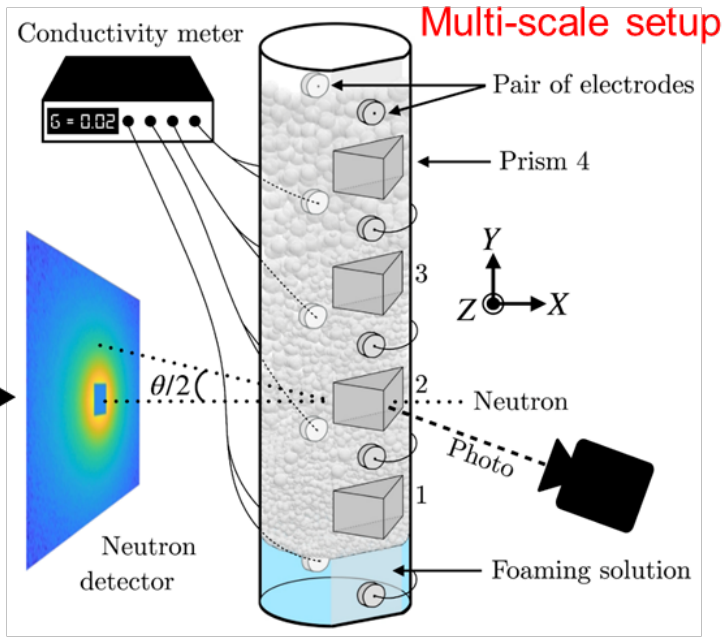
Julien Lamolinairie,[a] Benjamin Dollet,[b] Jean-Luc Bridot,[c] Pierre Bauduin,[d] Olivier Diat[d] and Leonardo Chiappisi *[a]

NEUTRONS FOR SOCIETY

A foam is : a multi-scale system

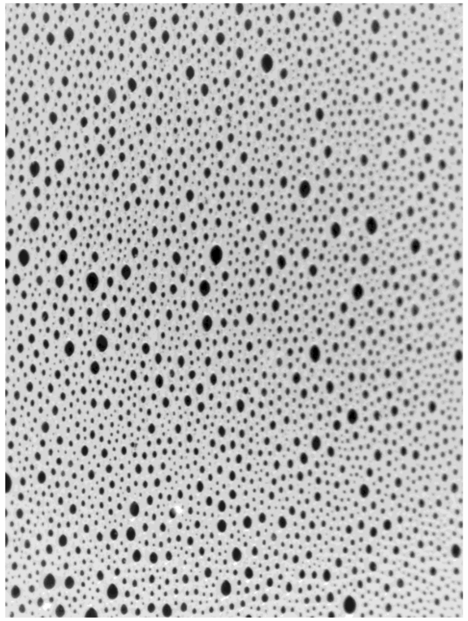
an out-of-equilibrium system

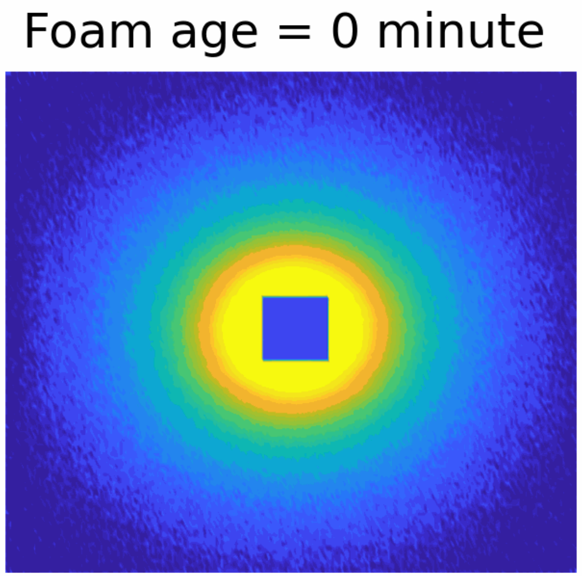


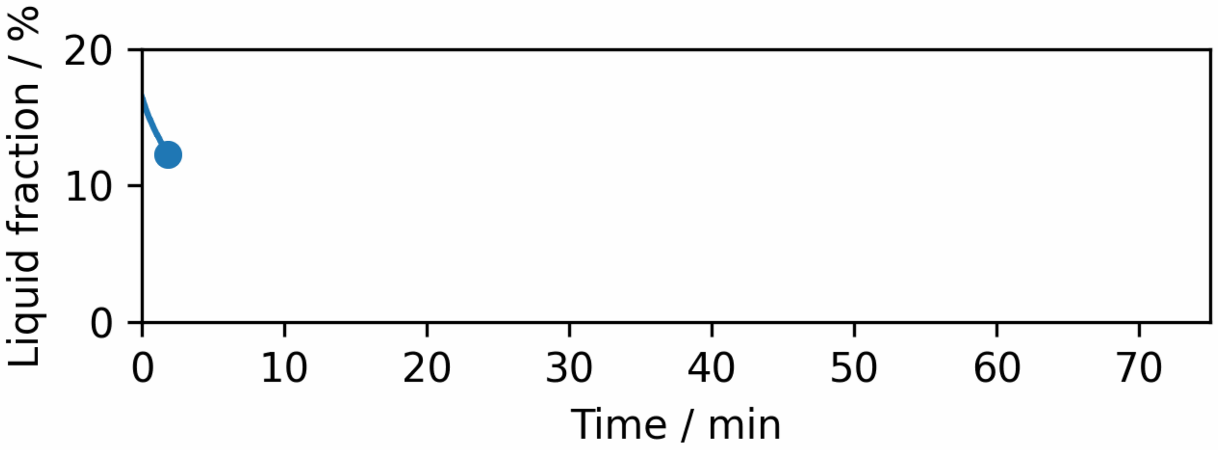


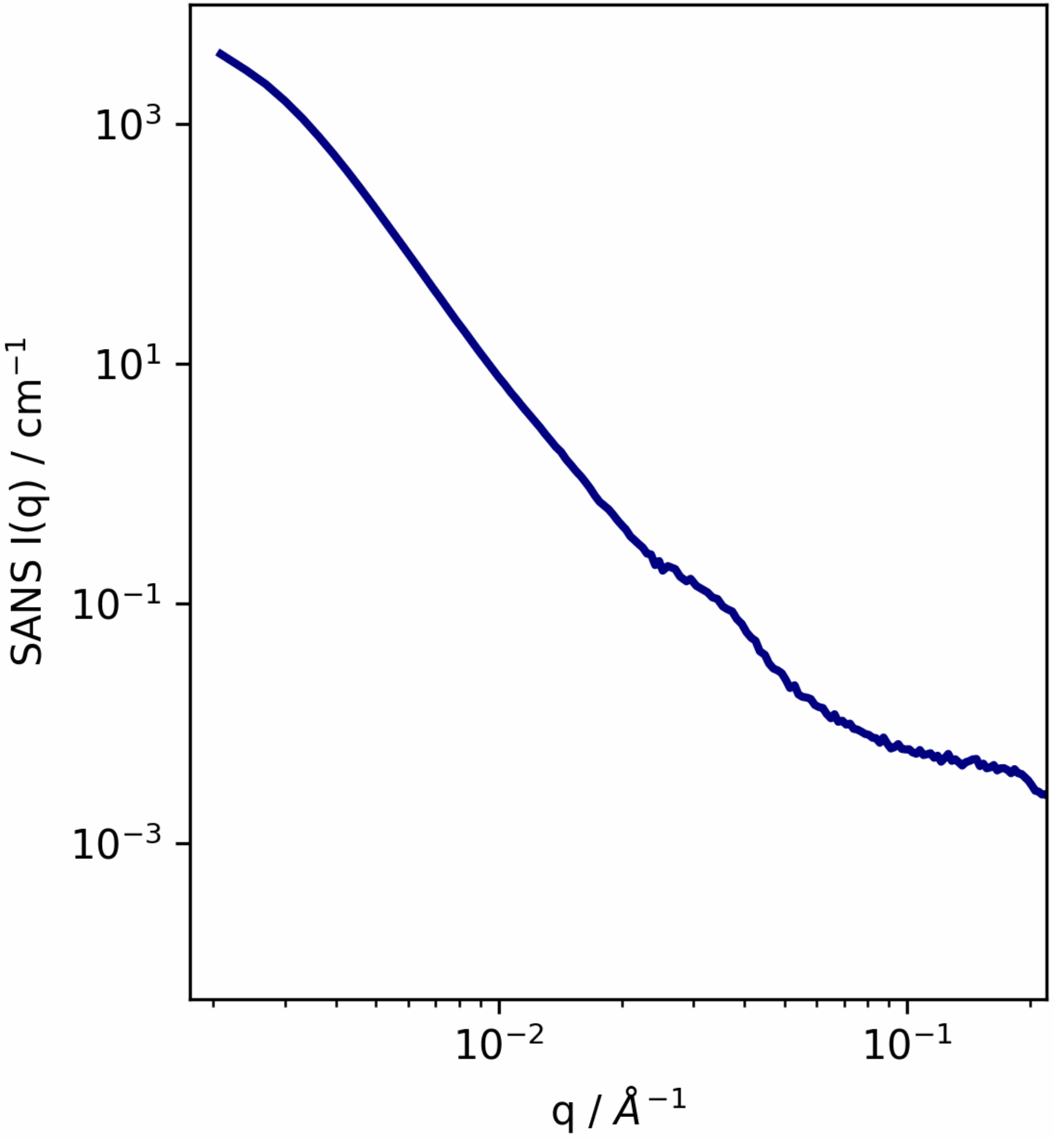
Development of a new device allowing the structural characterization of foam from the nanometer to the millimeter scale.

Simultaneous time-resolved analysis of liquid foams





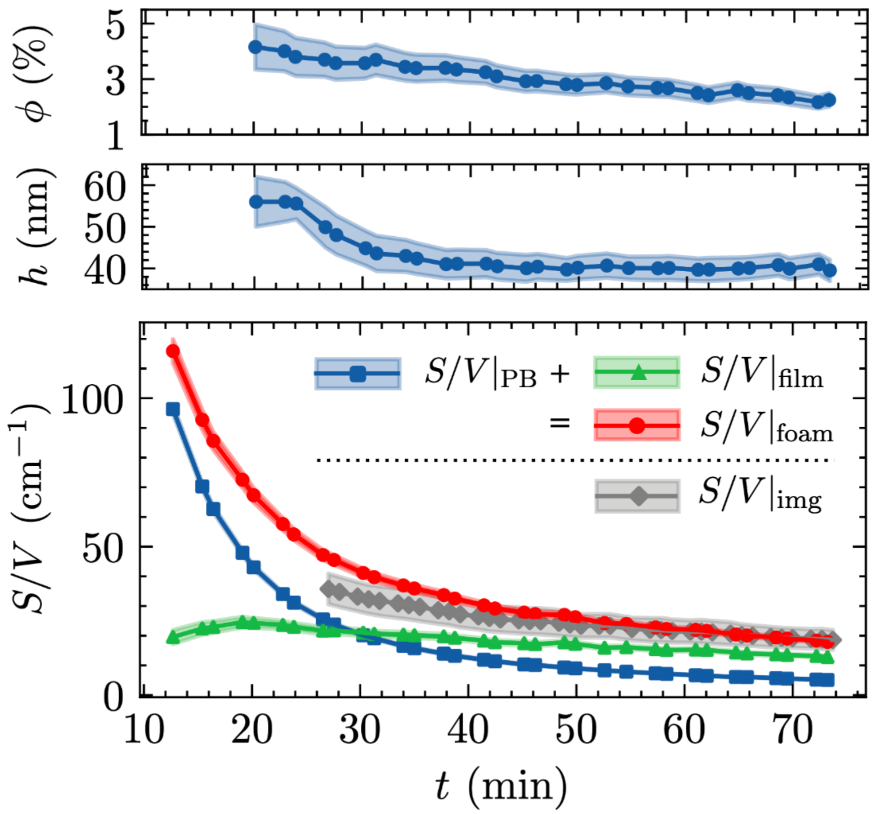




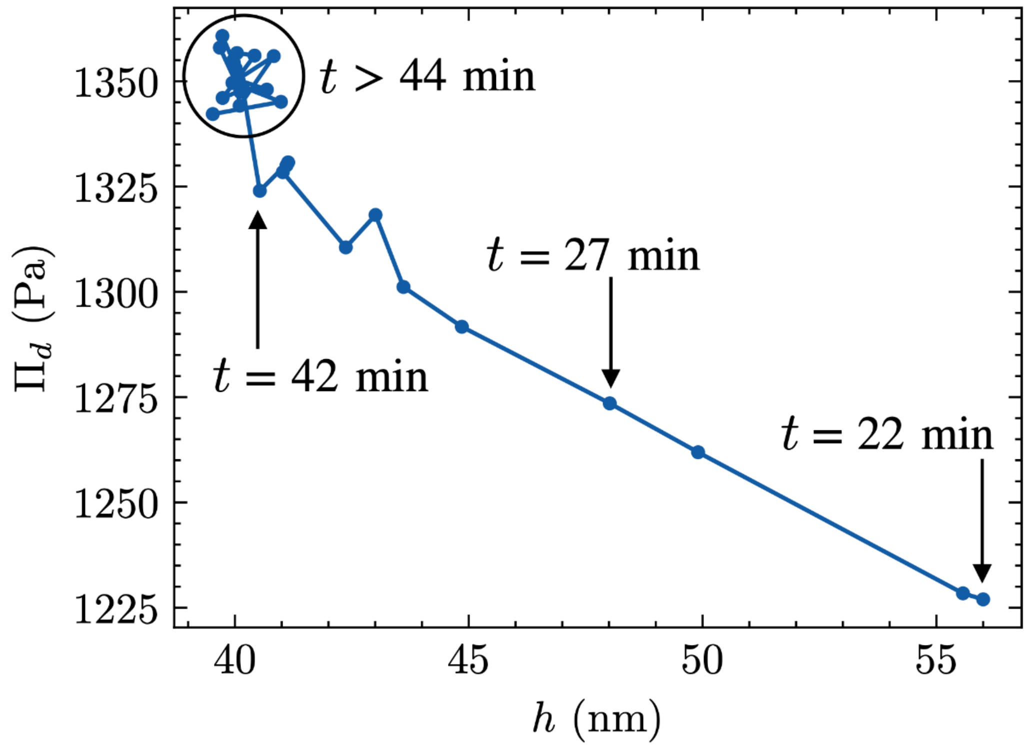
NEUTRONS FOR SOCIETY

Small Angle Neutron Scattering

Multi-scale analysis of liquid foams



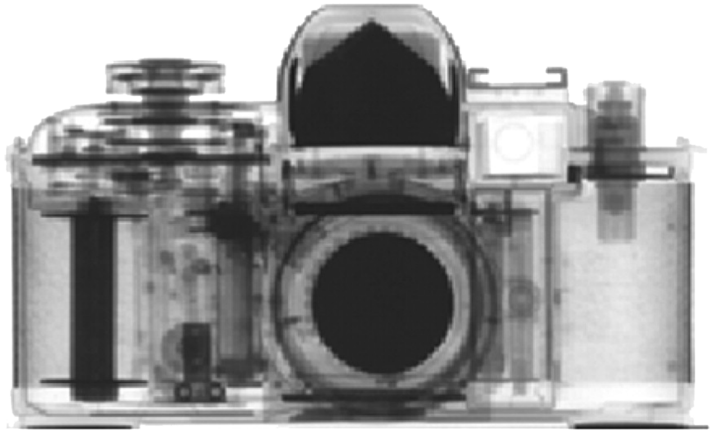
A new SANS model was developed and enables to extract the liquid fraction ϕ, the inter-bulles film thickness h and the specific surface area of the Plateau borders S/VPB and of the film $S/Vfilm$.



The information extracted from the image analysis and SANS data allows for the first time to determine the disjoining pressure $\prod_d$ vs thickness isotherm h in a real, draining foam.

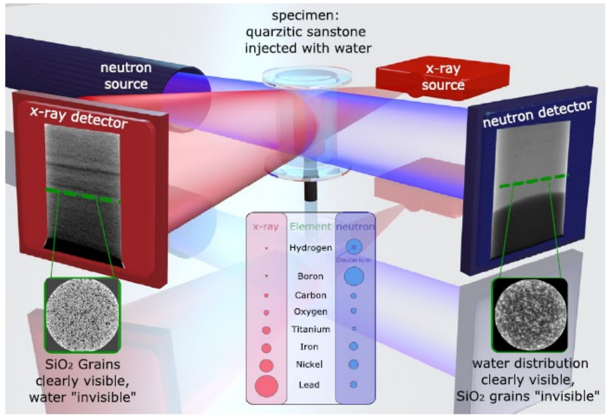
NEUTRONS FOR SOCIETY

Neutron imaging – Attenuation properties of the imaged object



NEUTRONS

X-RAYS

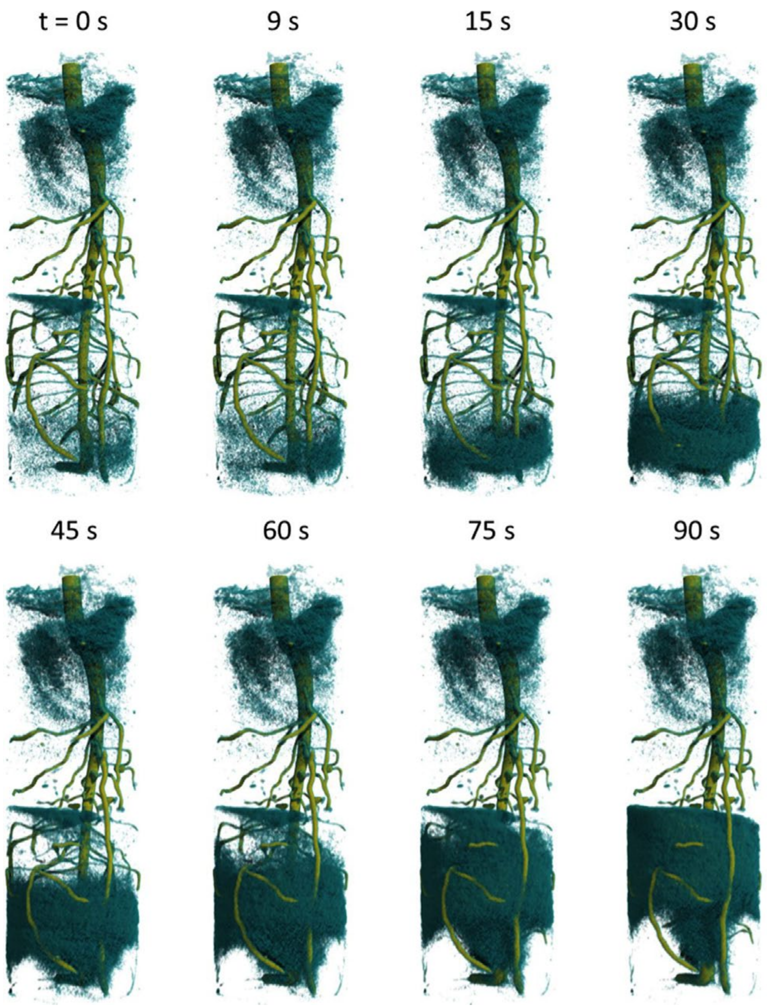


Next

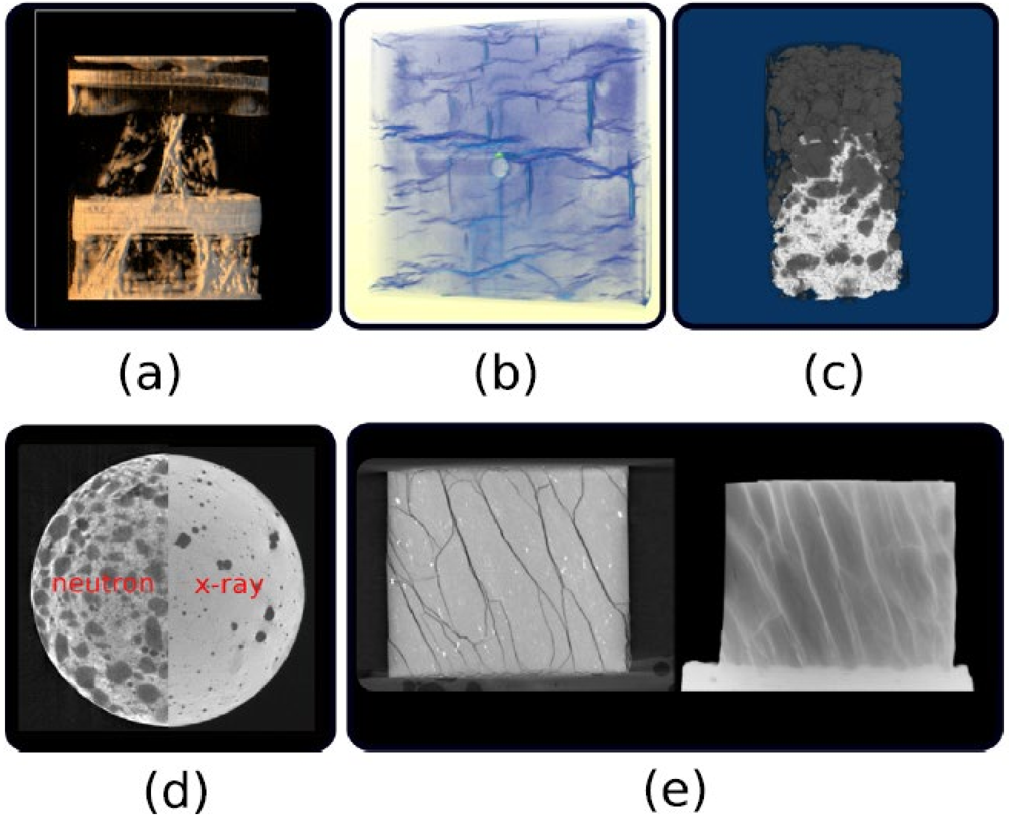
- Plastic components are well resolved by neutrons owing to their Hydrogen content while the metallic body with higher electronic density are well resolved by x-rays

Jeremy H. Lakey J. R. Soc. Interface 2009;6:S567-S573

Neutron imaging – 3D Tomography



Water front in lupine roots

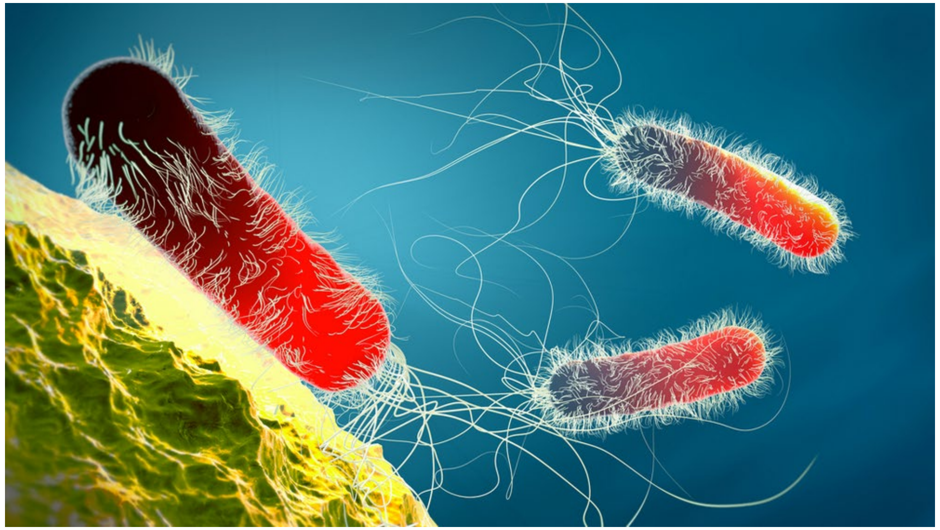


Concrete, Claystone, cultural heritage….

NEUTRONS HELP REVEAL DETAILS OF THE BINDING OF A HUMAN PATHOGEN TO OUR CELLS BY LAUE-DIFFRACTION

NEUTRONS FOR SOCIETY

- Pseudomonas aeruginosa is a human opportunistic **pathogen** that causes severe infections in immunocompromised patients. P. aeruginosa and other pathogenic bacteria use several virulence factors to promote their **infectivity**, including sugar-binding proteins
- **Neutron protein crystallography** and the production of deuterated protein and sugar have been used to study how Pseudomonas aeruginosa binds to host cells
- Pseudomonas aeruginosa attach to the cells and form a biofilm to colonize the tissue. The LecB protein from Pseudomonas aeruginosa binds specifically to fucose, a small sugar present on the surface of the host cells via hydrogen-bonding and calcium coordination
- Neutron data from LecB/fucose complex revealed details of **H-bonding networks, hydrophobic interactions, protonation**, and **hydration**.
- Development of LecB inhibitors to block the binding process (new drugs)

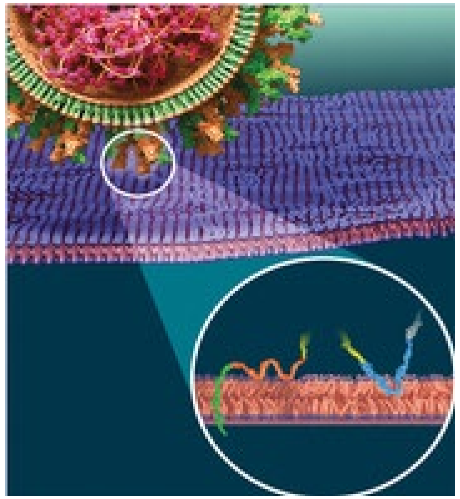


nature COMMUNICATIONS

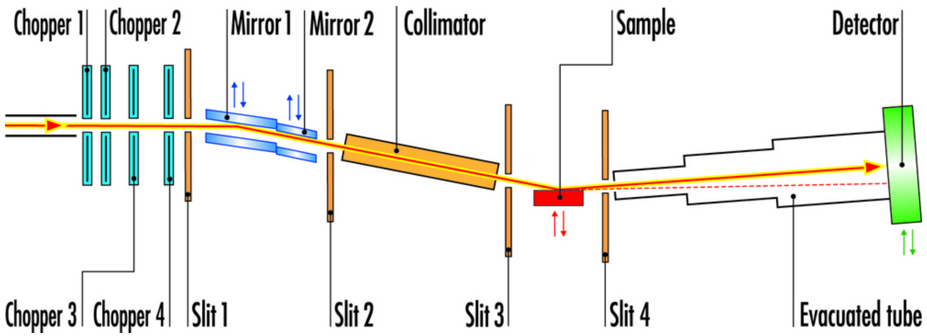
Nature Communications volume 13,194 (2022)

NEUTRON SCATTERING TECHNIQUES REVEAL THE ROLES OF SARS-COV-2 FUSION PEPTIDES DURING INFECTION BY NEUTRON REFLECTOMETRY

NEUTRONS FOR SOCIETY



- Understanding of the mechanisms of **cellular infection** by β-coronaviruses
- The ILL experiments on **Spike fusion** peptides provided direct structural information from specular **neutron reflectometry** to determine the molecular mechanisms of infectivity. Membranes were modelled using natural lipid extracts
- Peptides present within the fusion domain were found to interact primarily with lipid headgroups. The peptides act a bridge between the host and viral membranes and promote membrane fusion. The intracellular calcium levels may therefore provide an indication to where and how the viral and host membranes fuse during SARS-CoV-2 infection.



Figaro

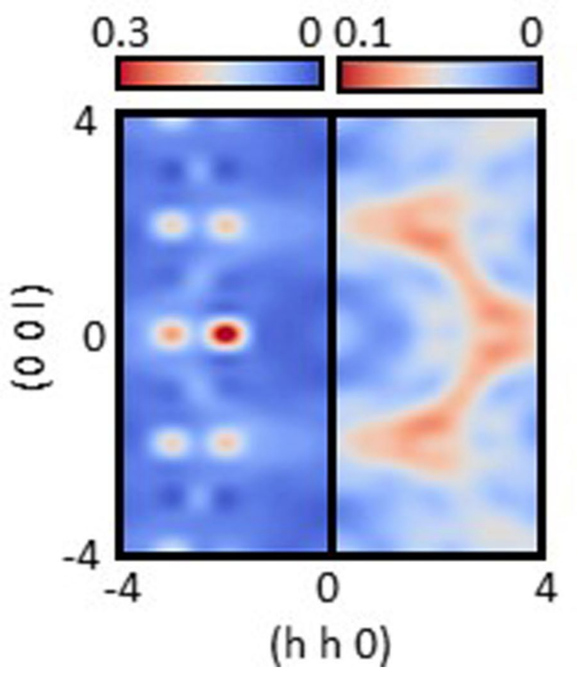
JACS
JOURNAL OF THE AMERICAN CHEMICAL SOCIETY

J. Am. Chem. Soc. 2022, 144, 2968−2979

Neutron spin interacts with unpaired electrons → magnetism

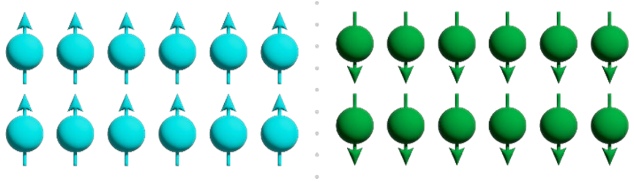
NEUTRONS FOR SOCIETY

Neutrons probe directly the complex magnetic structure and excitations of materials – polarized neutron beams and magnetic fields facilitate these investigations by Neutron Diffraction (Powder or Single crystal) and Inelastic measurements.

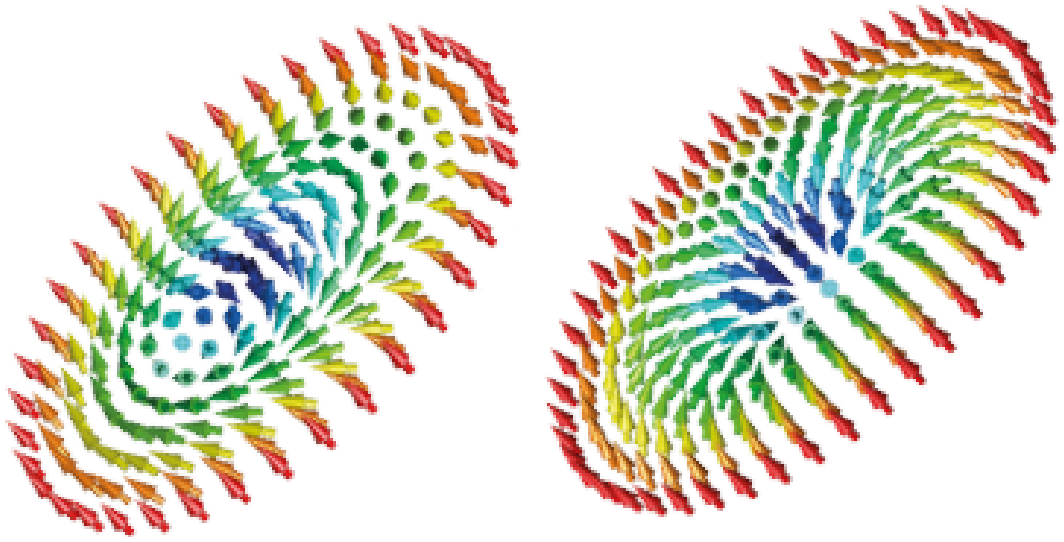


Spin liquids

enigmatic magnetic state



Arrangement of spins in two skyrmion structures



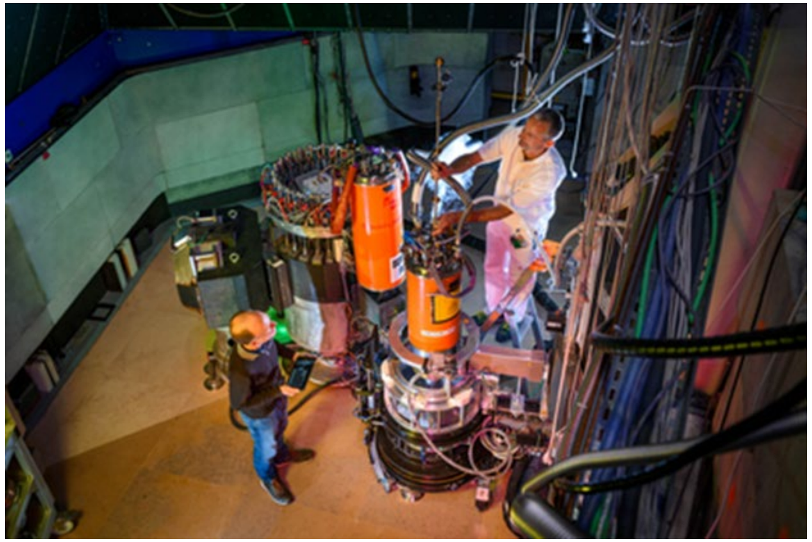
If theses **smaller spin structures** can be reliably stabilised and manipulated, they could be used as information carriers in next-generation devices

I. Kezsmarki et al., Nature Materials, 2015, **14**, 1116; DOI: 10.1038/nmat4402ptions.

NEXT GENERATION ENERGY EFFICIENCY: THE POTENTIAL OF SUPERCONDUCTIVITY

NEUTRONS FOR SOCIETY

- Climate change and the energy crisis have highlighted the need to rapidly accelerate progress on global energy efficiency. While **superconductivity** holds immense potential to revolutionize energy storage and transmission, the complexity of the domain requires multidisciplinary research in order to understand the physics of superconductors and how they can be enhanced.
- Superconductivity describes the ability of certain materials to conduct an electric current with zero resistance and thus extremely low energy losses.
- The ultimate ambition, however, is to achieve superconductivity at **room-temperature**, enabling an energy-efficiency revolution through the lossless transmission and **storage of electrical energy**.
- A major breakthrough came in 1986 with the discovery of high-temperature superconductivity in **cuprates** – a new class of material made of layers of copper and oxygen atoms separated by layers of other elements.
- One key question is whether charge density waves (CDW) and spin density waves (SDW) simply coexist or are directly coupled in cuprate materials and how their fluctuations may give rise to high-temperature superconductivity.

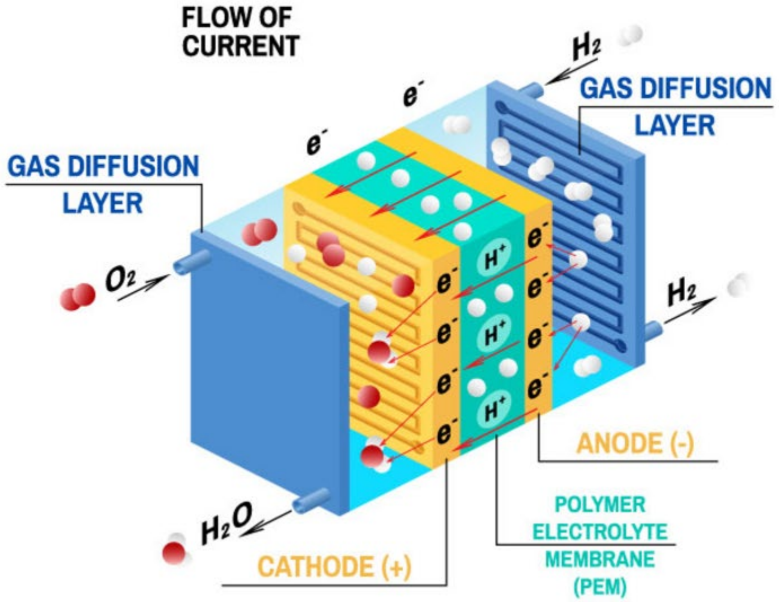


Thales TAS Spectrometer

TOWARDS THE IDEAL FUEL CELL

NEUTRONS FOR SOCIETY

- **Semipermeable polymeric membranes** that selectively allow the passage of negative ions (anions) play a key role in several important technologies including **fuel cells**. Neutron studies untangle the **complex dynamics** in an anion exchange membrane when employed in a fuel cell setting.
- There is therefore a great deal of interest in understanding and optimising the various **transport processes** across these membranes while maintaining their stability.
- Quasi-elastic neutron scattering provides the means of unpicking these subtly coupled effects. Neutrons can reveal motions and dynamical changes in molecules like polymers and water because they can interact with these motions at given energies. The resulting characteristic energy changes can then be measured by **Time-Of-Flight** and **backscattering** spectrometers (Sharp+, IN16B).

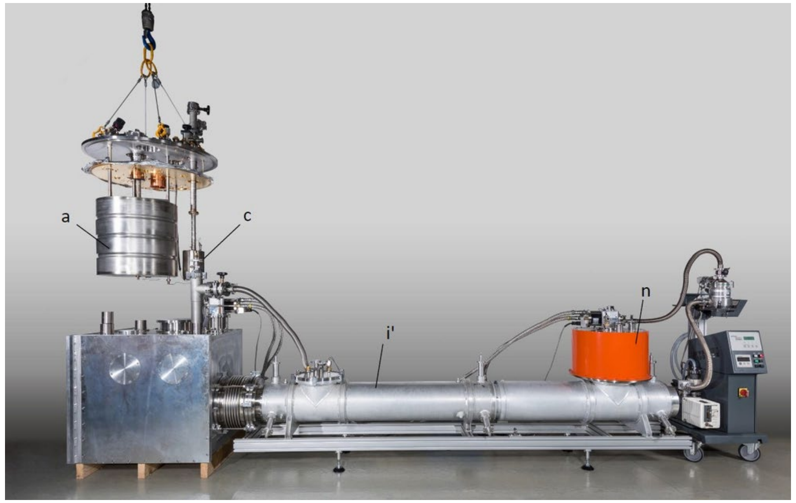


PARTICLE PHYSICS – FUNDAMENTAL PARTICLES AND FORCES

NEUTRONS FOR SOCIETY

- Cosmological evolution – Theory of particles and forces – Stellar astrophysics – Quantum Mechanics - Nuclear fission – Metrology
- The cold or ultra-cold neutrons produced at the ILL can tell us a great deal about the **'symmetry'** characteristics of particles and their interactions – perhaps helping to explain, for example, how the Universe came to contain mainly **matter and not antimatter**, even though created in equal amounts.
- Determination of the **Electric Dipole Moment** (EDM) of the neutron which is (almost) zero
- The ILL is also able to create exotic nuclei with high numbers of neutrons to explore the pathways by which elements are made in the stars.

PF2

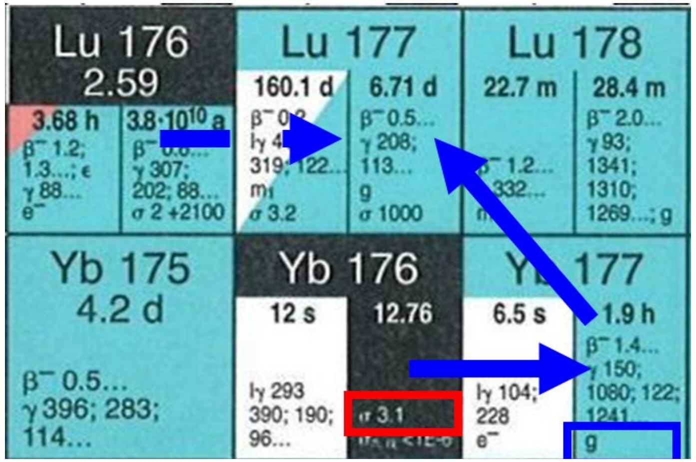


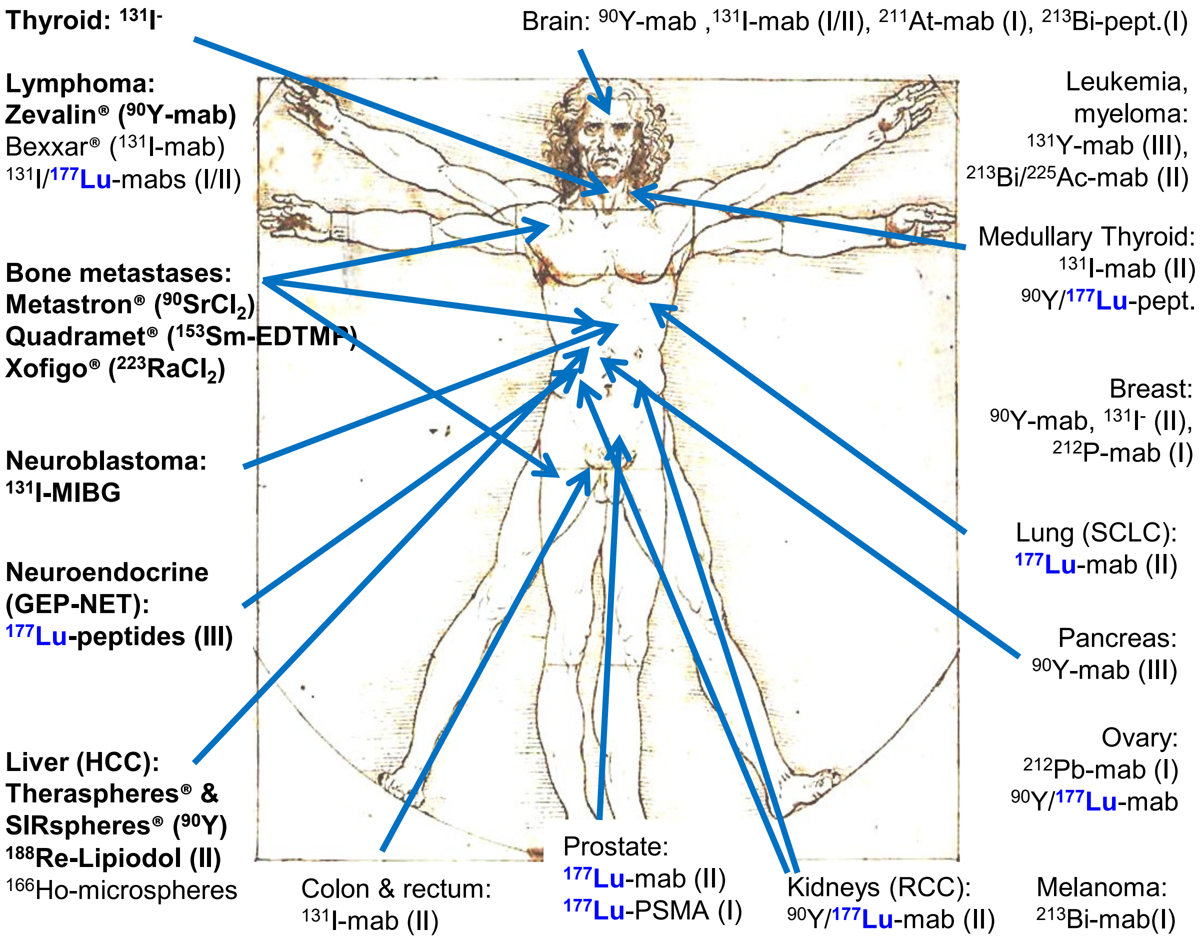
Supersun

NEUTRONS FOR SOCIETY

Radioisotopes Production

Understand and produce, pure short-lived (~weeks) isotopes for therapeutic applications



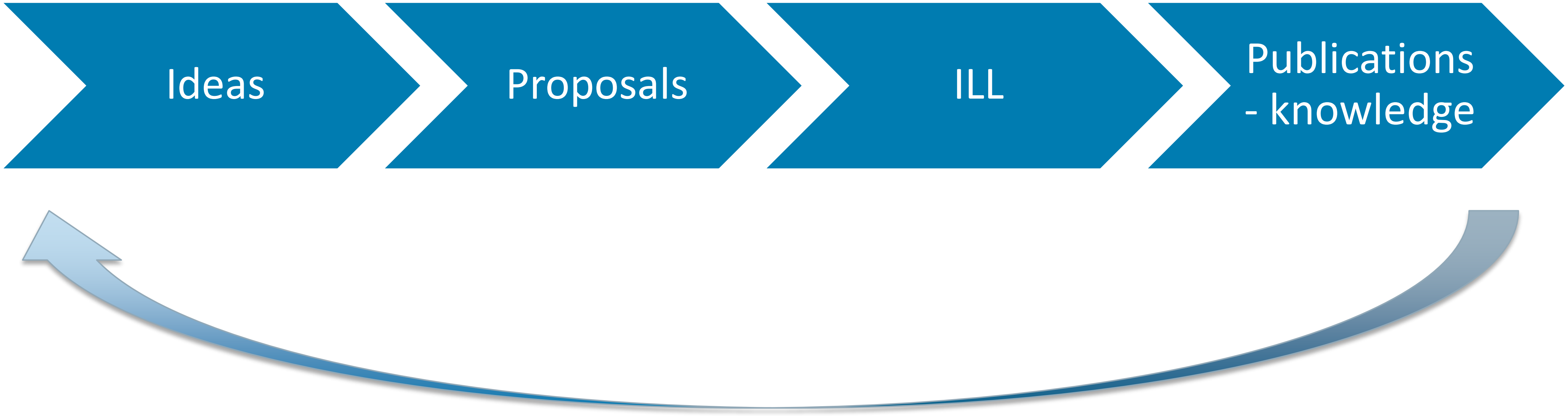


Lu 177 emit gamma rays on a few millimeters and enable to treat small metastasis

NEUTRONS FOR SOCIETY

How do we achieve this?

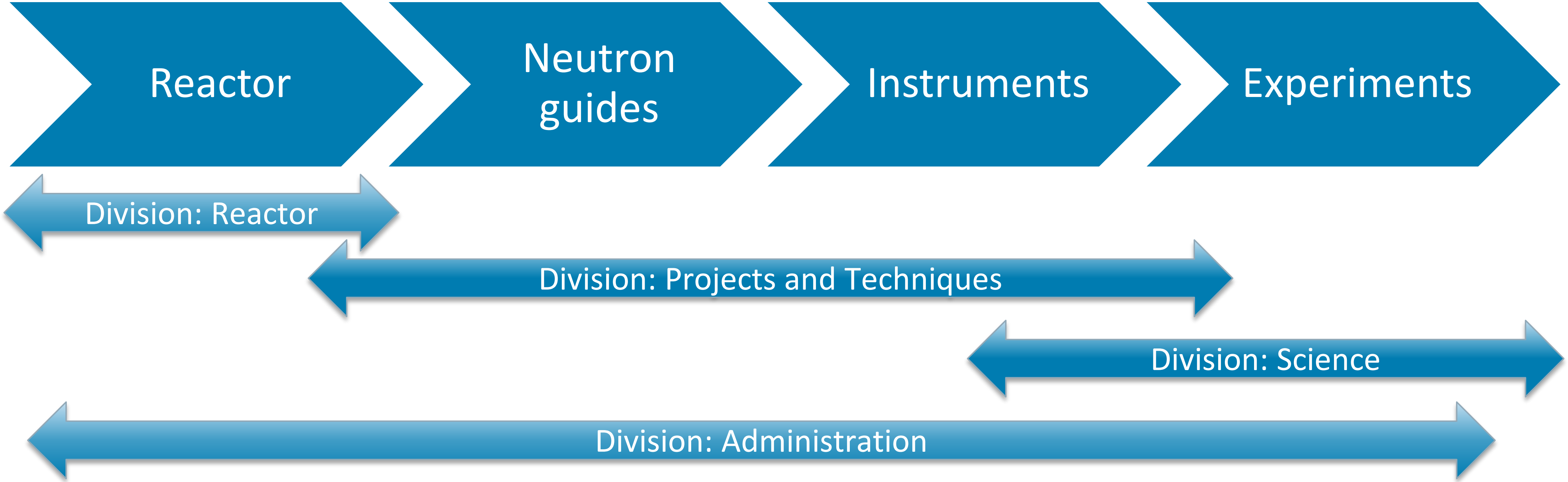
In the scientific community



NEUTRONS FOR SOCIETY

How do we achieve this?

TEAMWORK @ ILL



BEAM TIME AVAILABILITY

NEUTRONS FOR SOCIETY

Access to neutron via proposal system or scientific collaboration

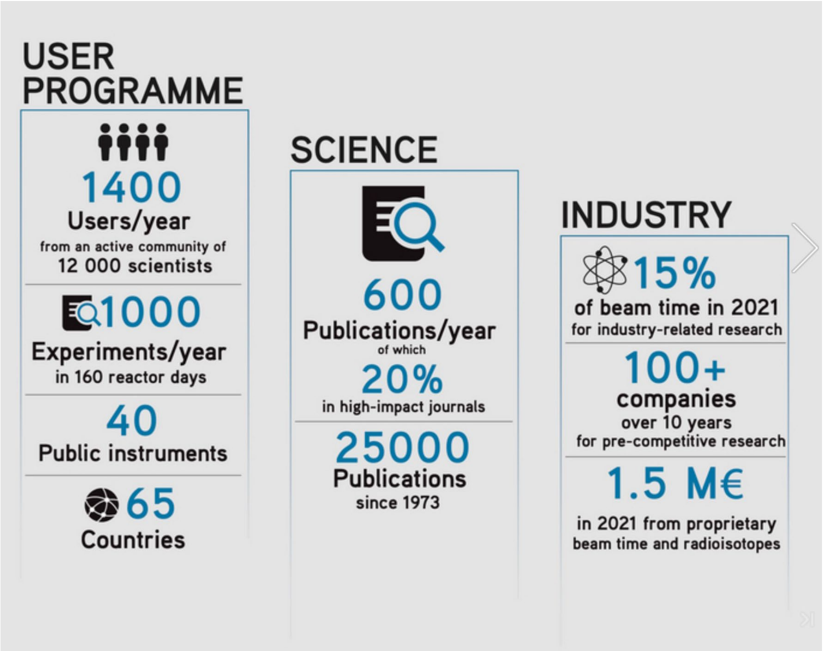
Normal path for academic users:

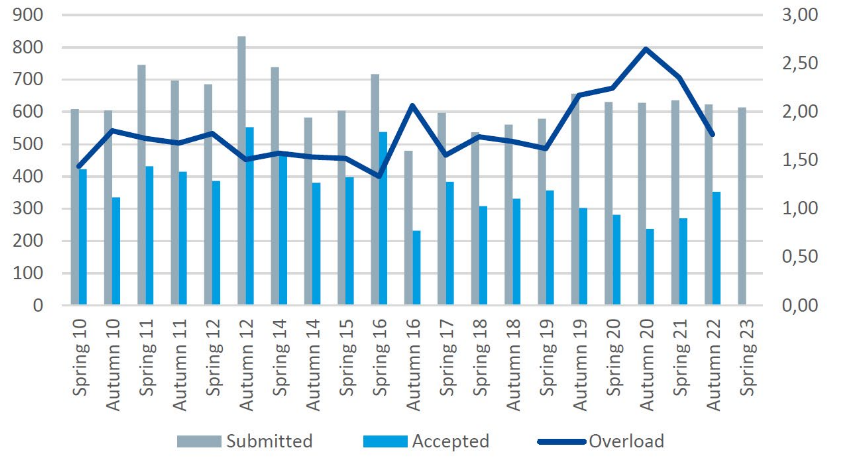
- Application two times / year
- Review by scientific subcommittees
- Quick access possible

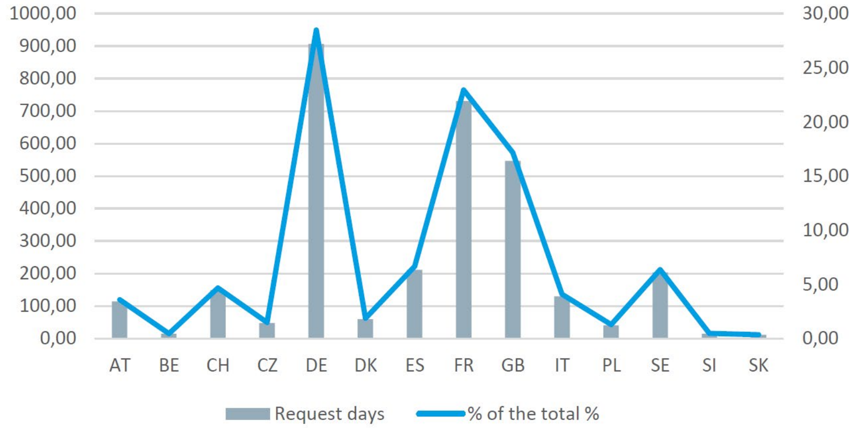
Data public after 2 years embargo period

Industrial beam time:

- Direct access to beam time
- Confidentiality for experiment and data



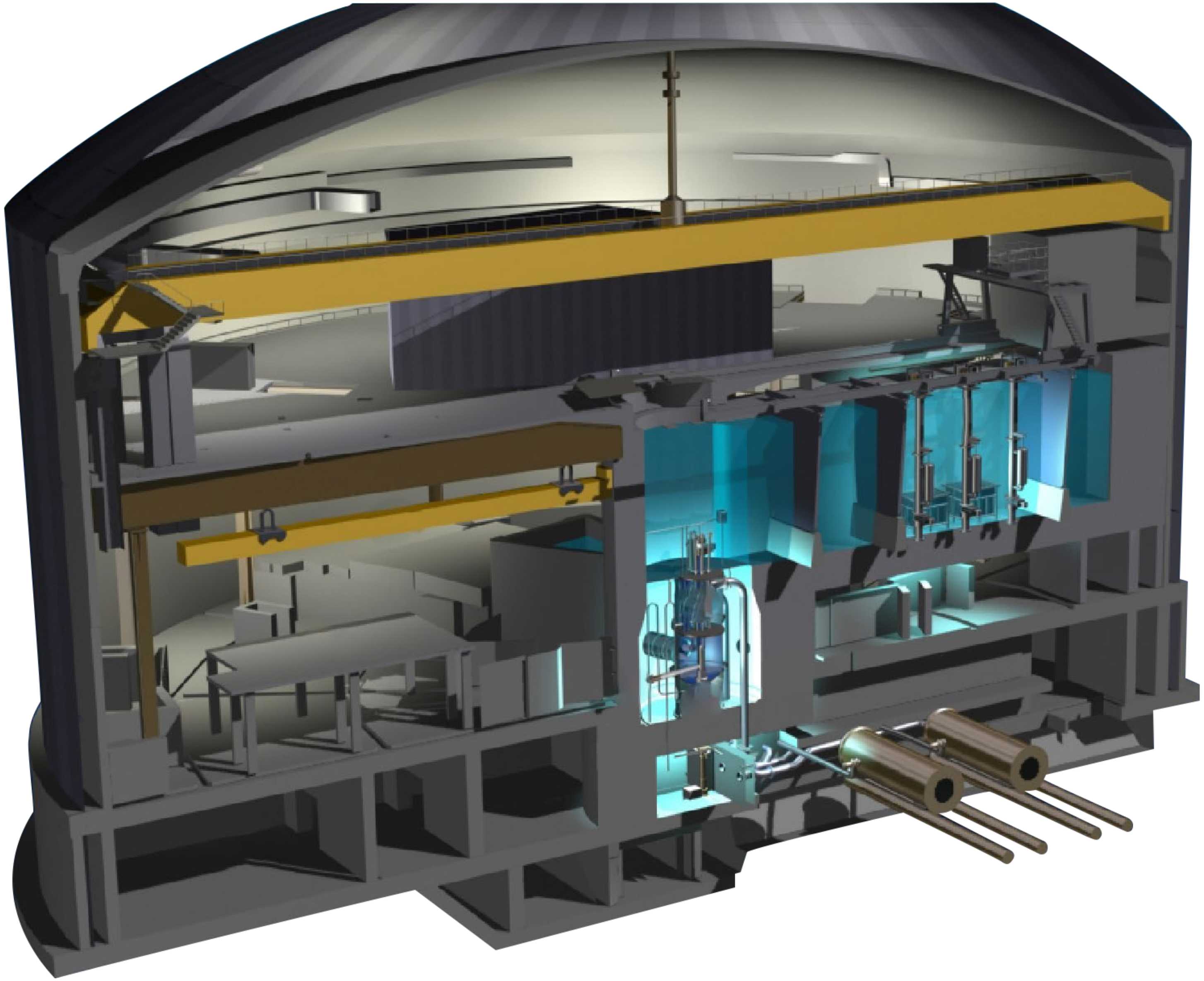


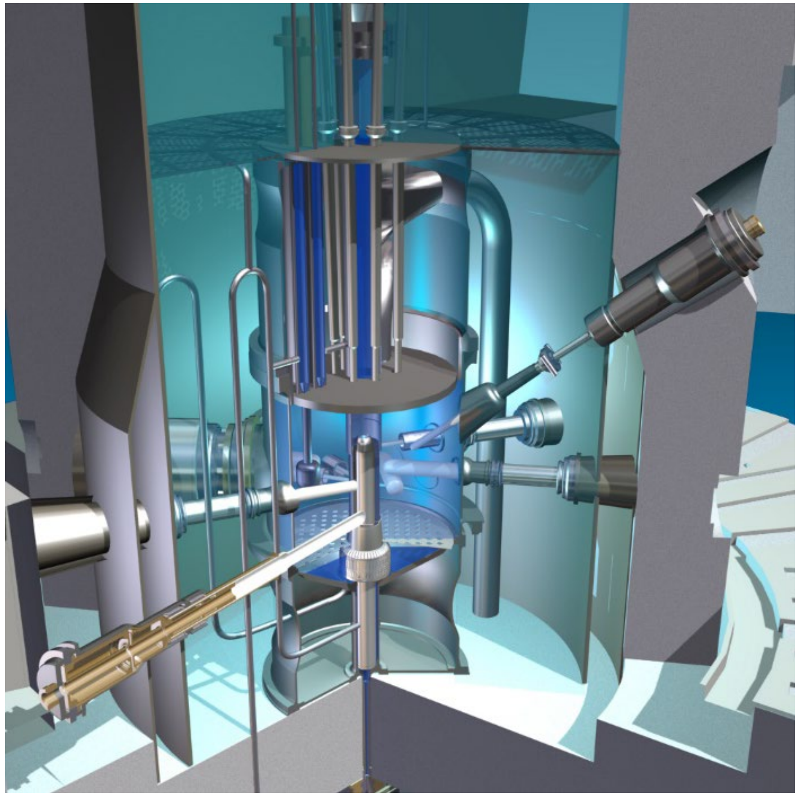


Year					Operating days
2024				POLAR CRANE	110
2025	POLAR CRANE			CRANE C	160
2026	CRANE C				160
2027					160/170
2028					160/170
2029					160/170
2030					160/170

THE ILL REACTOR

NEUTRONS
FOR SOCIETY





A neutron source generating

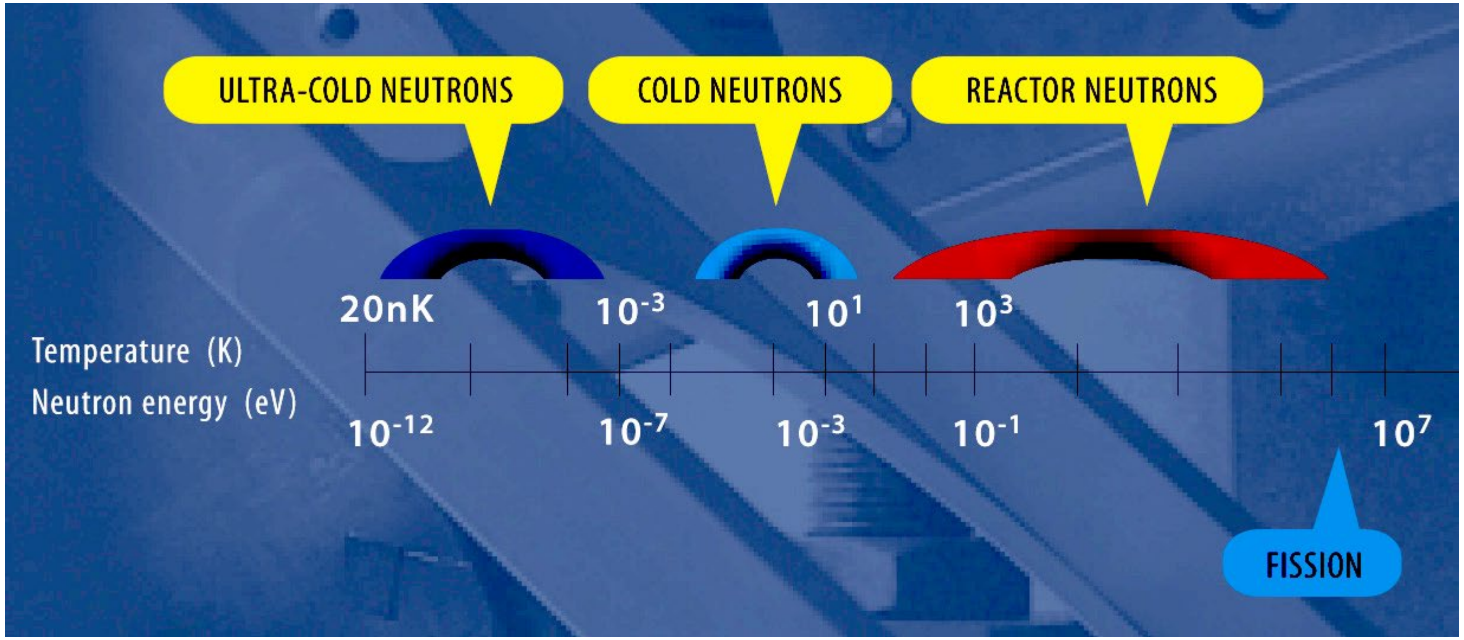
~10^{15} neutrons/cm^2/sec

at a max power of 57 MW

The neutron

As a probe

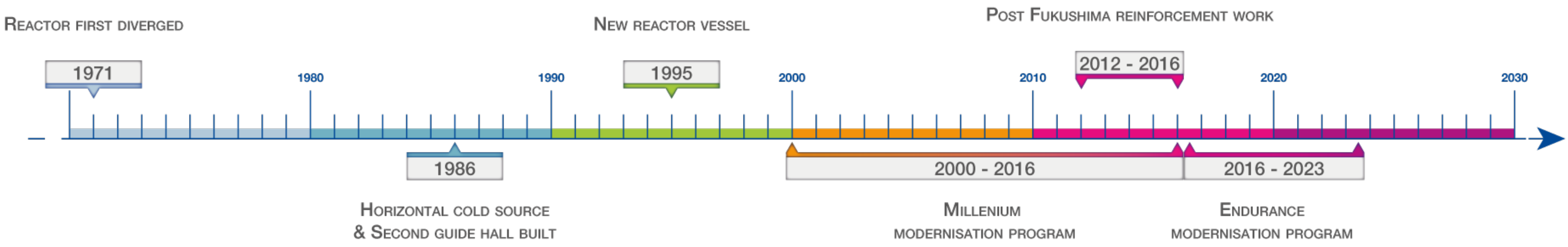
	Energy	Temperature (K)	Wavelength (nm)	velocity (m/s)
Ultra cold neutrons	< 10 μeV	< 0.05	> 30	< 15
Cold neutrons	100 - 5000 μeV	1 - 60	0.4 - 3	150 - 1000
Thermal neutrons	5 - 50 meV	60 - 600	0.13 - 0.4	1000 - 4000
Hot neutrons	0.05 - 0.5 eV	600 - 6000	0.04 - 0.13	4000 - 10000



Modernisation programmes

NEUTRONS FOR SOCIETY

Replacement of critical reactor components, H1-H2 beamtube and final phase of Endurance instrument upgrade program with two new large guides systems (H24 and H15)



Millenium: 85 M € invested in 25 new or upgraded instruments, providing x25 gains in efficiency

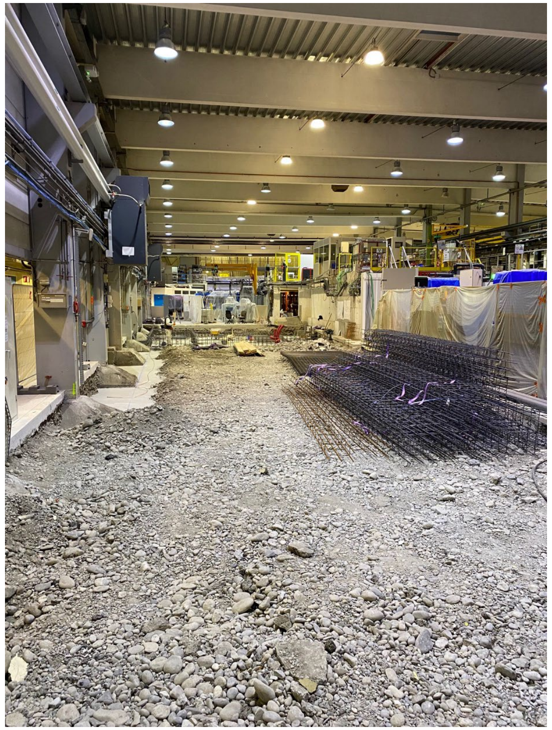
Endurance: 60 M € invested in 20 new or upgraded instruments, improved data treatment software, new sample environment

NEUTRONS FOR SOCIETY

H1-H2 Long Shutdown

- high complexity of the H1-H2 shutdown works, tight schedule and interdependent sequences of works
- limitations imposed by the covid pandemic such as a reduced number of staff on-site
- H1-H2 *project,* including the rollout of Endurance instrumentation and infrastructure

maximum destruction February 2022



ILL7 guide hall - Chartreuse

ILL7 guide hall - Vercors

ILL22 guide hall - NEXT

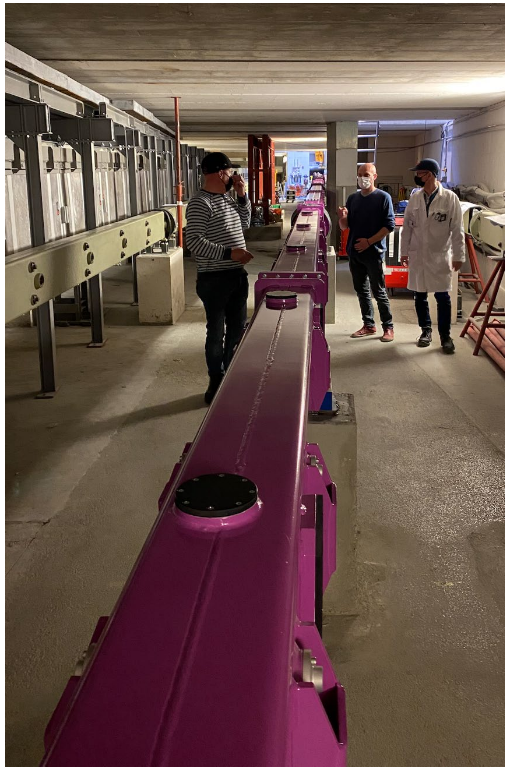
ILL5 H1H2

NEUTRONS FOR SOCIETY

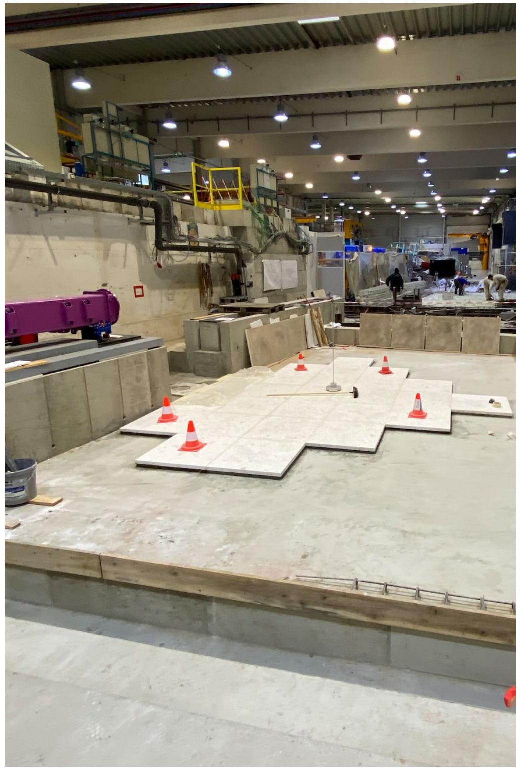
H1-H2 Long Shutdown

- high complexity of the H1-H2 shutdown works, tight schedule and interdependent sequences of works
- limitations imposed by the covid pandemic such as a reduced number of staff on-site
- H1-H2 *project,* including the rollout of Endurance instrumentation and infrastructure

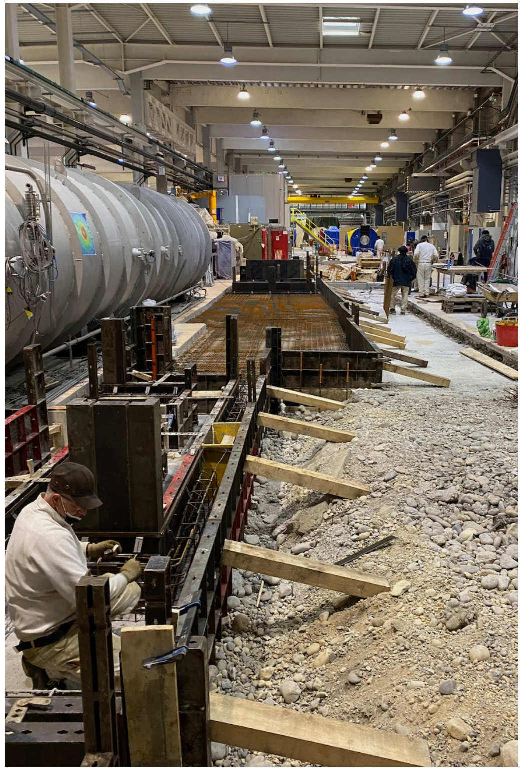
April 2022



ILL7 H24 guide



ILL7 guide hall – D10+



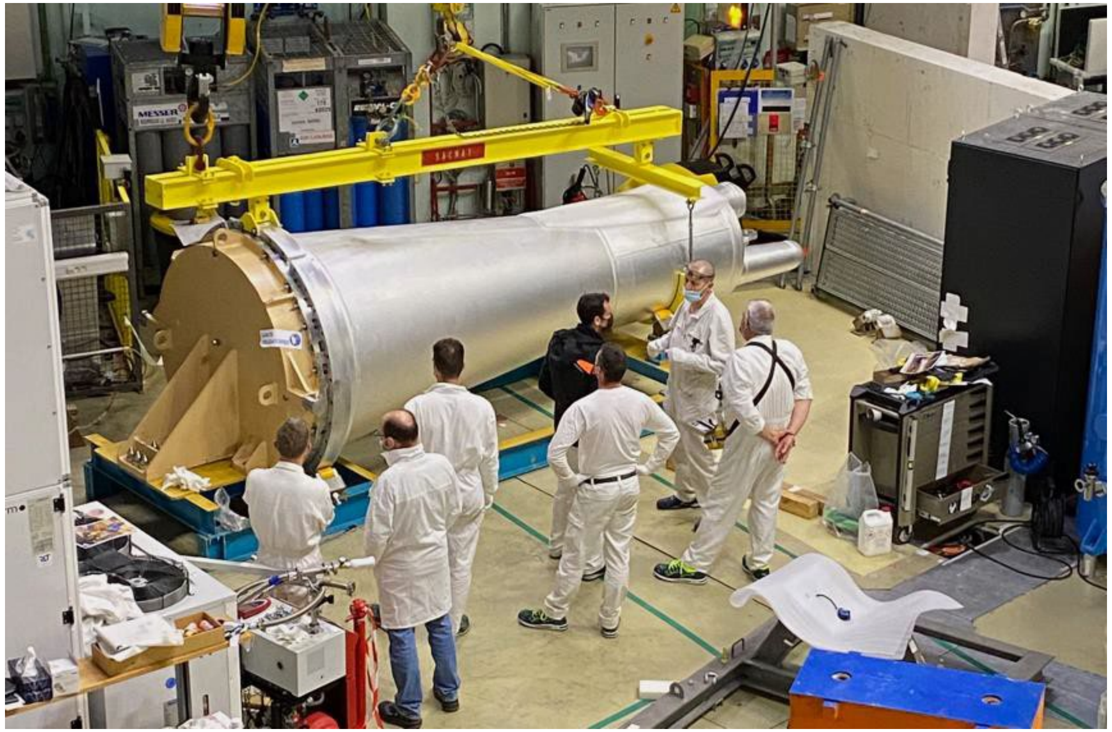
ILL7 guide hall - SAM

ILL22 guide hall – D16

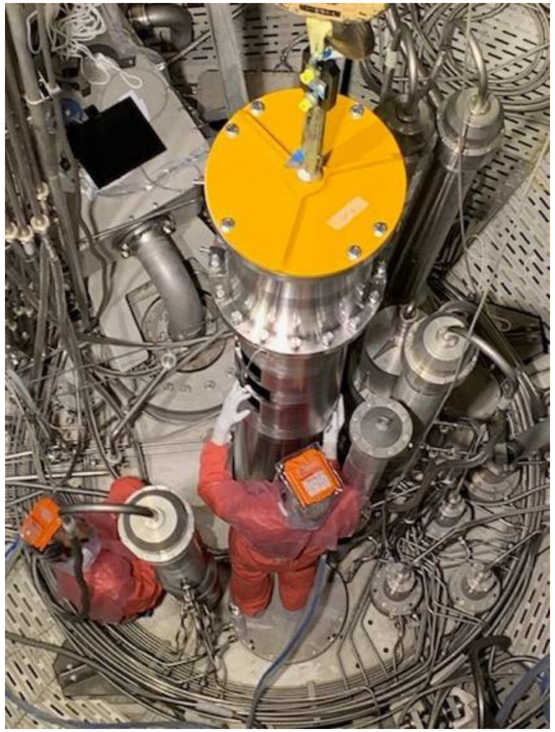
NEUTRONS FOR SOCIETY

H1-H2 Long Shutdown and ILL20-23

- excellent, comprehensive project management; creative adaption of planning and execution
- good ILL working spirit, high internal mobility; high efficiency of mounting operations
- reactor restart on March 1th , 2023 – on time and within budget



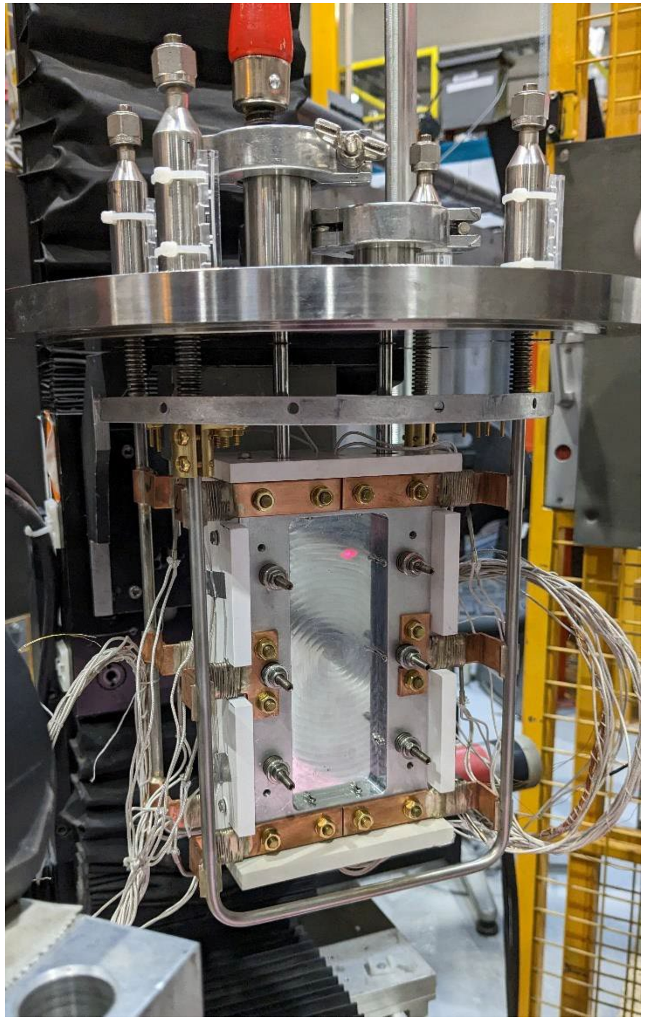
April 2022: installation of H1-H2 beamtube



May: replacement of chimney

H24 Endurance CRG Instruments

in commissioning: XtremeD – IN13 backscattering



alignment of IN13 mono on T13c

- XtremeD: a new diffractometer for extreme sample environments: magnetic field, pressure, levitation, …
- IN13: new temperature gradient monochromator at the thermal backscattering instrument

NEUTRONS FOR SOCIETY

Endurance Instruments

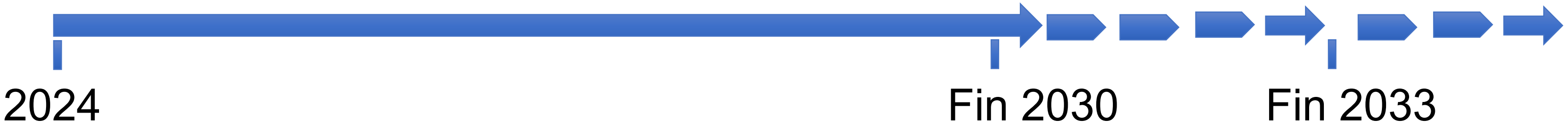
H15 cold-neutron guide + instruments: T3, D(00)7, D11+, SAM, SHARP+

March 2023

- H15 guide installation continues during 2023
- project proceeds as planned

Ch. Dewhurst, B. Giroud, G. Manzin, J. Beaucour

TODAY: ILL STRATEGY – STRATEGY WORKING GROUP



Core Priorities as determined by working group:

- Continuing the safe and compliant operation of the reactor
- Delivering high-quality beam time
- Optimally exploiting the increased performance following ENDURANCE
- Maximizing science output
- Consolidating the instrument suite, based on its instrument review
- Supporting in-house research and development
- Strengthening the user community
- Attracting staff
- Reinforcing knowledge transfer
- Educating the next generation of neutron researchers (PhD & Post-docs)

→ Development of a **Science Strategy** for ILL with the Scientific Council

Welcome to the Summer School 2023 and Welcome to the ILL