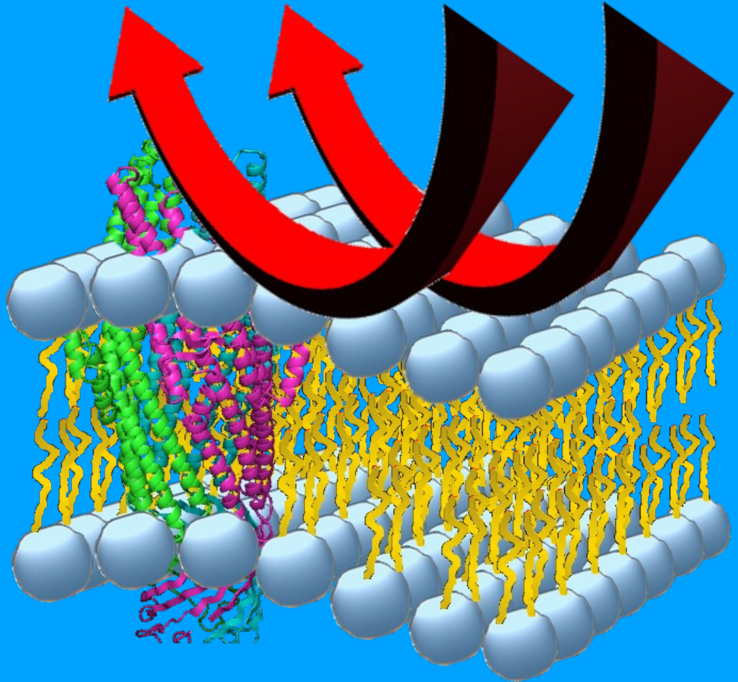
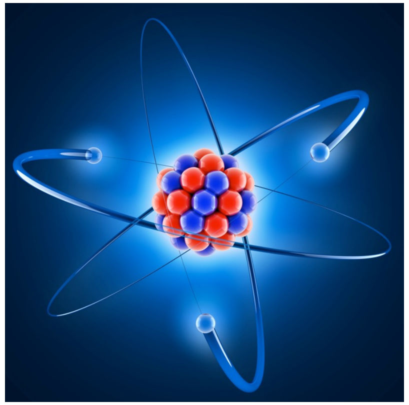
Neutrons for soft and biological matter

Giovanna Fragneto
European Spallation Source ERIC





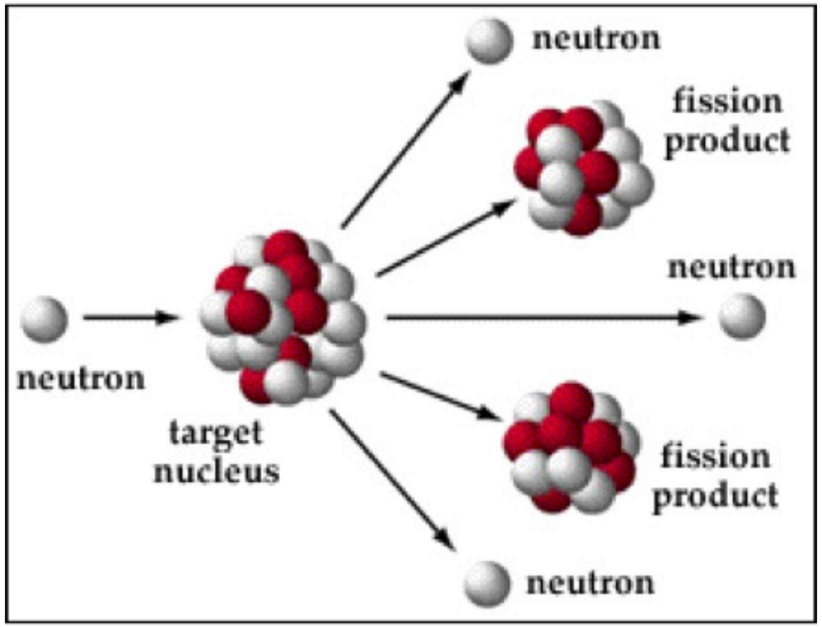
Neutrons

- Subatomic particles found in atomic nuclei
- Discovered in 1932 by Chadwick
- Mass slightly higher than that of protons (~1.67×10^{-27} kg)
- Uncharged
- Lifetime ~15 mins
- Wave-particle duality ($v = 2.2$ km/s at RT)
- Wavelength similar to atomic distances ($\lambda = 0.18$ nm at RT)
- Energies similar to motion of molecules (~ 0.025 eV)
- Possess a spin

Generating neutrons : Fission

Element (e.g. ^{235}U) that readily decays with neutron release and upon bombardment with a neutron then splits to release more neutrons generating a chain reaction

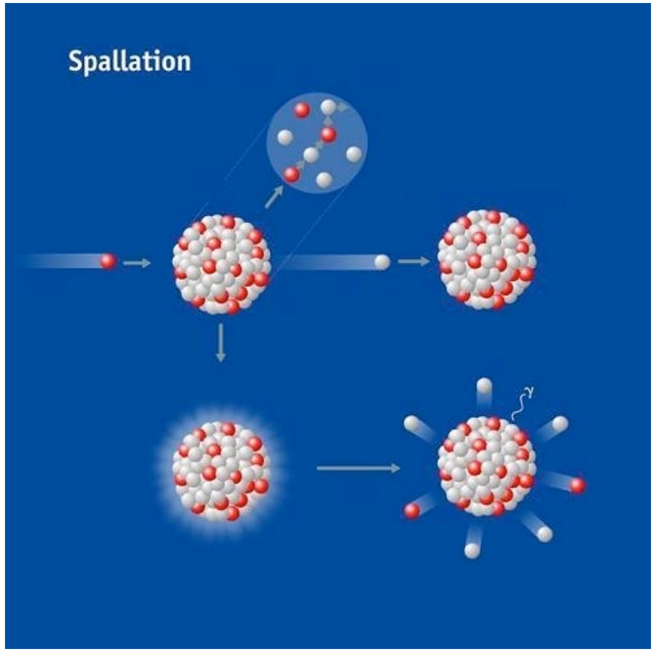
In nuclear reactors, the rate of the reaction is controlled with absorbing materials that remove some of the produced neutrons

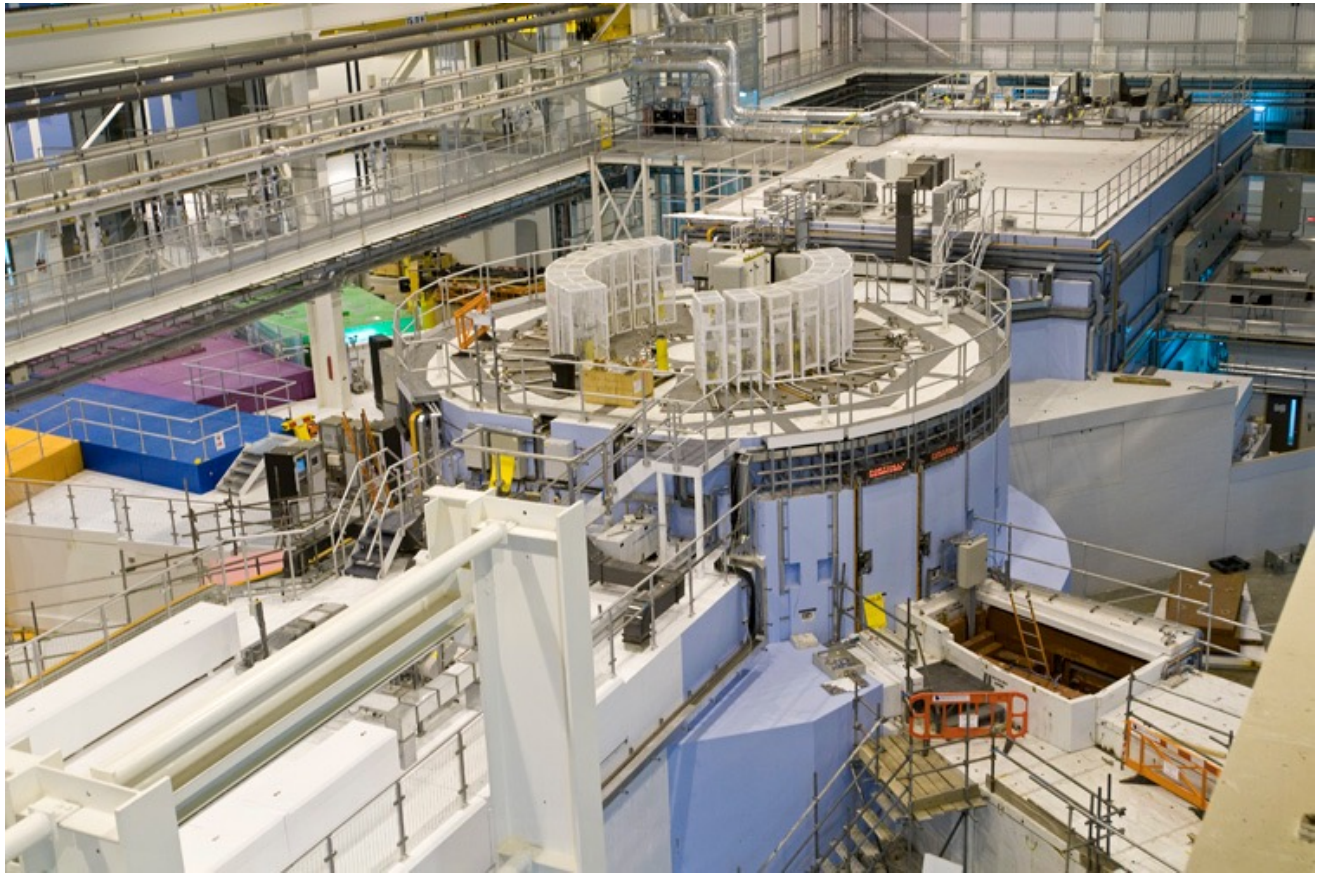


Generating neutrons : Spallation

A high energy pulsed electron or proton beam is used to bombard a heavy metal target.

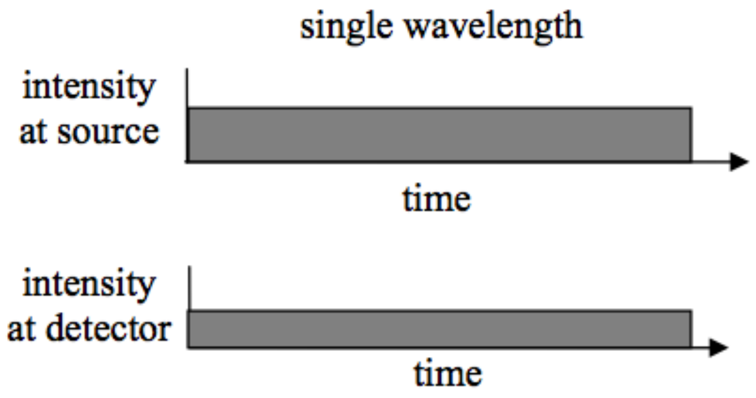
20 - 30 neutrons produced per proton.



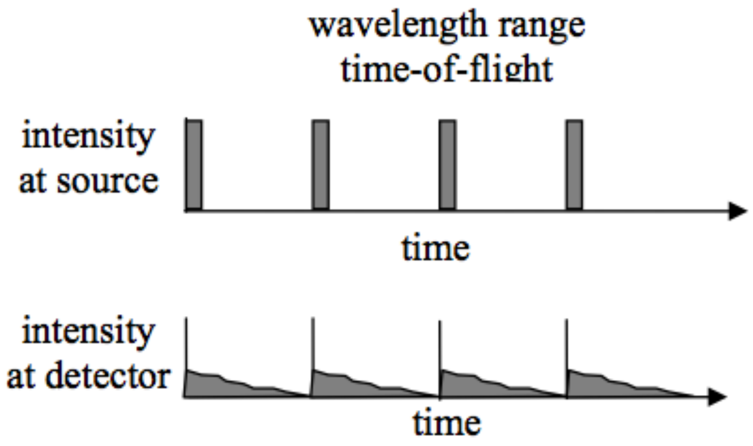


ISIS Facility, Rutherford-Appleton Lab, UK

"Monochromatic" vs Time-of-flight
Reactor versus spallation



Some of the neutrons all of the time



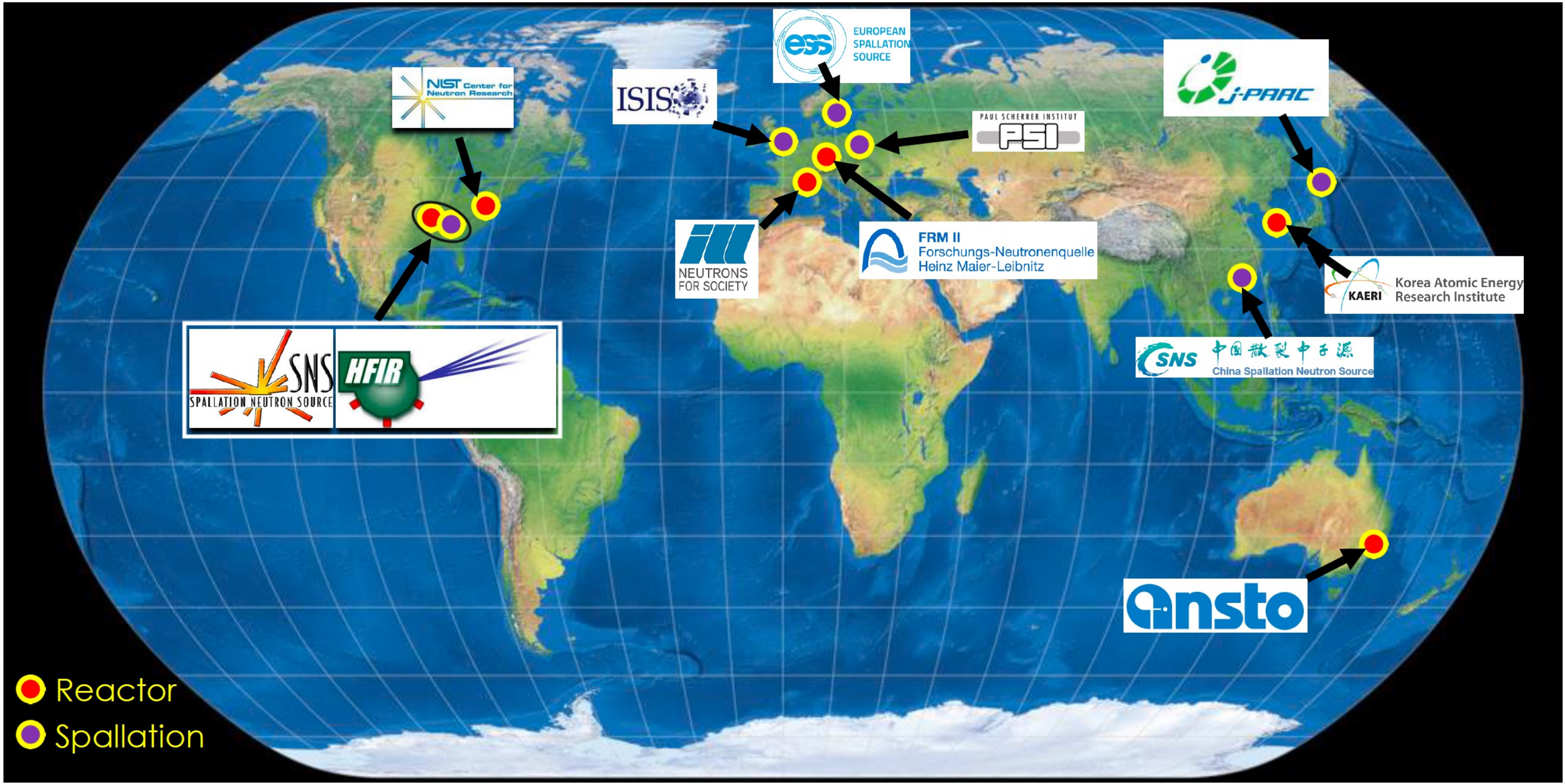
All of the neutrons some of the time

$$Q = \frac{4\pi}{\lambda} sin\theta$$

Varying **angle** to access different Q values

Varying **angle and wavelength** to access different Q values

Neutron Sources around the world



Global neutron source landscape

Continuous Sources

Fission reactors :

ILL (France) – 58 MW thermal, 50-day fuel cycle, 4 cycles / year

HFIR (USA) – 83 MW thermal, 23-day fuel cycle, 6-7 cycles / year

Cyclotron *accelerator-based*:

SINQ (PSI/Switzerland) – 1,4 MW proton beam power producing muons and spallation neutrons

Pulsed Sources

Long-pulse driven by linear accelerator *pulse length 2,86* ***milli****seconds*

ESS (SE/DK) – 14 Hz, 0,8 – 2 GeV, 2-5 MW proton beam power

ESS bridges the space between continuous and short-pulsed sources and opens up new techniques and opportunities

Short-pulse driven by rapid-cycling synchrotron accelerators (RCS)*, all beam structures less than 1* ***micro****second*

J-PARC MLF (Japan) – 25 Hz, 3 GeV RCS up to 1 MW proton beam power – **Hg** target

ISIS (RAL/UK) – 50 Hz, 0,8 GeV RCS up to 200 kW proton beam power providing muons and spallation neutrons divided between TS-1 (40 Hz) and TS-2 (10 Hz) – **W** target

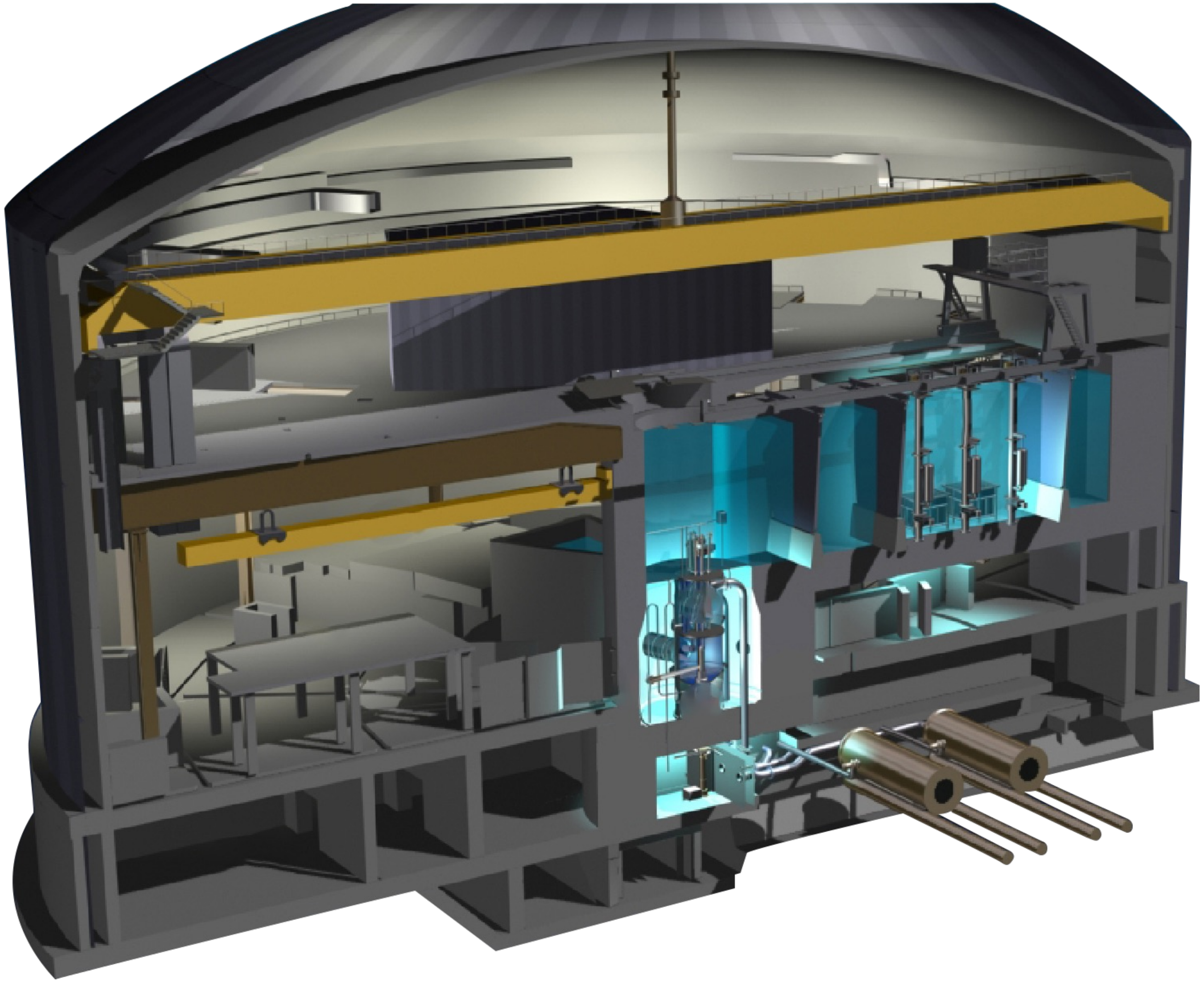
CSNS (China) – 25 Hz, 1,6 GeV RCS up to 100 kw proton beam power **–** **W** target

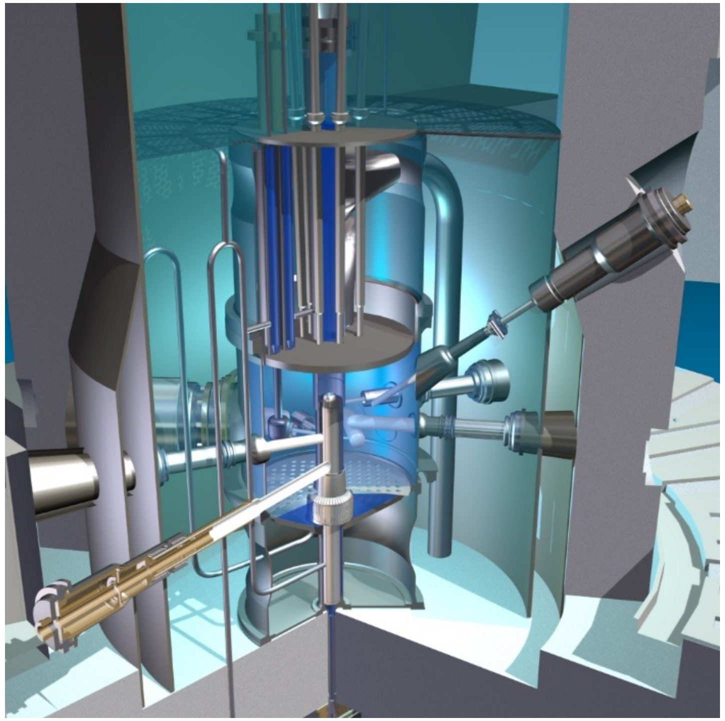
Short-pulse driven by linear accelerators and accumulator rings*, all beam structures less than 1* ***micro****second*

SNS (USA) – 60 Hz, 1,05 GeV 1,7 MW proton beam power - **Hg** target

LANSCE (USA) – 20 Hz, 0,8 GeV 80 kW proton beam power – **W** target

The ILL benefits from the world's most intense continuous neutron source operating since 1971



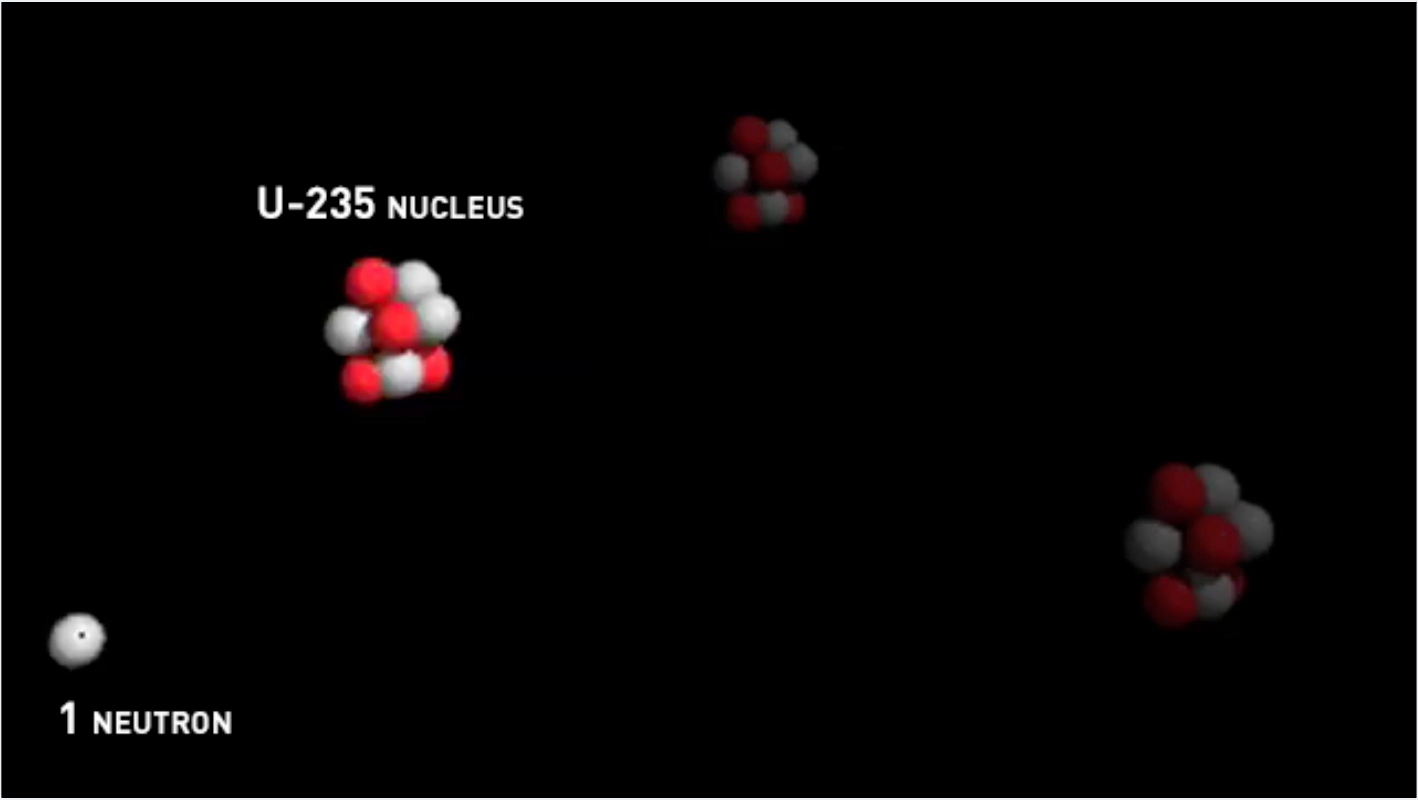


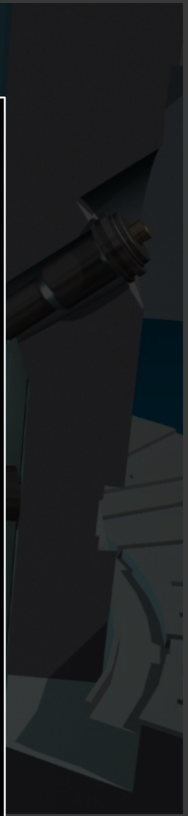
A neutron source generating

5 x 10^{18} fast neutrons/sec

at a max power of 58 MW

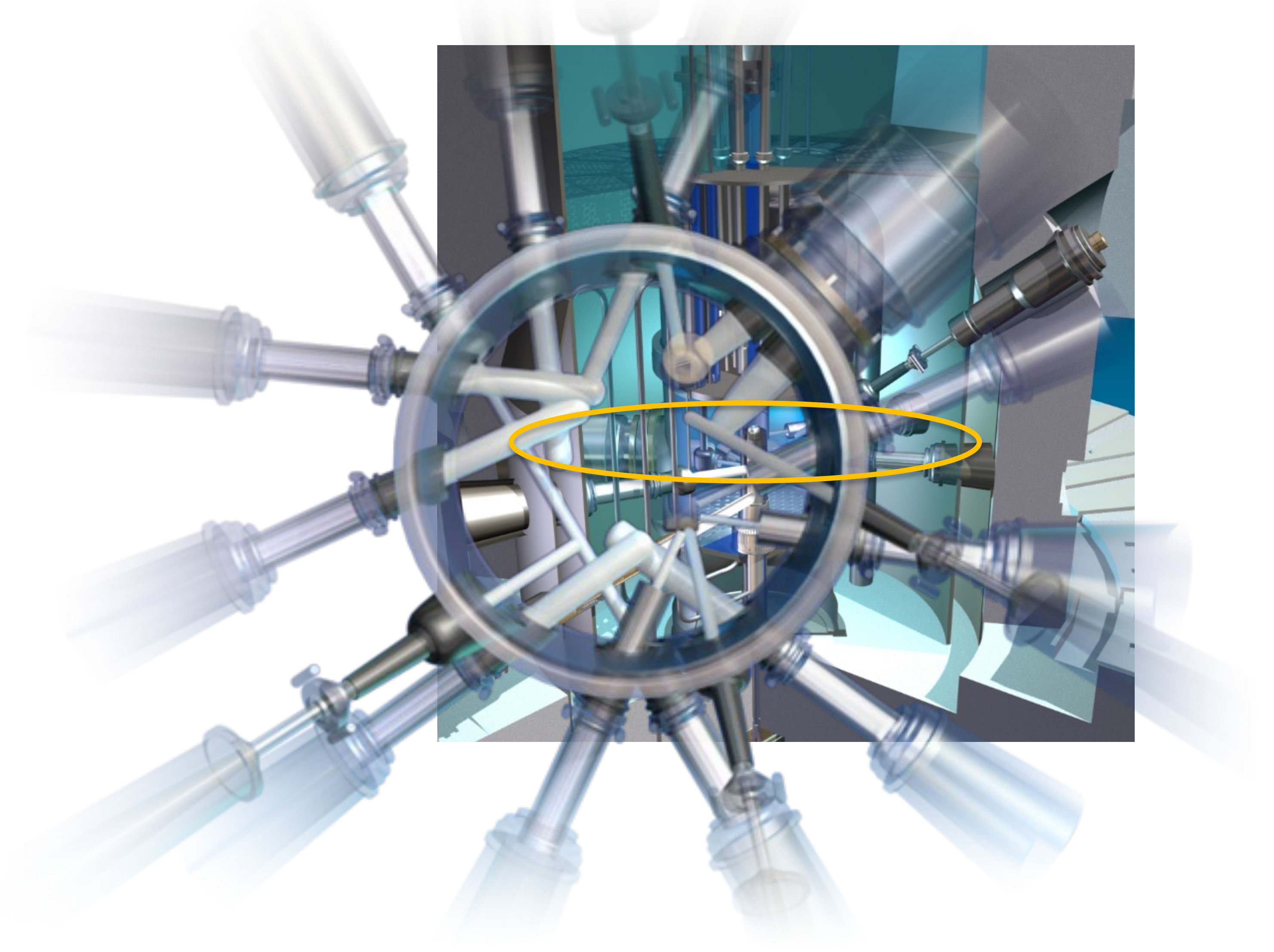
NEUTRONS PRODUCTION BY CONTROLLED CHAIN REACTIO



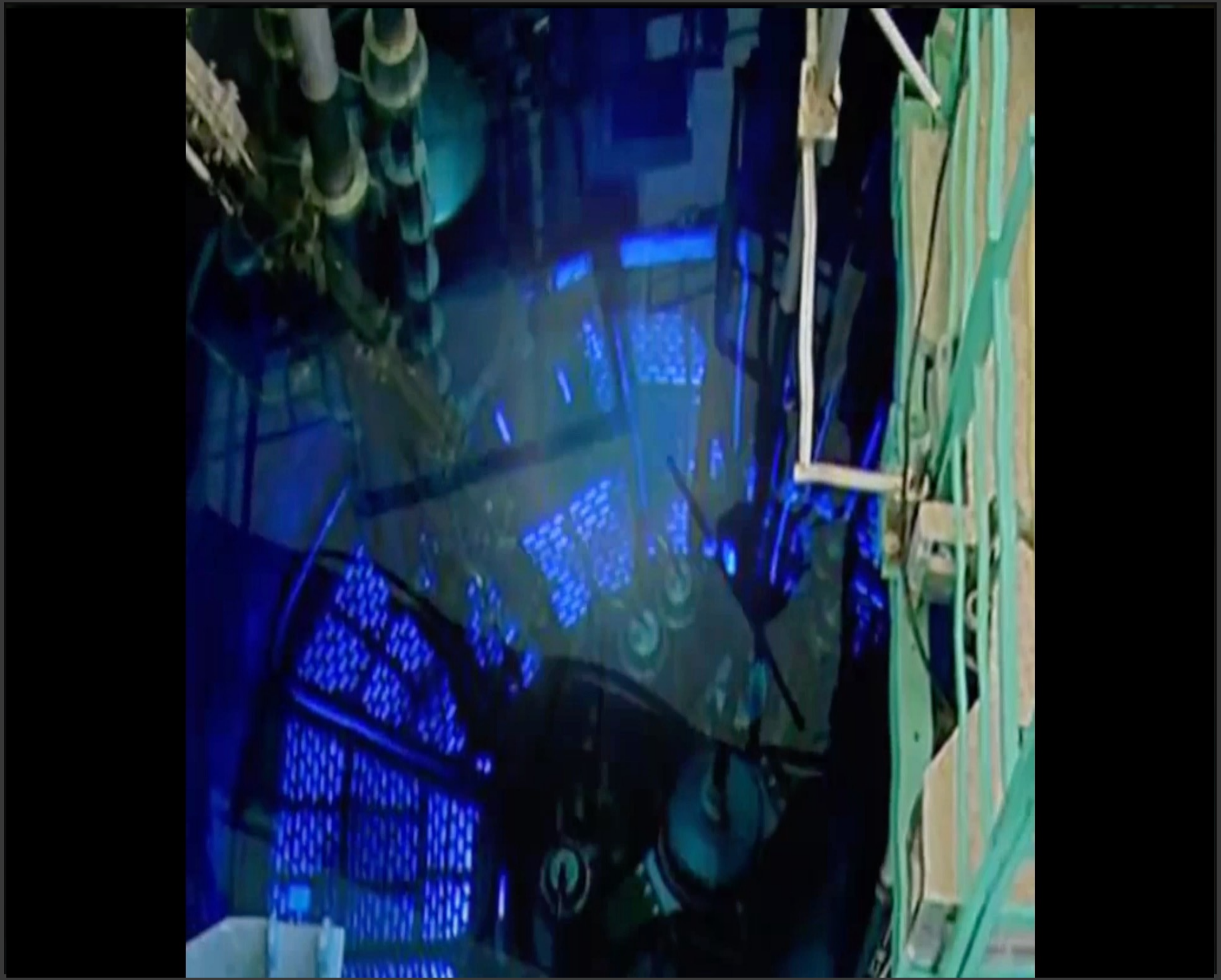


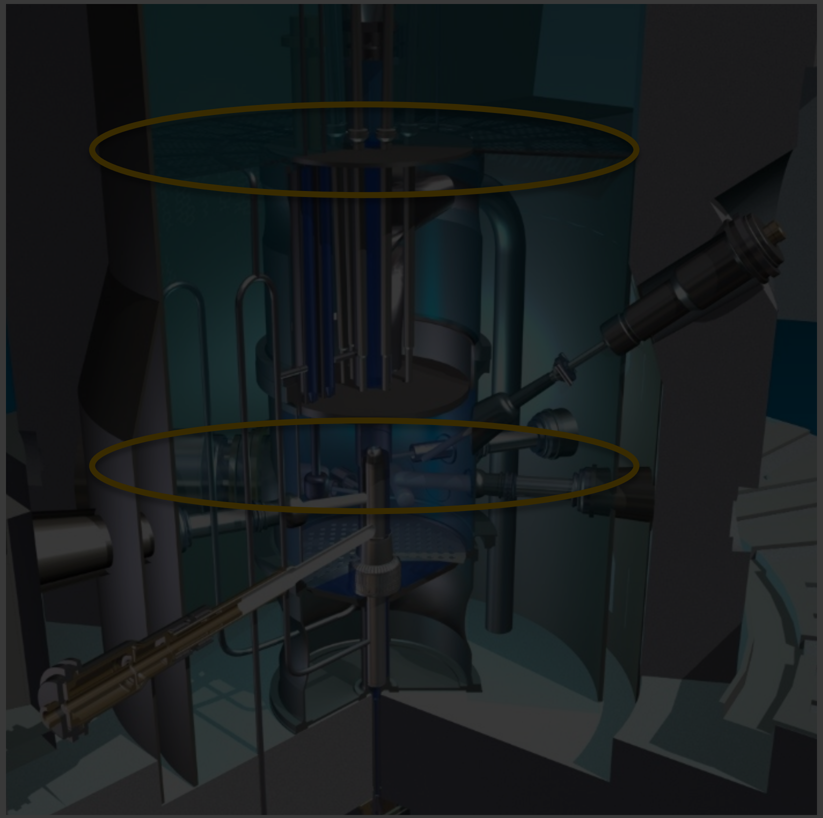
A neutron source generating
5×10^{18} fast neutrons/sec
at a max power of 58 MW

HOW NEUTRONS ARE EXTRACTED AND GUIDED



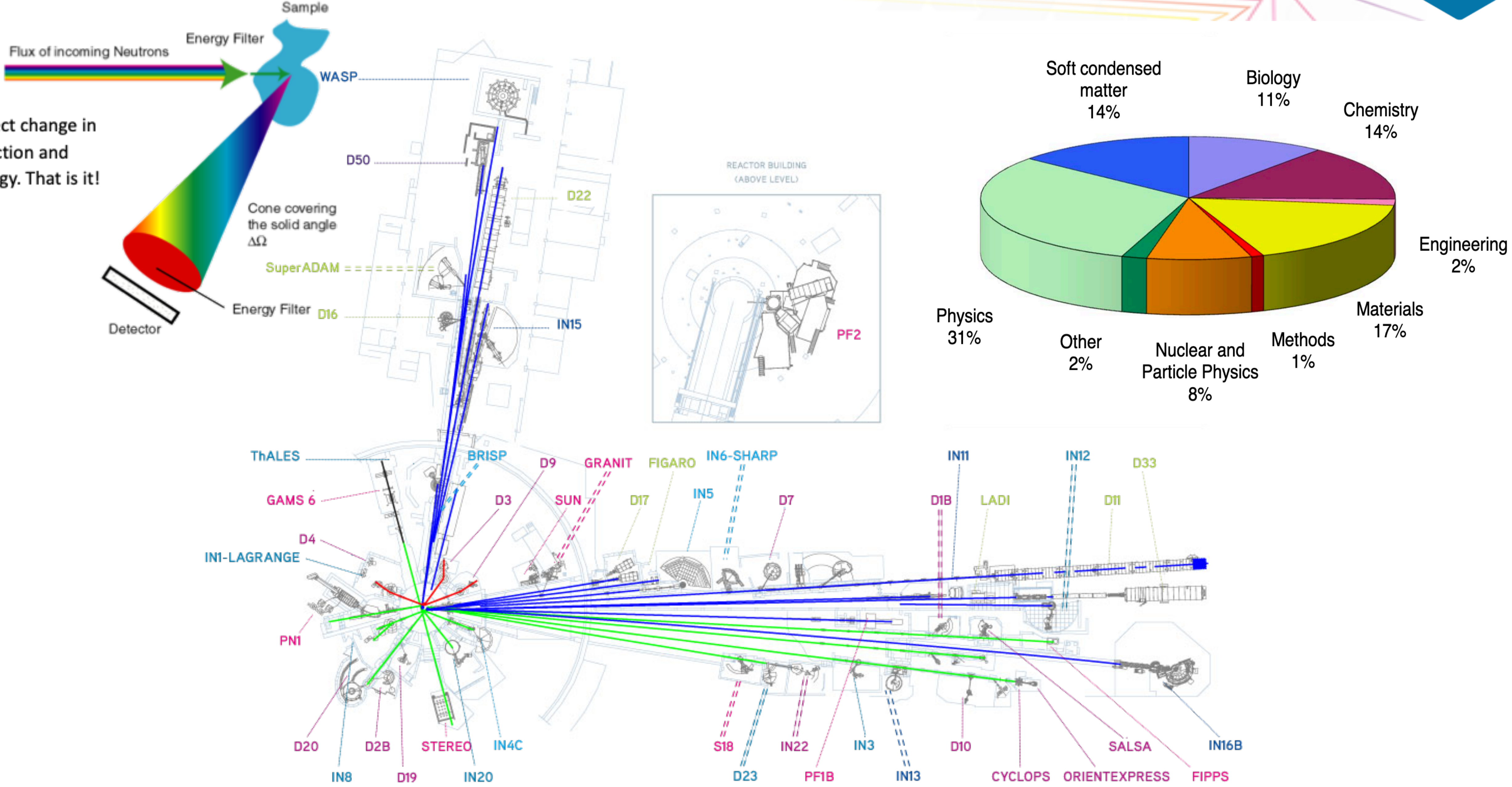
How neutrons feed the instrument suite



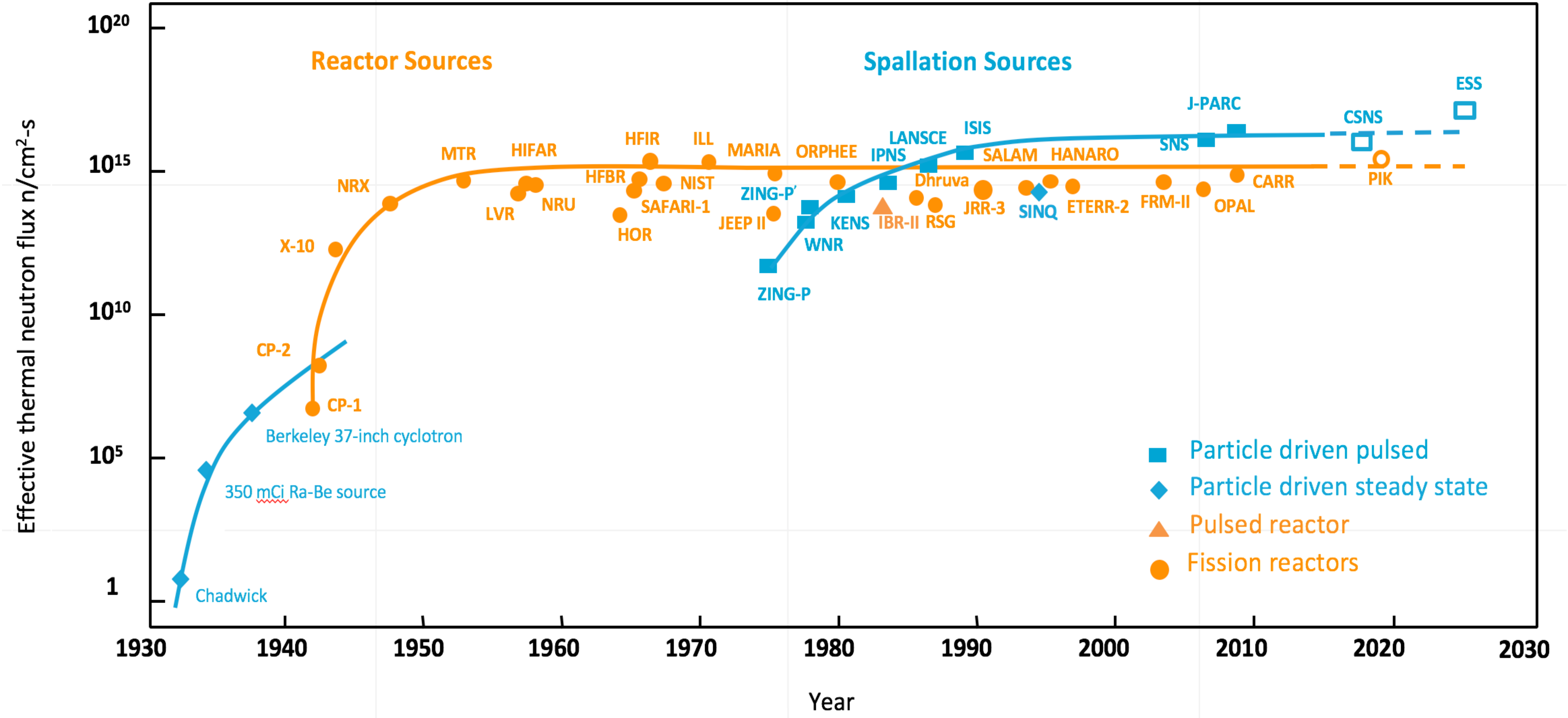


THE ILL'S INSTRUMENT SUITE

Detect change in direction and energy. That is it!



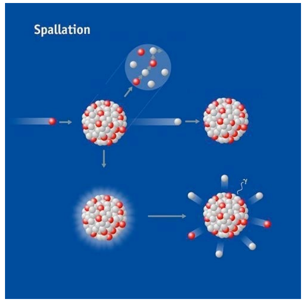
Neutron Source Brightness

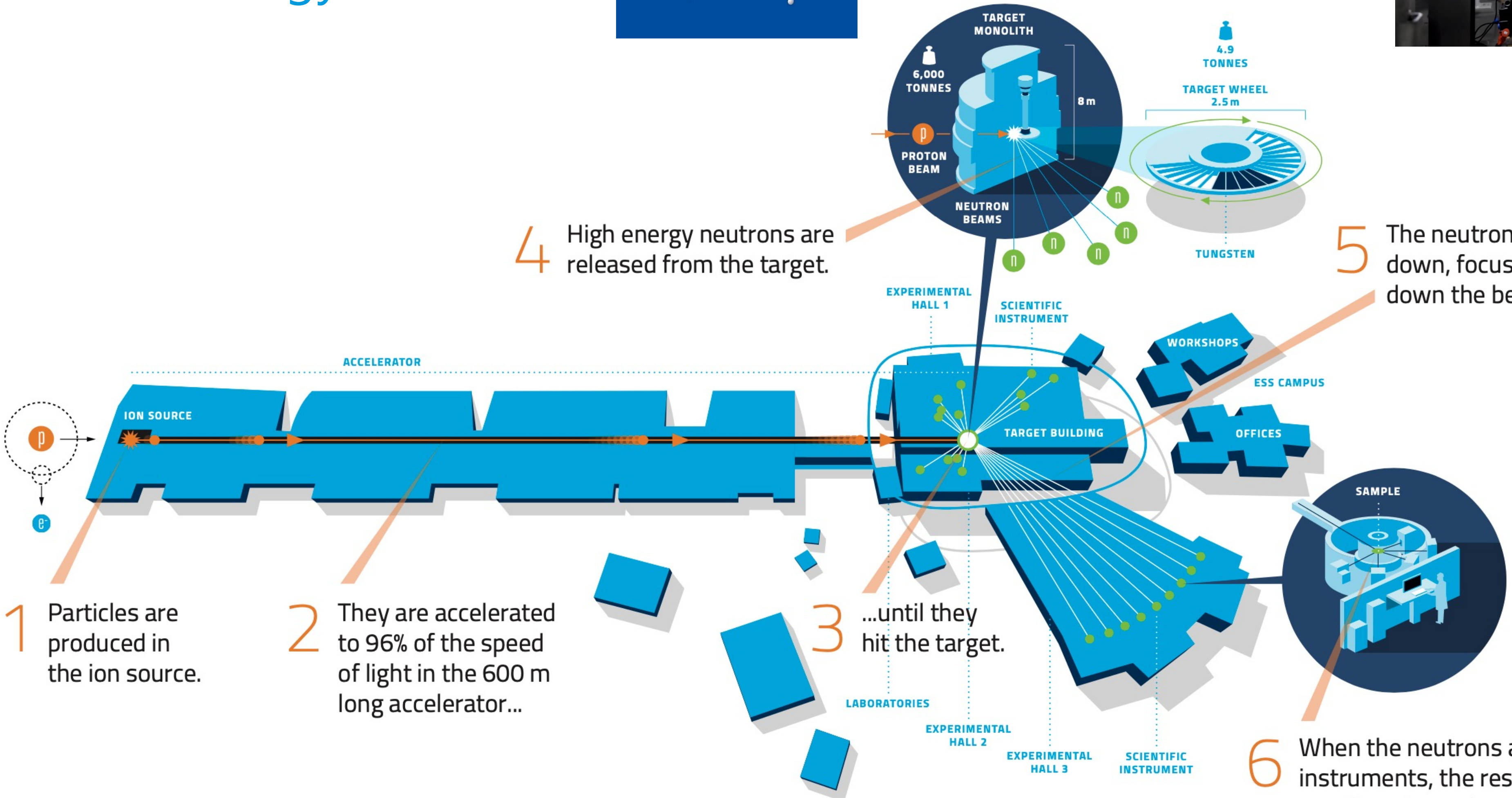


(Updated from *Neutron Scattering*, K. Skold and D. L. Price, eds., Academic Press, 1986)

How ESS works

The technology





1 Particles are produced in the ion source.

2 They are accelerated to 96% of the speed of light in the 600 m long accelerator…

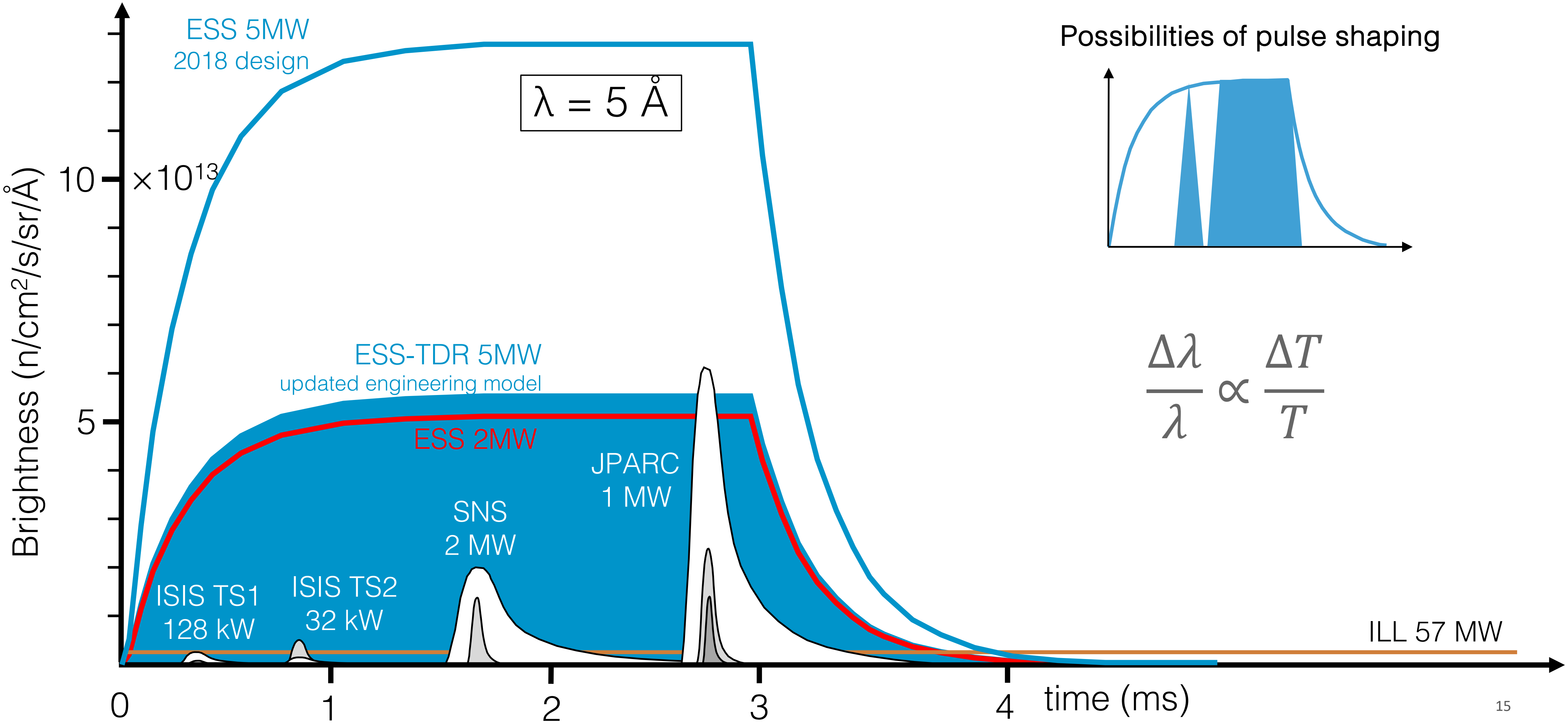
3 …until they hit the target.

4 High energy neutrons are released from the target.

5 The neutrons are slowed down, focused and sent down the beamlines.

6 When the neutrons arrive at the instruments, the researchers can use them to explore materials down to an atomic level.

Long-pulse Performance and Flexibility



Possibilities of pulse shaping

$$\frac{\Delta\lambda}{\lambda} \propto \frac{\Delta T}{T}$$

Time-of-Flight Neutron Scattering

de Broglie relation (tof (muS) = 252.78*λ(Å)*L(m))

We use time-distance diagrams to visualise chopper operation.

Slope of lines is neutron velocity = wavelength

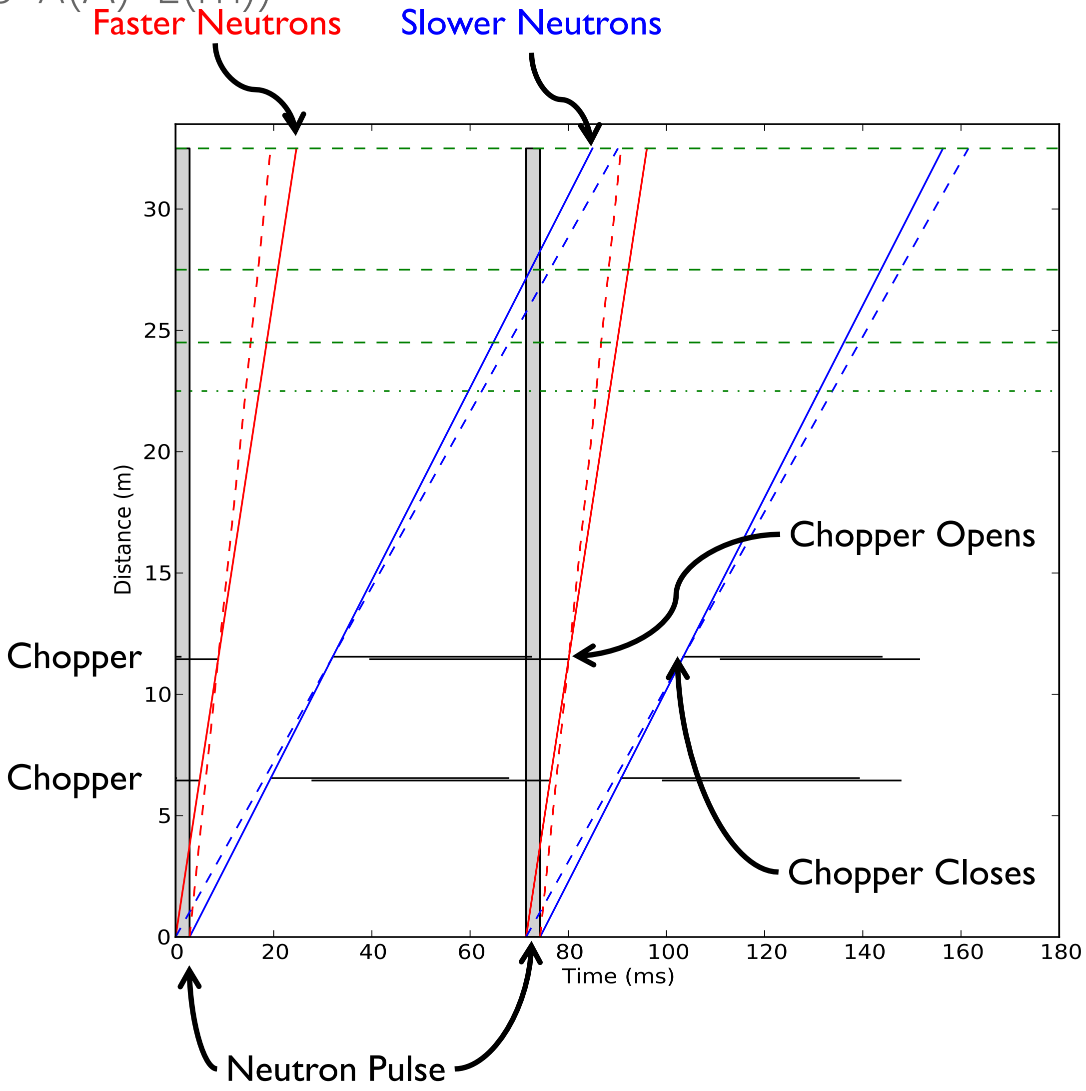
$$\tau = \frac{L}{v}$$

$$\lambda = \frac{h}{mv}$$

$$\tau = \frac{m}{h} L\lambda$$

$$\tau[ms] = \frac{L[m]\lambda[\mathring{A}]}{3.956}$$

$$\Delta\tau[ms] = \frac{L[m]\Delta\lambda[\mathring{A}]}{3.956}$$



Spallation and time of flight at ESS
Broad energy range from spallation & moderation process
Effective for 0.2-200 meV.

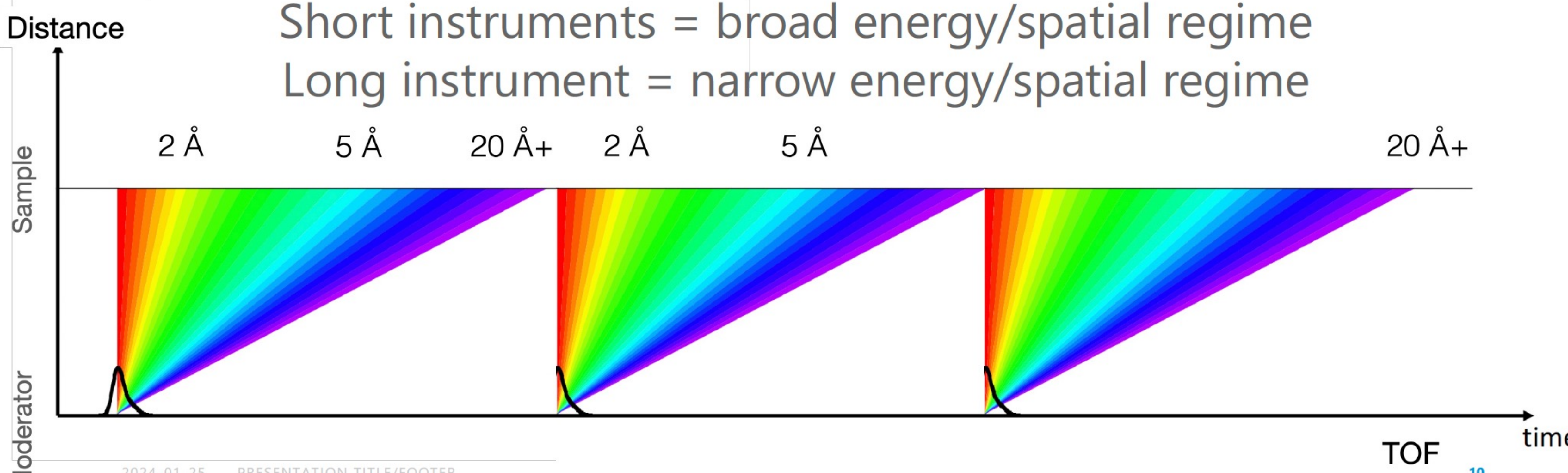
Length of instruments determined by science case.

14 Hz pulses. $\Delta T \cong 71$ ms

1) Short instruments = broad $\Delta\lambda$, long instrument = narrow $\Delta\lambda$

Short instruments = broad energy/spatial regime

Long instrument = narrow energy/spatial regime



Neutron Instruments

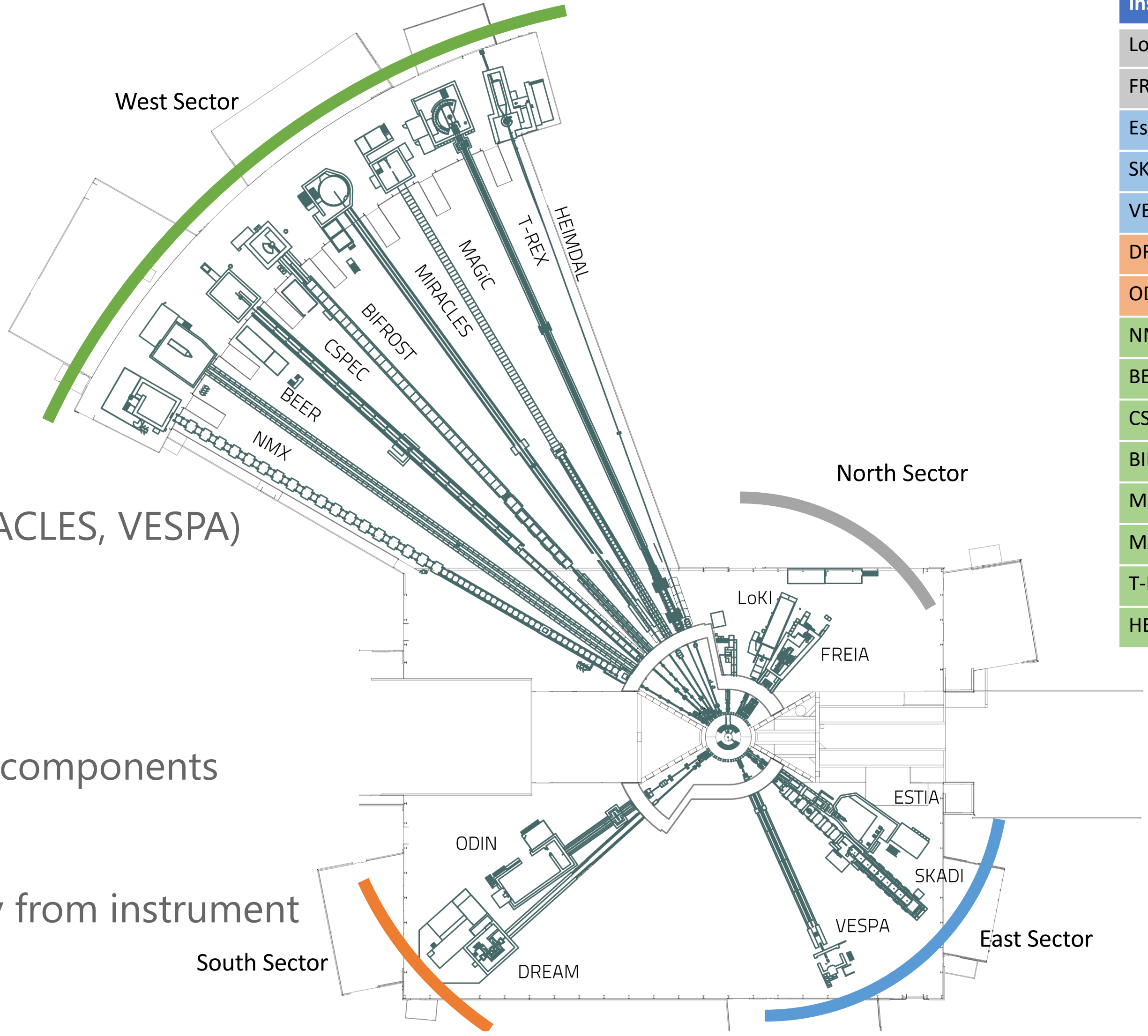
Andersen, K. H.; Argyriou, D. N.; Jackson, A. J. et al. The Instrument Suite of the European Spallation Source. *Nuclear Instruments and Methods in Physics Research Section A:* **2020**, *957*, 163402. https://doi.org/10.1016/j.nima.2020.163402.

15 instruments + Test Beamline

Diffractometers (DREAM, MAGiC, HEIMDAL)
SANS (LoKI, SKADI)
Reflectometers (Estia, FREIA)
Imaging (ODIN)
Engineering Diffraction (BEER)
Macromolecular Crystallography (NMX)
Spectrometers (CSPEC, T-REX, BIFROST, MIRACLES, VESPA)

Novel detector technologies and geometries
Complex pulse-shaping

Shared neutron bunker – common space for components
Common timing system for facility
Single controls infrastructure (EPICS)
Control and data recording running remotely from instrument



Instrument	Beamport
LoKI	N7
FREIA	N5
Estia	E2
SKADI	E3
VESPA	E7
DREAM	S3
ODIN	S2
NMX	W1
BEER	W2
CSPEC	W3
BIFROST	W4
MIRACLES	W5
MAGiC	W6
T-REX	W7
HEIMDAL	W8

Neutron Instruments for soft/bio science

Andersen, K. H.; Argyriou, D. N.; Jackson, A. J. et al. The Instrument Suite of the European Spallation Source. *Nuclear Instruments and Methods in Physics Research Section A:* **2020**, *957*, 163402. https://doi.org/10.1016/j.nima.2020.163402.

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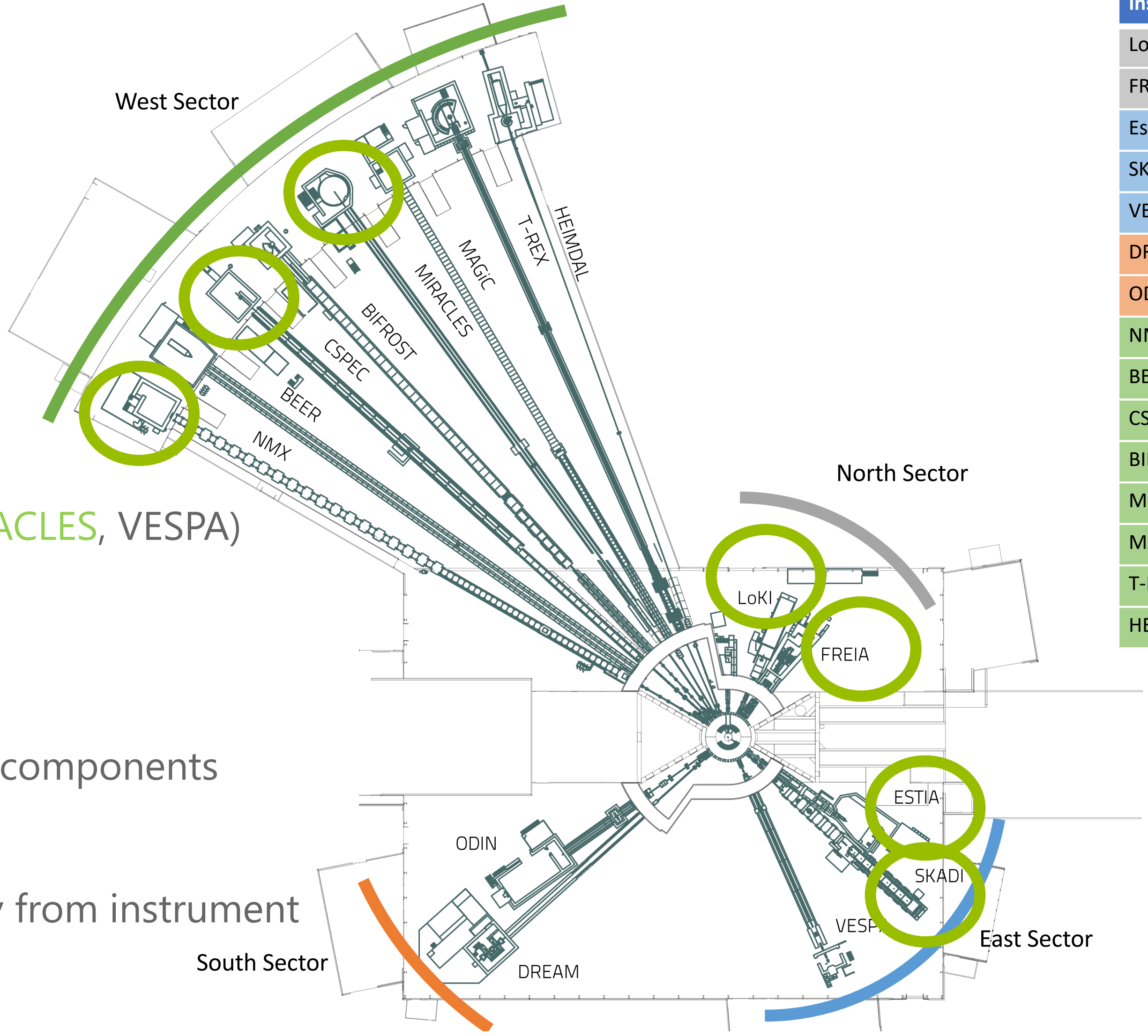

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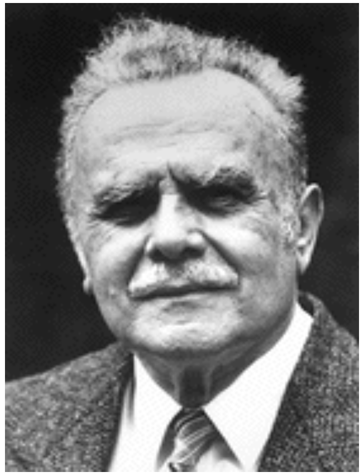
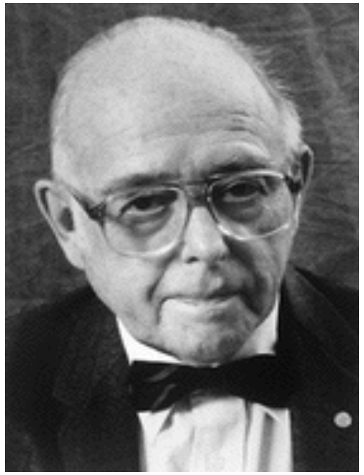
T-REX	W7
HEIMDAL	W8

Nobel Prize in Physics, 1994

A unique probe of ‘where atoms are and what atoms do’ - *to paraphrase the citation for the Nobel Prize in Physics awarded to Brockhouse and Shull in 1994*



Bert Brockhouse
Dynamics
(Neutron Spectroscopy)



Cliff Shull
Structure
(Neutron Diffraction)

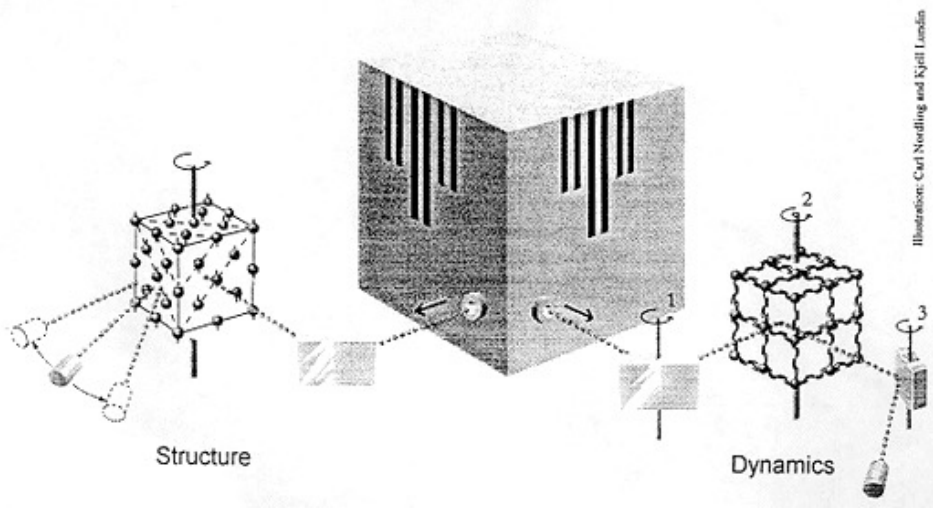
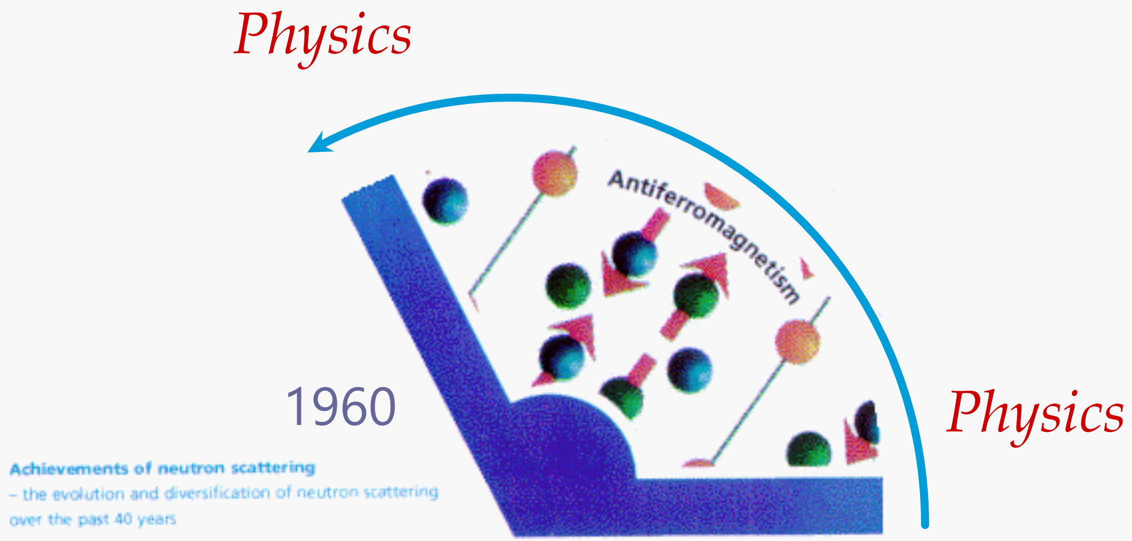


Illustration: Carl Nordling and Kjell Lundin

12 Oct 1994
Press Release

(…) Both methods are based on the use of neutrons flowing out from a nuclear reactor. When the neutrons bounce against (are scattered by) atoms in the sample being investigated, their *directions* change, depending on the atoms’ relative positions. This shows how the atoms are arranged in relation to each other, that is, the structure of the sample. Changes in the neutrons’ *velocity*, however, give information on the atoms’ movements, e.g. their individual and collective oscillations, that is their dynamics.

Science with neutrons



Physics

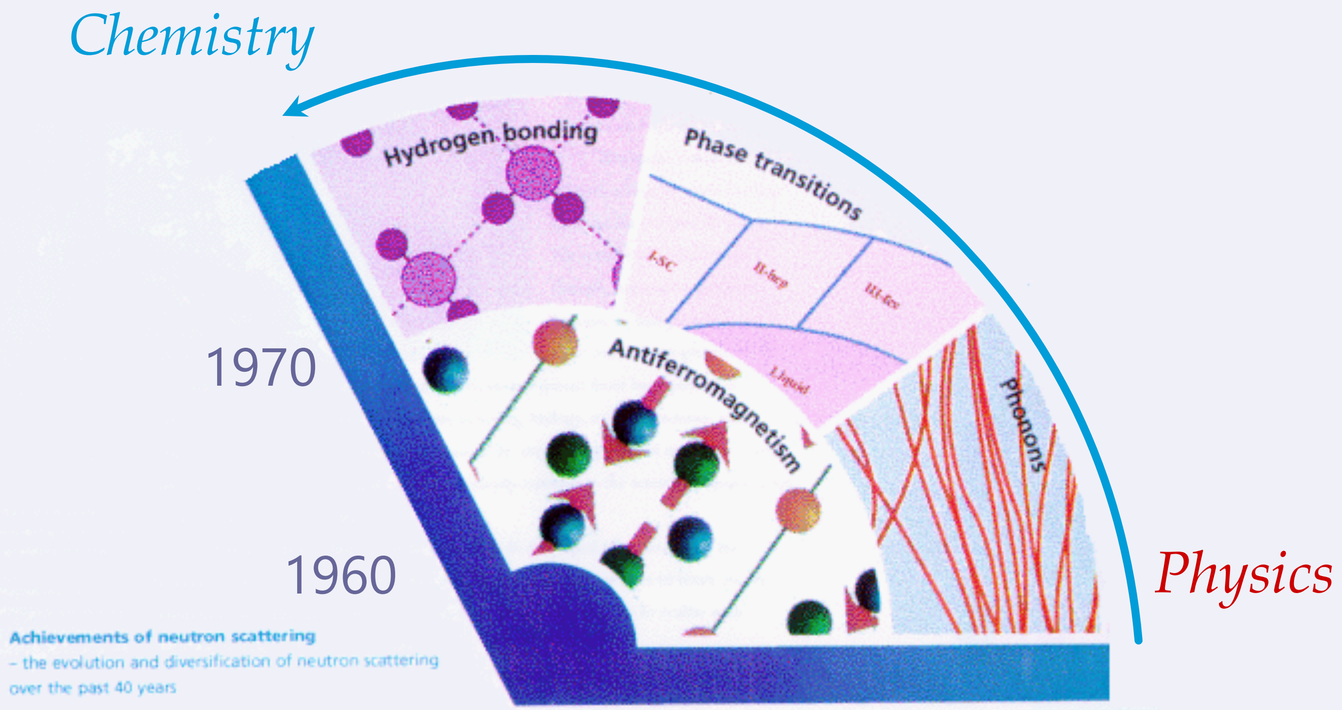
Physics

1960

Achievements of neutron scattering
– the evolution and diversification of neutron scattering over the past 40 years

Courtesy of ISIS

Science with neutrons



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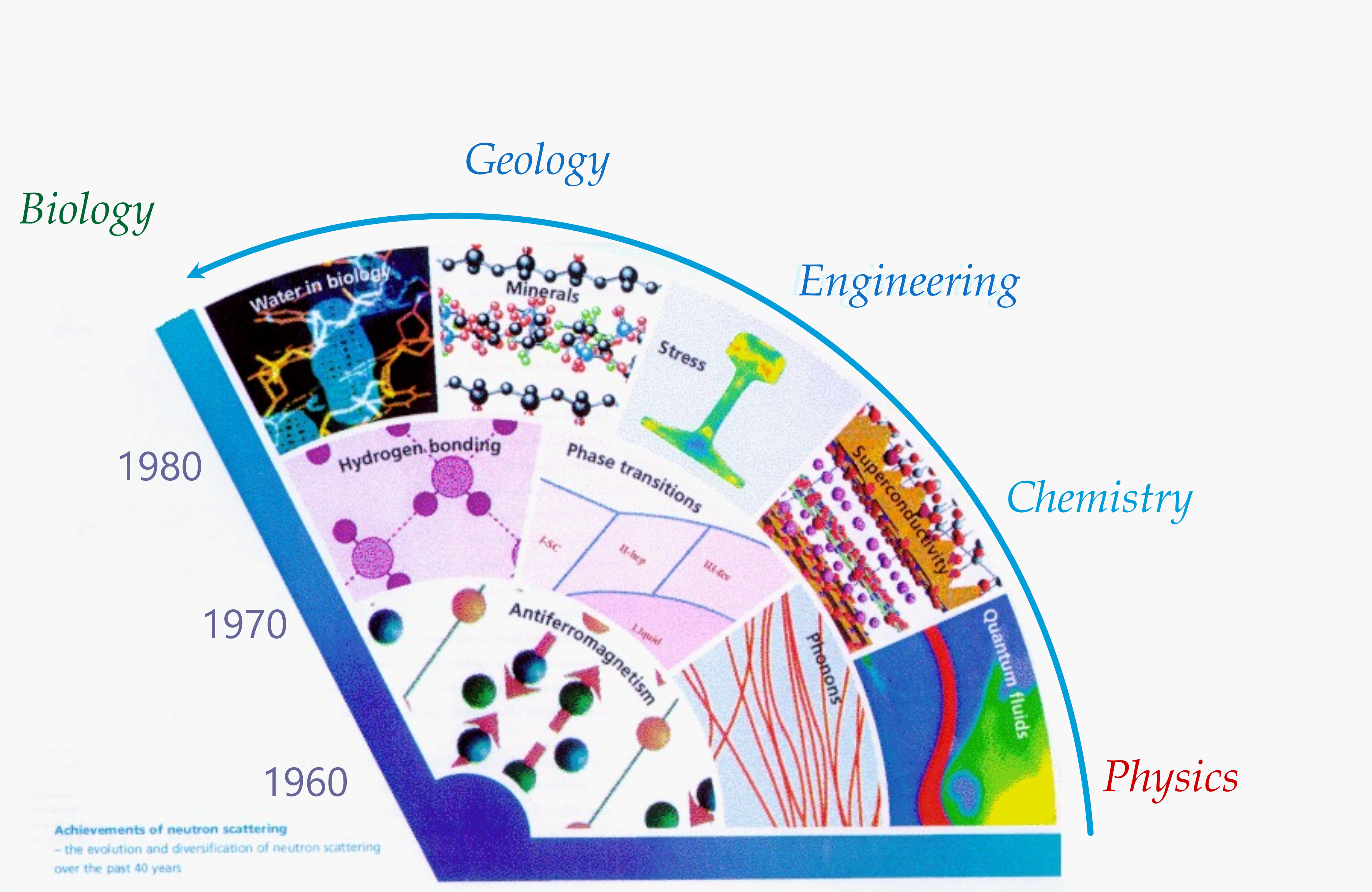

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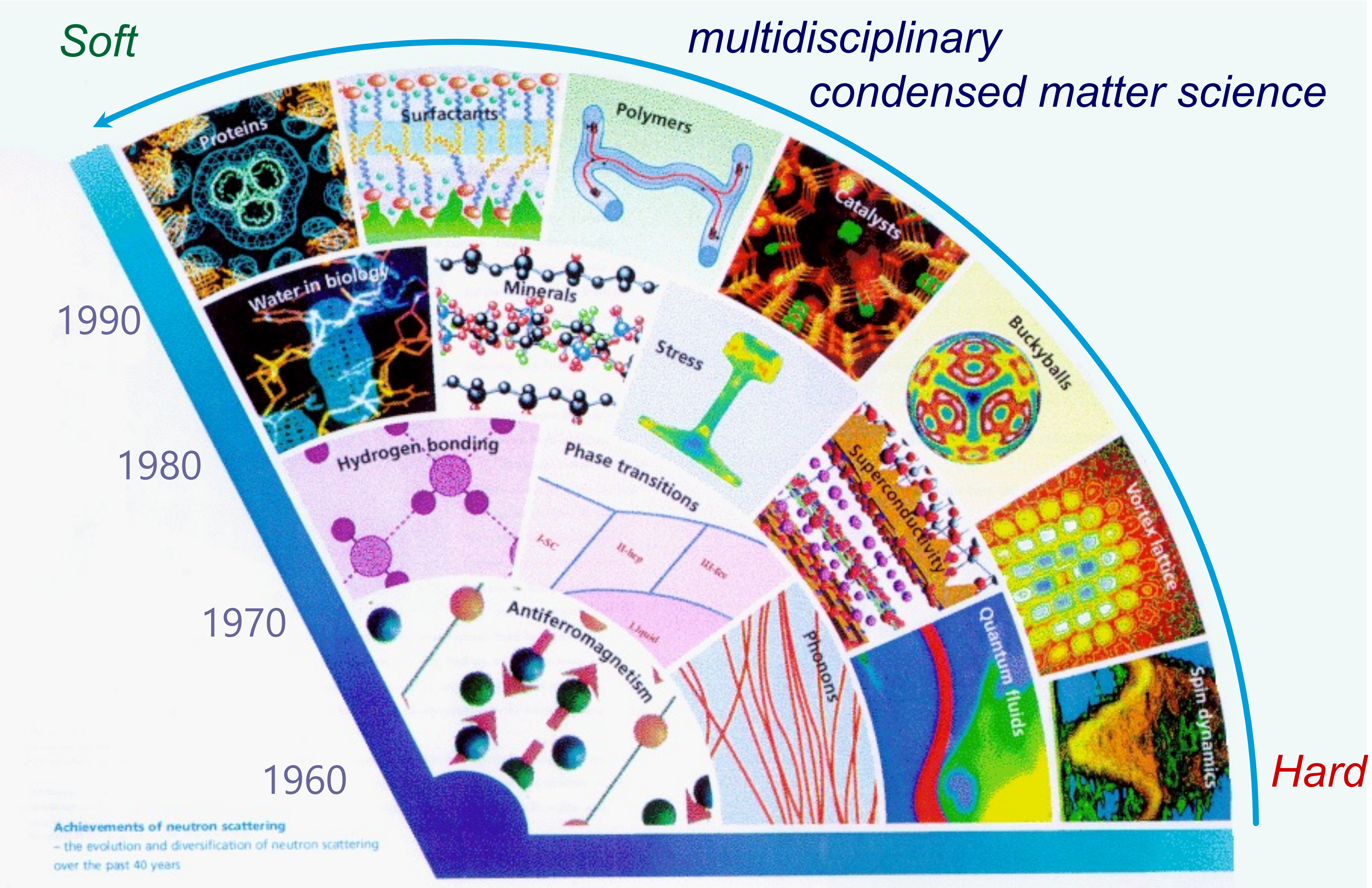
Science with neutrons



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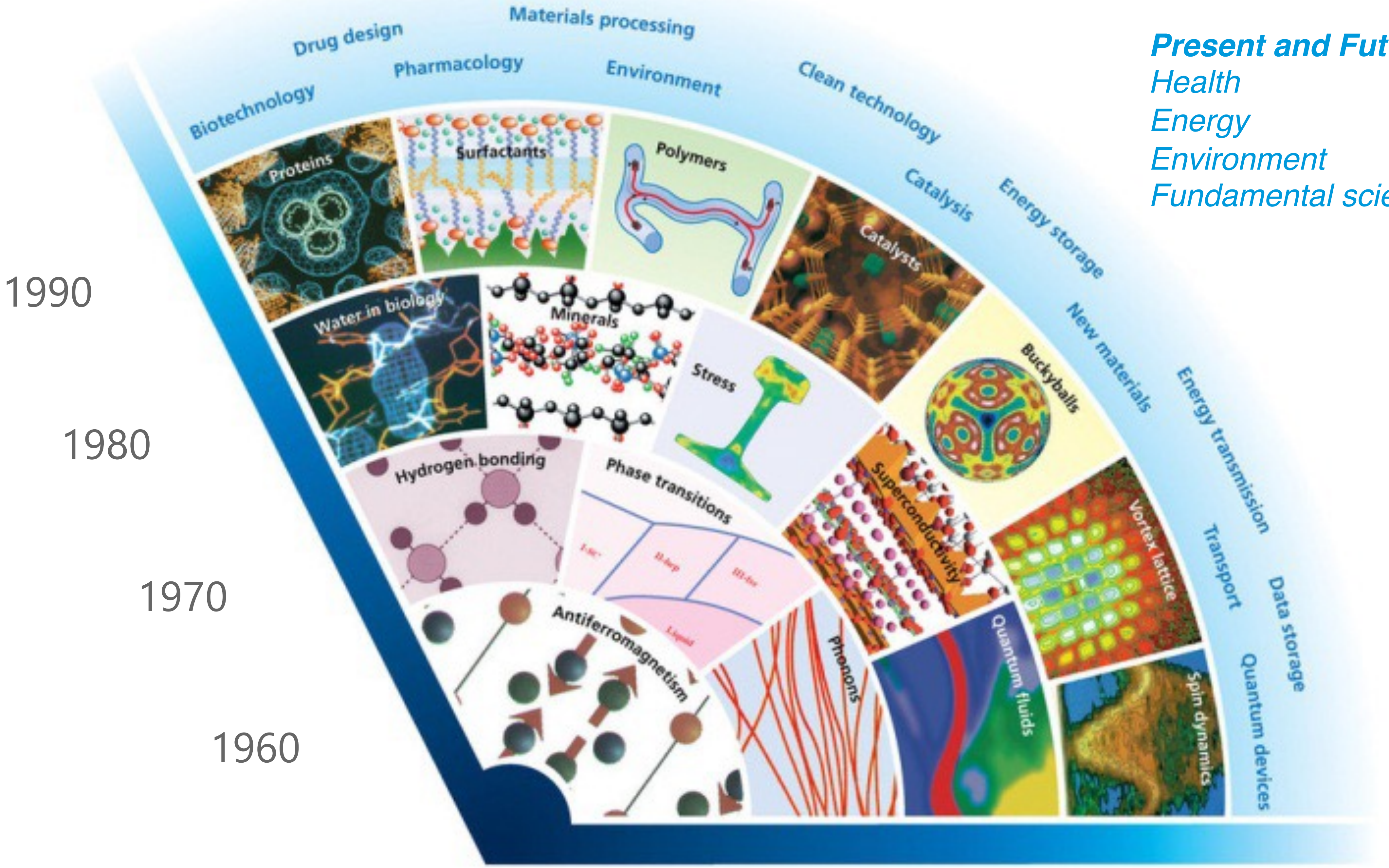
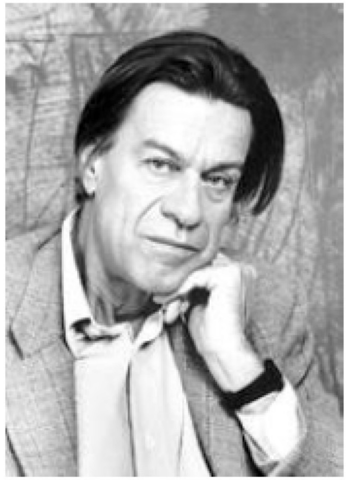


Present and Future:
Health
Energy
Environment
Fundamental science

SOFT MATTER

"Molecular systems giving a strong response to very weak command signal"



deGennes (1991)

"founding father of soft matter"

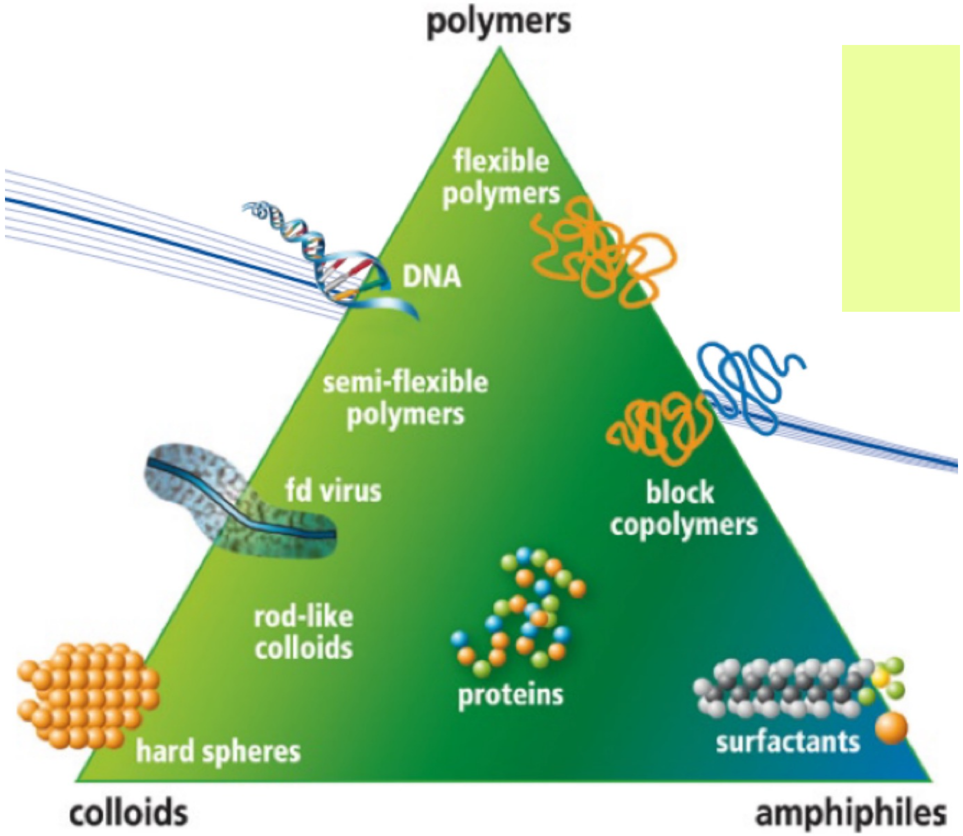
Condensed matter: states are easily deformed by small external fields, including thermal stresses and thermal fluctuations.

Relevant energy scale comparable with room temperature **thermal energy (E~kT).**

Structures in the size range of **nanometres to a few micrometres.**

Complex fluids : including colloids, polymers, surfactants, foams, gels, liquid crystals, granular and biological materials.

"Anything you can't take in an airplane" - Daan Frankel



www.eu-softcomp.net

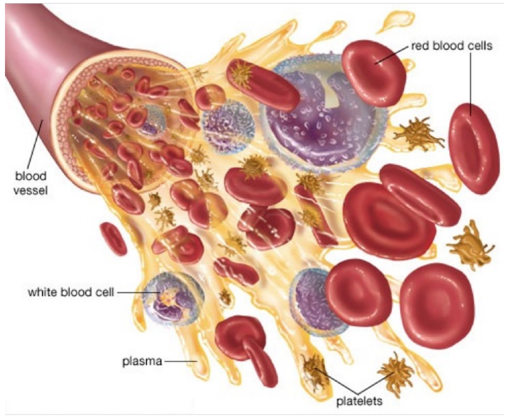
Food

Heinz (http://www.heinz.co.uk/)

Consumer goods

P&G (http://www.pg.co.uk//)

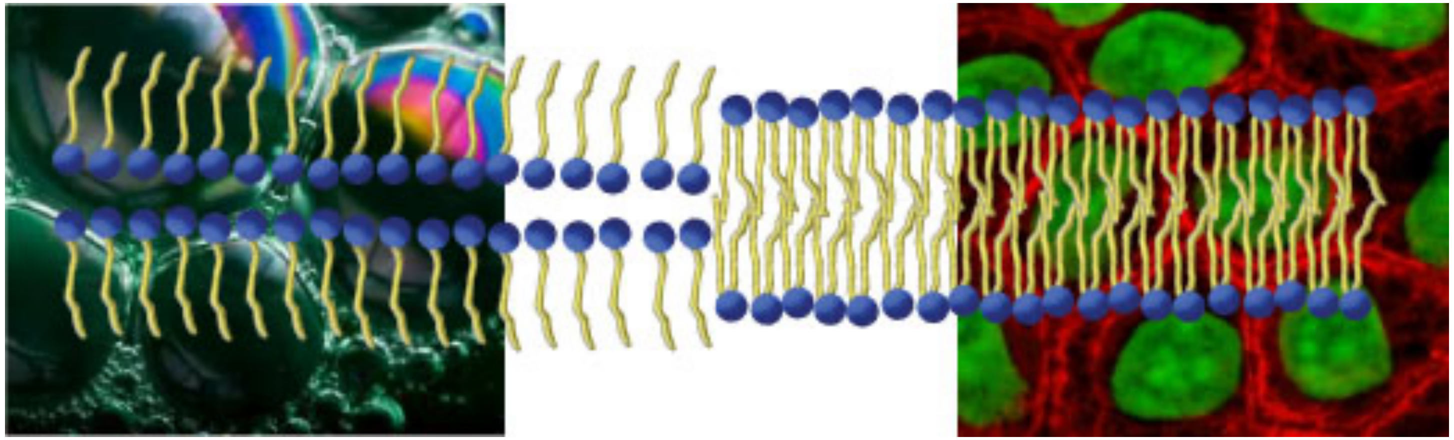
Biological matter



Encyclopedia Britannica

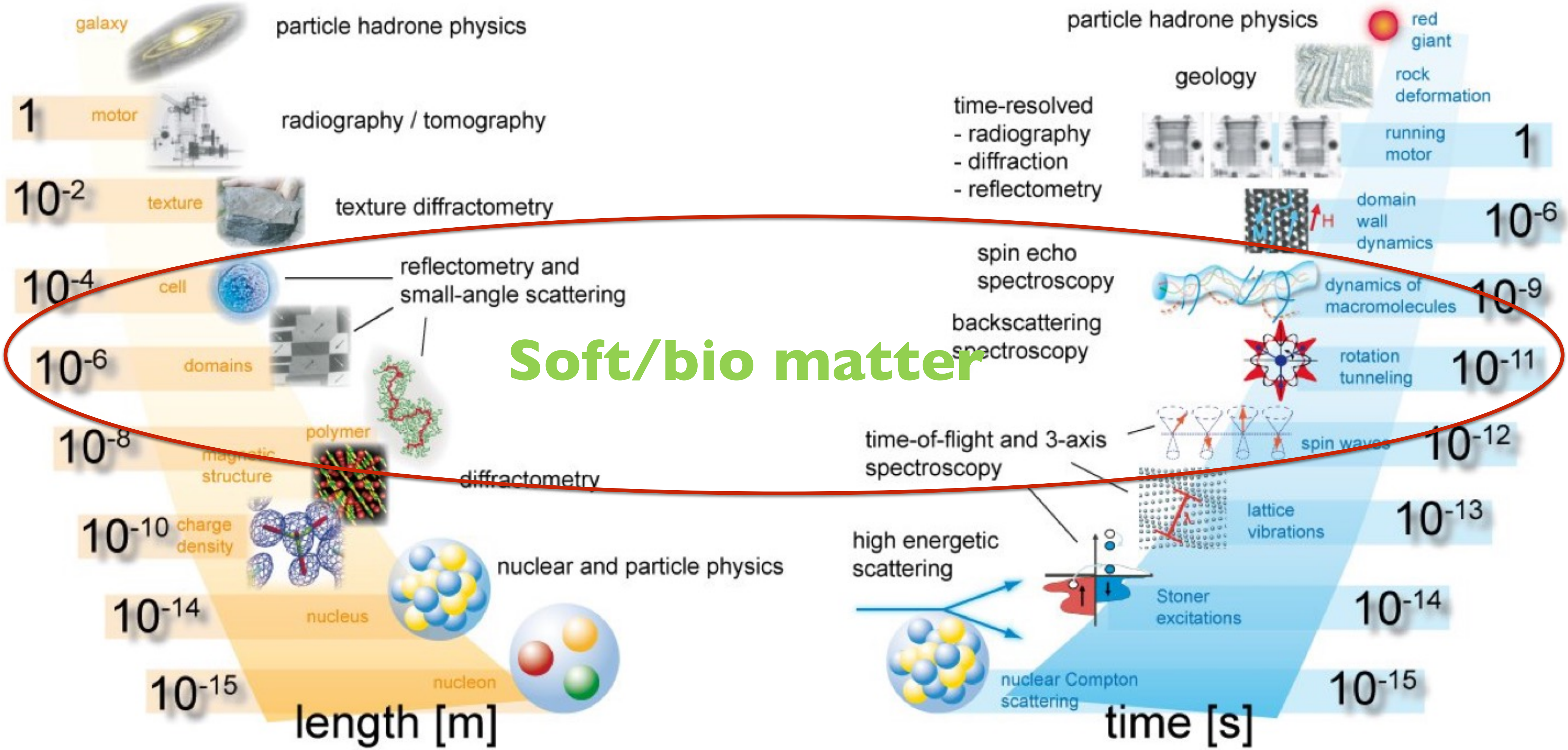
Soft matter plays an important role in nearly every aspect of our daily life and soft matter research is a driving force in a broad range of innovation fields.

Soft and biological materials have very different functions but share common structural features

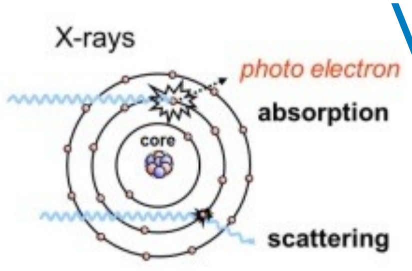


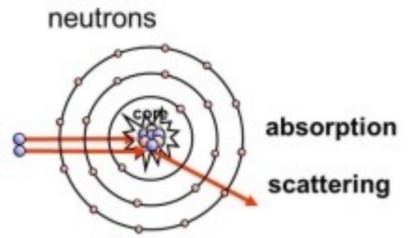
Soap bubbles and cell membranes are formed by **amphiphilic** molecules able to **self-assemble**, a few **nanometer** thick and which **structure** and **dynamics** can be determined by **scattering** techniques

Why Neutron Scattering?



Why use neutrons to study soft and biological material?



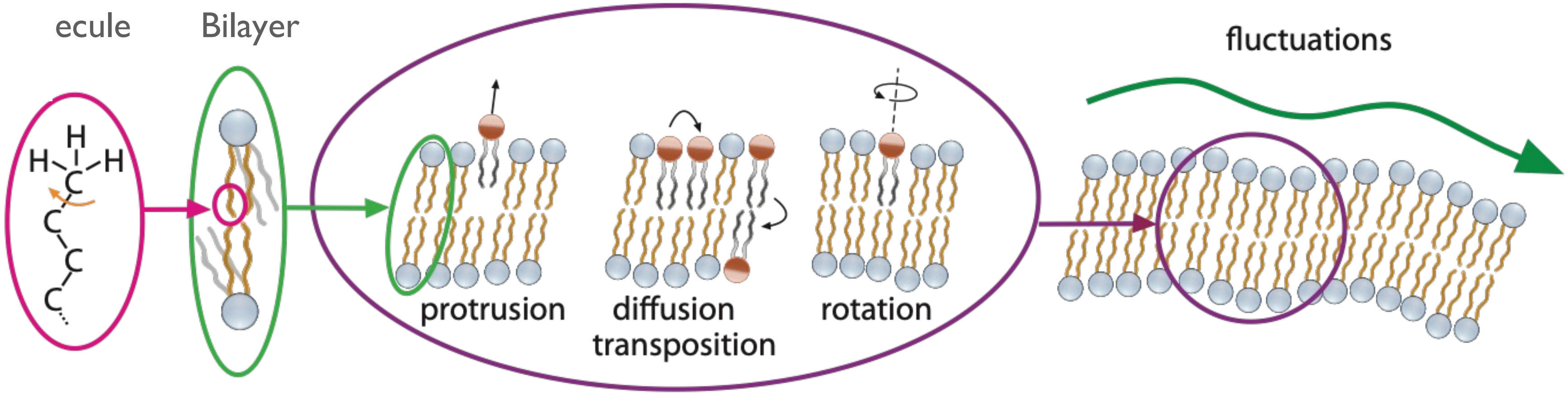


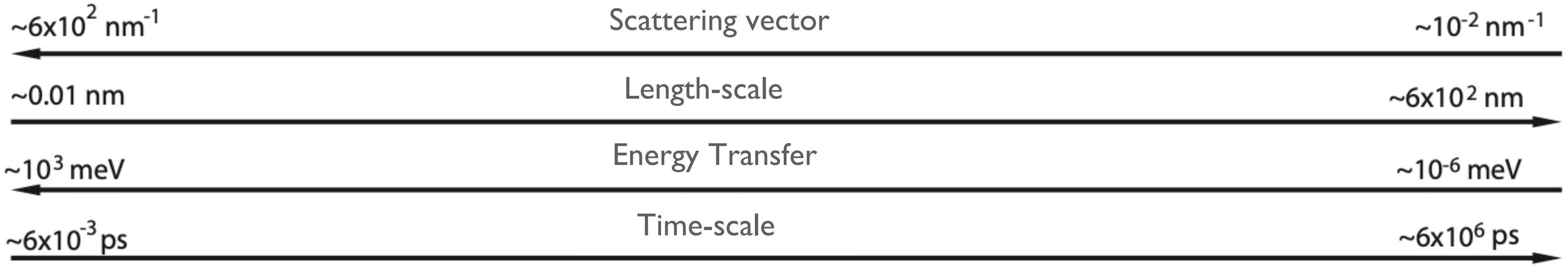
Access structure and composition

Like X-rays thermal neutrons possess the right wavelengths.

In addition neutrons possess the ideal energies for spectroscopy of thermal fluctuations.

Probe lengths (Å to μm) and time-scales (ps to *hr*)





~$6x10^2$ nm^{-1} Scattering vector ~10^{-2} nm^{-1}

~0.01 nm Length-scale ~$6x10^2$ nm

~10^3 meV Energy Transfer ~10^{-6} meV

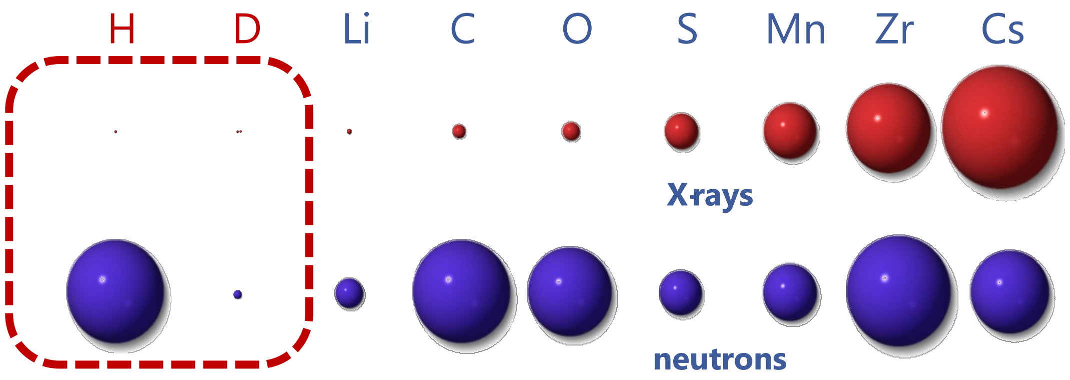
~$6x10^{-3}$ ps Time-scale ~$6x10^6$ ps

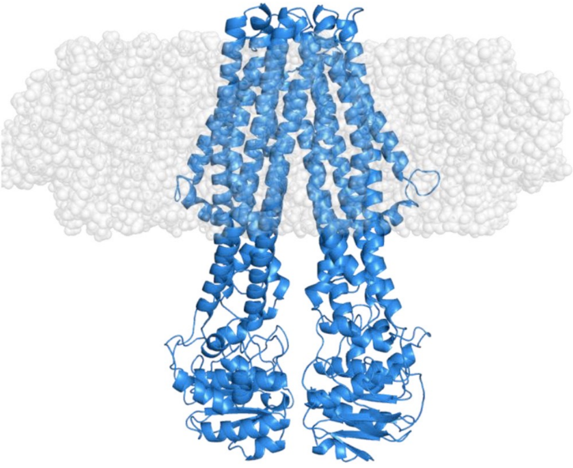
Fragneto G., Etudier la structure des membranes biologiques: l'intérêt des systèmes modèles et des neutrons, Reflets de la Physique, 41, oct 2014

Why use neutrons to study soft an biological material?

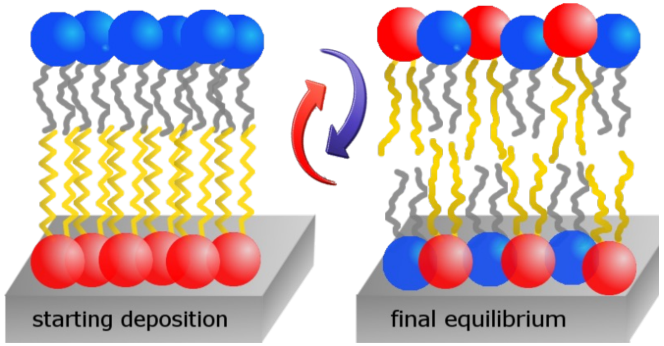
Neutrons interact with nuclei

- are sensitive to light atoms, particularly hydrogen
- can exploit isotopic substitution, especially H/D
- ‘see‘ materials differently to X-rays, complementary



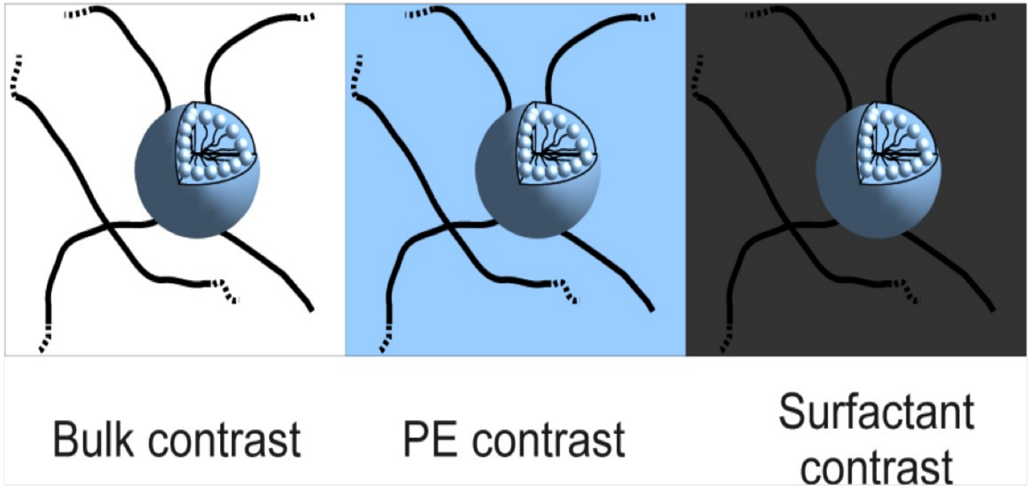


Josts et al. Structure 2018



Gerelli Y., et al., Langmuir 2012

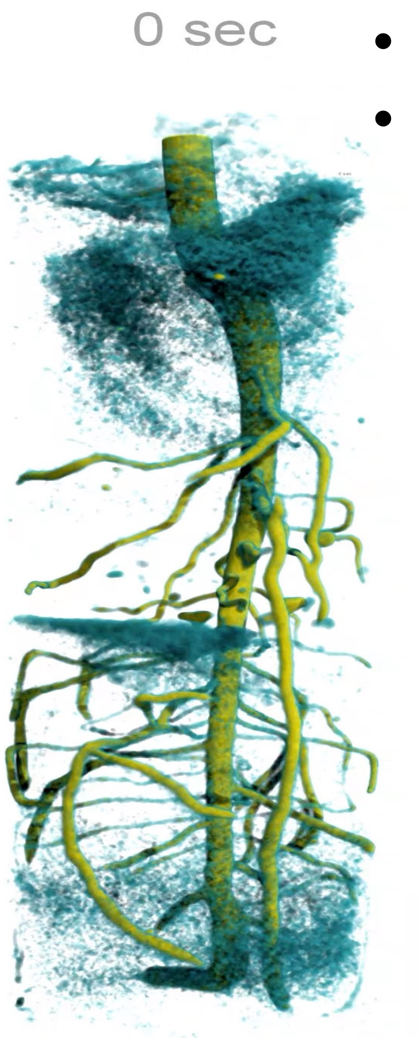
Polyelectrolyte + surfactant complex

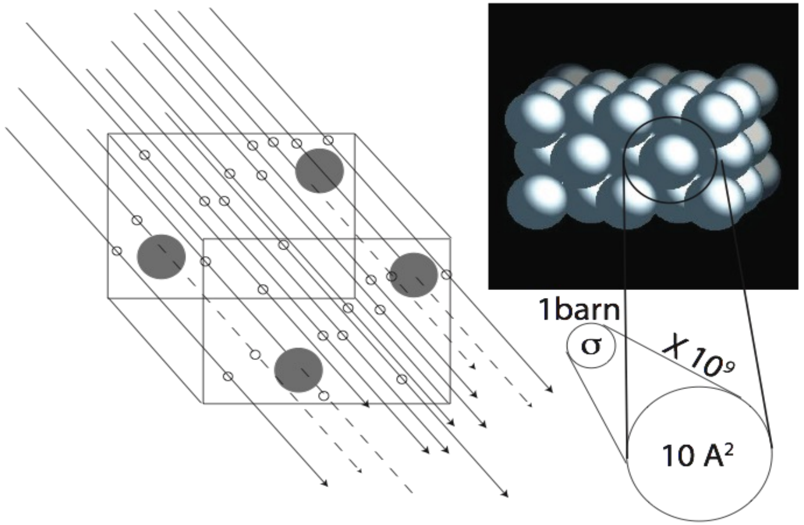


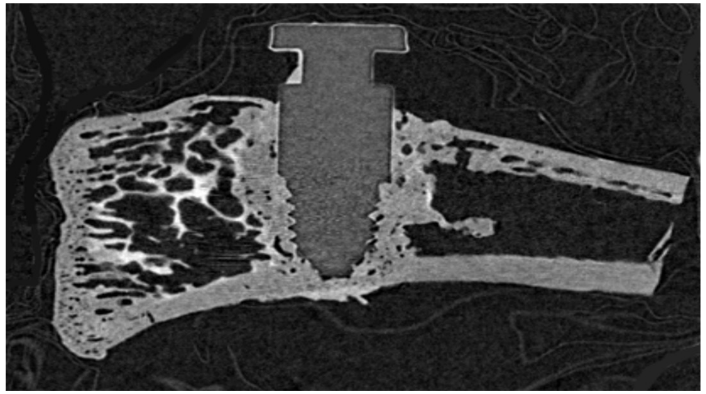
I. Hoffmann et al. J. Chem. Phys. 2015.

Neutrons are a neutral particle

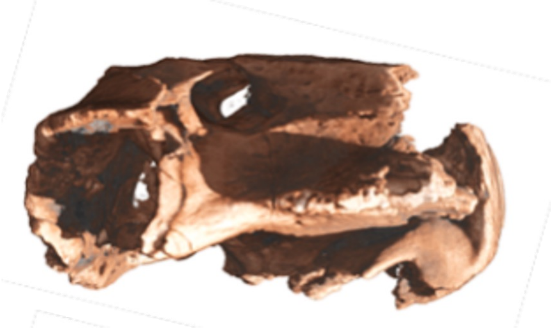
- are highly penetrating - imaging of light elements deeply buried in materials
- can be used as non-destructive probes





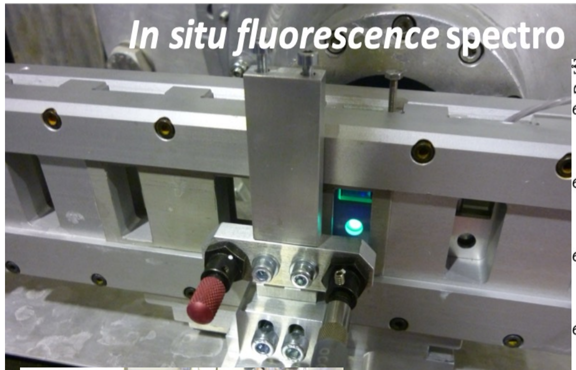


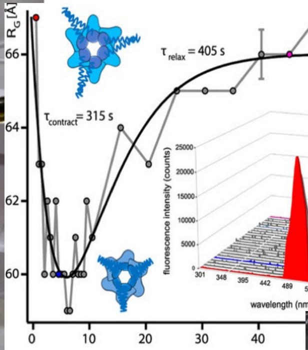
Bone Structures
+ implants



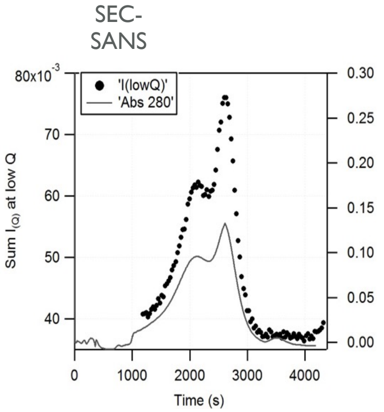
Neutrons are a neutral particle

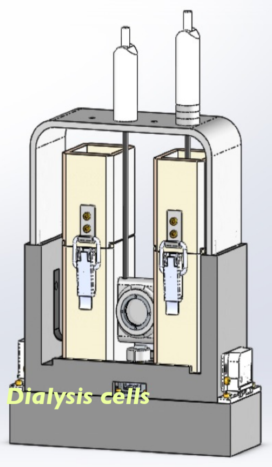
- are highly penetrating → *buried interfaces*
- can be used to study samples in extreme environments and allow use of in-situ complementary techniques

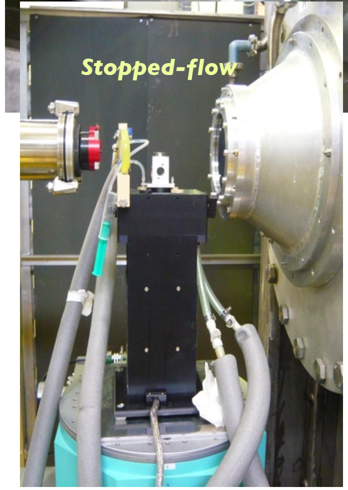


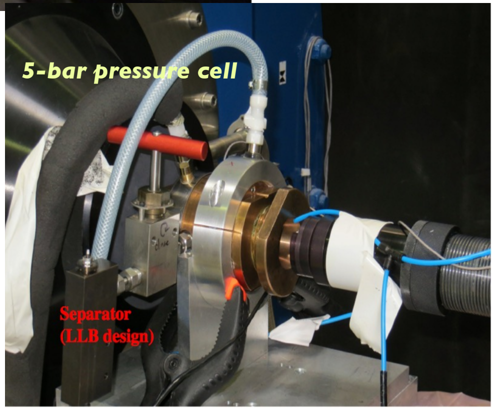


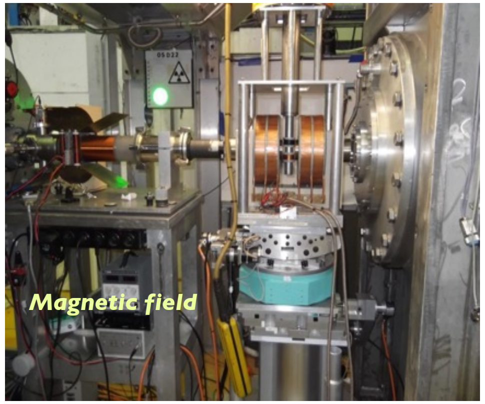
Scientific Reports 2017

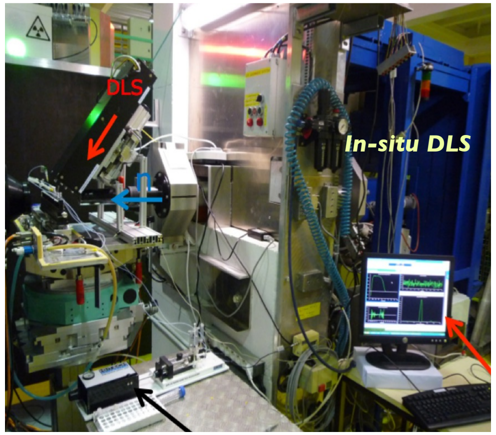












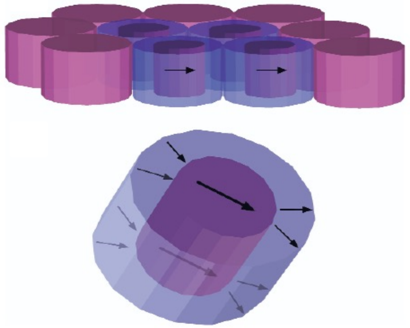
Why use neutrons to study soft and biological material?

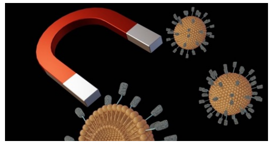
Non destructive

Possibility to work in physiological conditions

Neutrons **vs.** **x-rays**

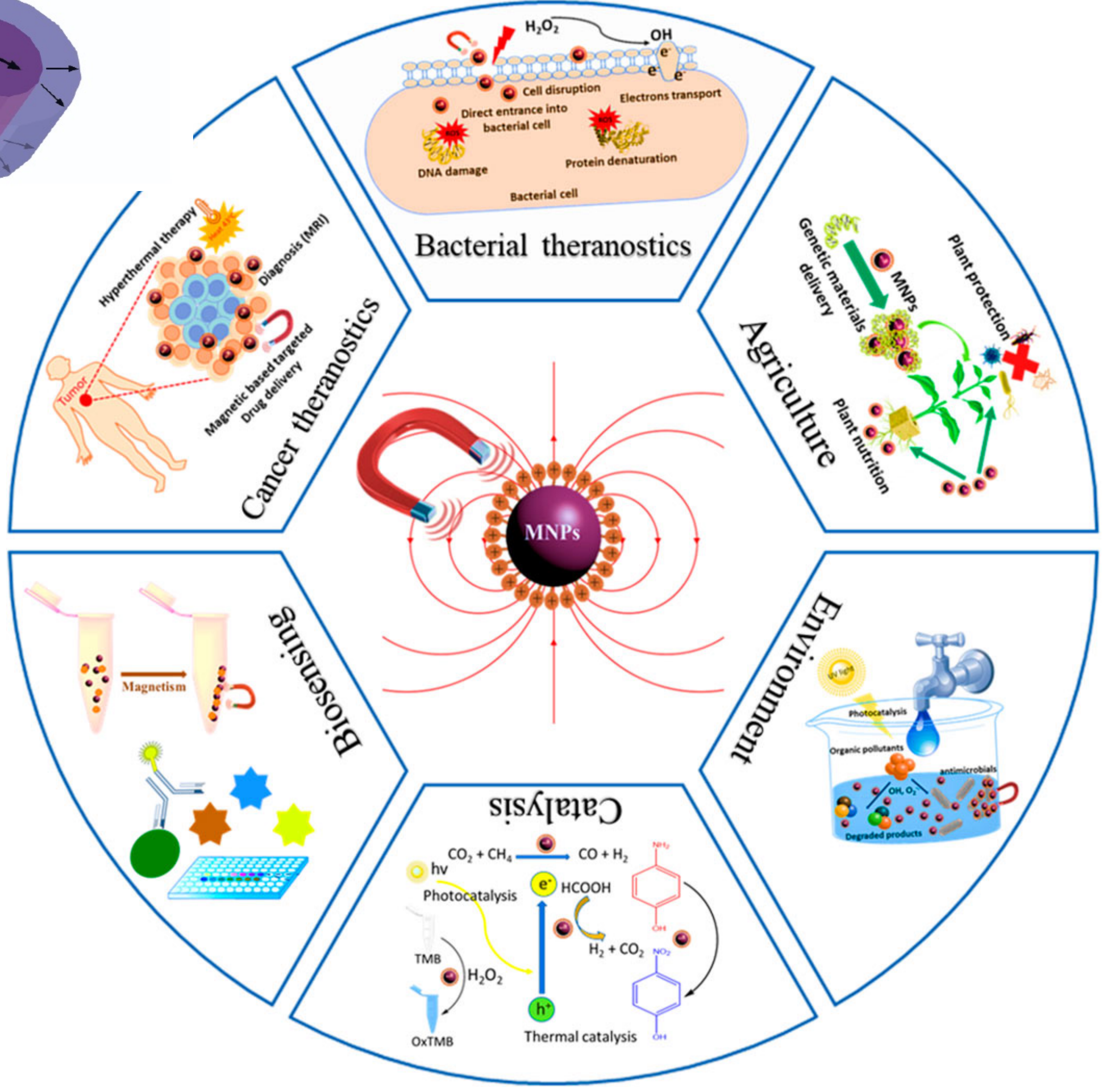
Neutrons have a magnetic moment and spin

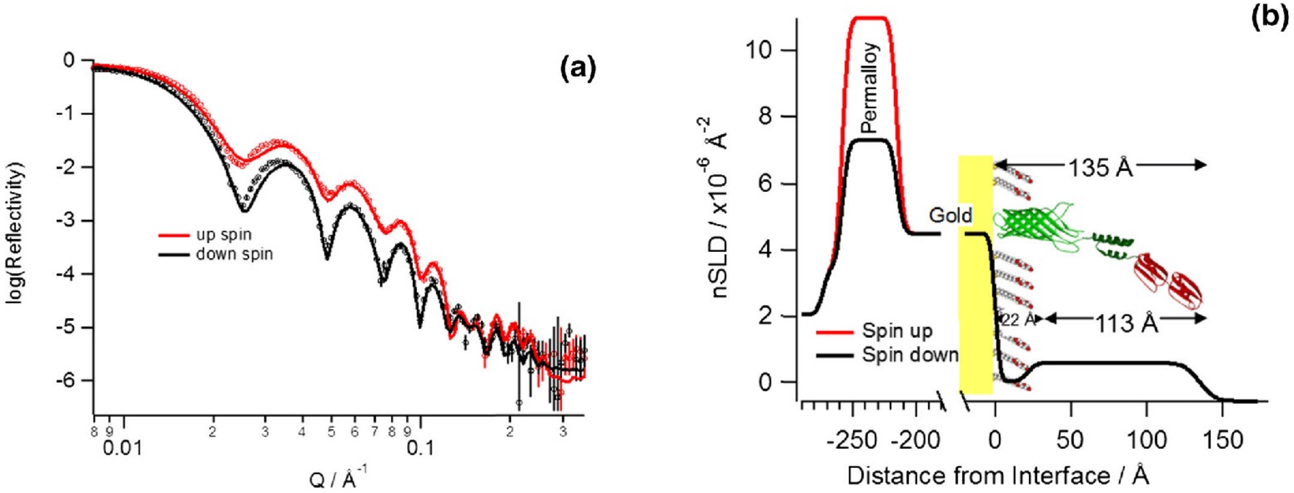




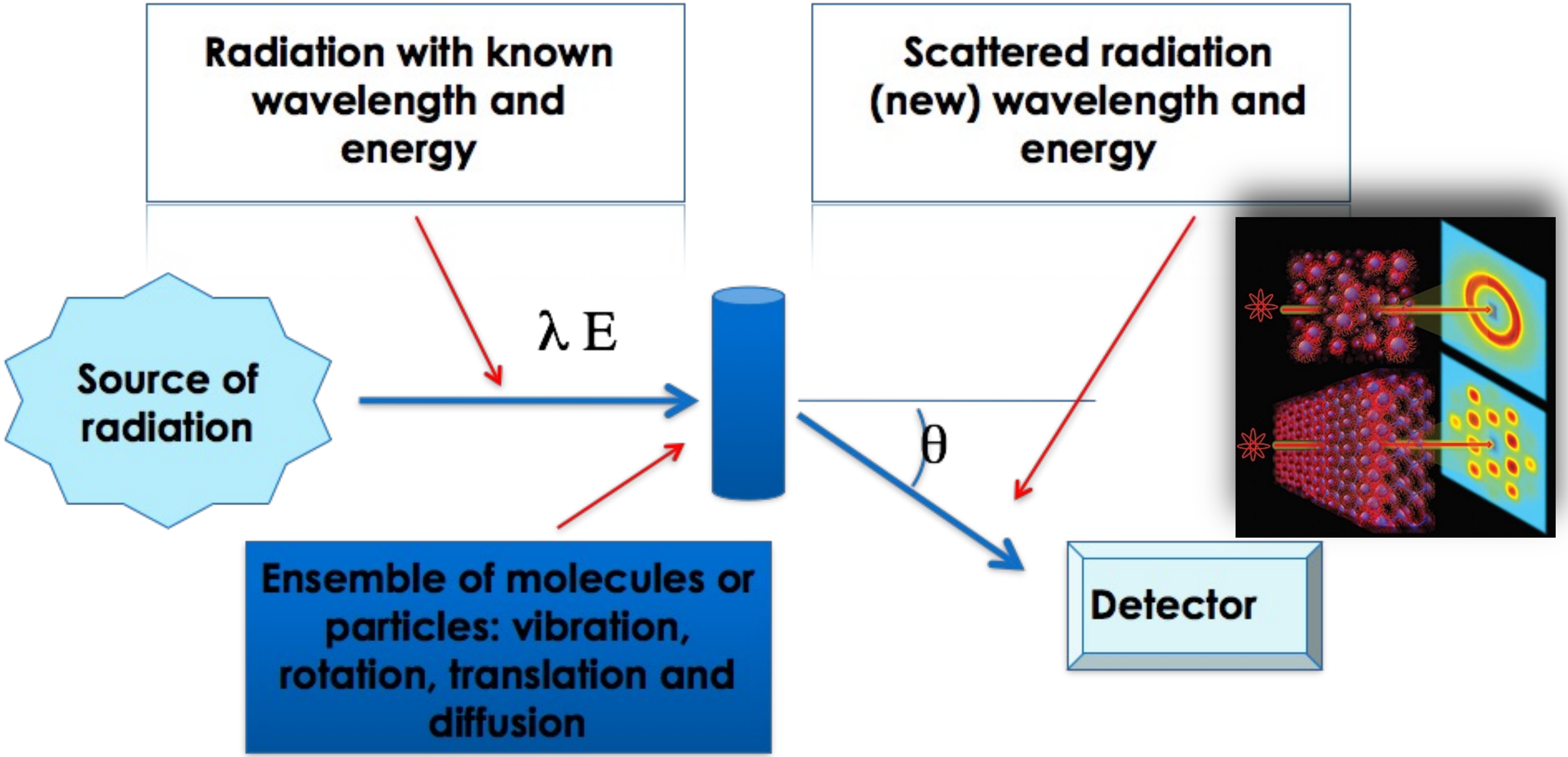
- study microscopic magnetic structures
- study magnetic fluctuations , and
- develop magnetic materials
- formed into polarised beams,
- study nuclear (atomic) orientation, and
- separate coherent from incoherent scattering

- *magnetic systems in soft matter (magnetic nanoparticles)*
- *magnetic contrast in reflectometry*





PRINCIPLE OF A SCATTERING EXPERIMENT



Radiation with known wavelength and energy

Scattered radiation (new) wavelength and energy

Source of radiation

Ensemble of molecules or particles: vibration, rotation, translation and diffusion

Detector

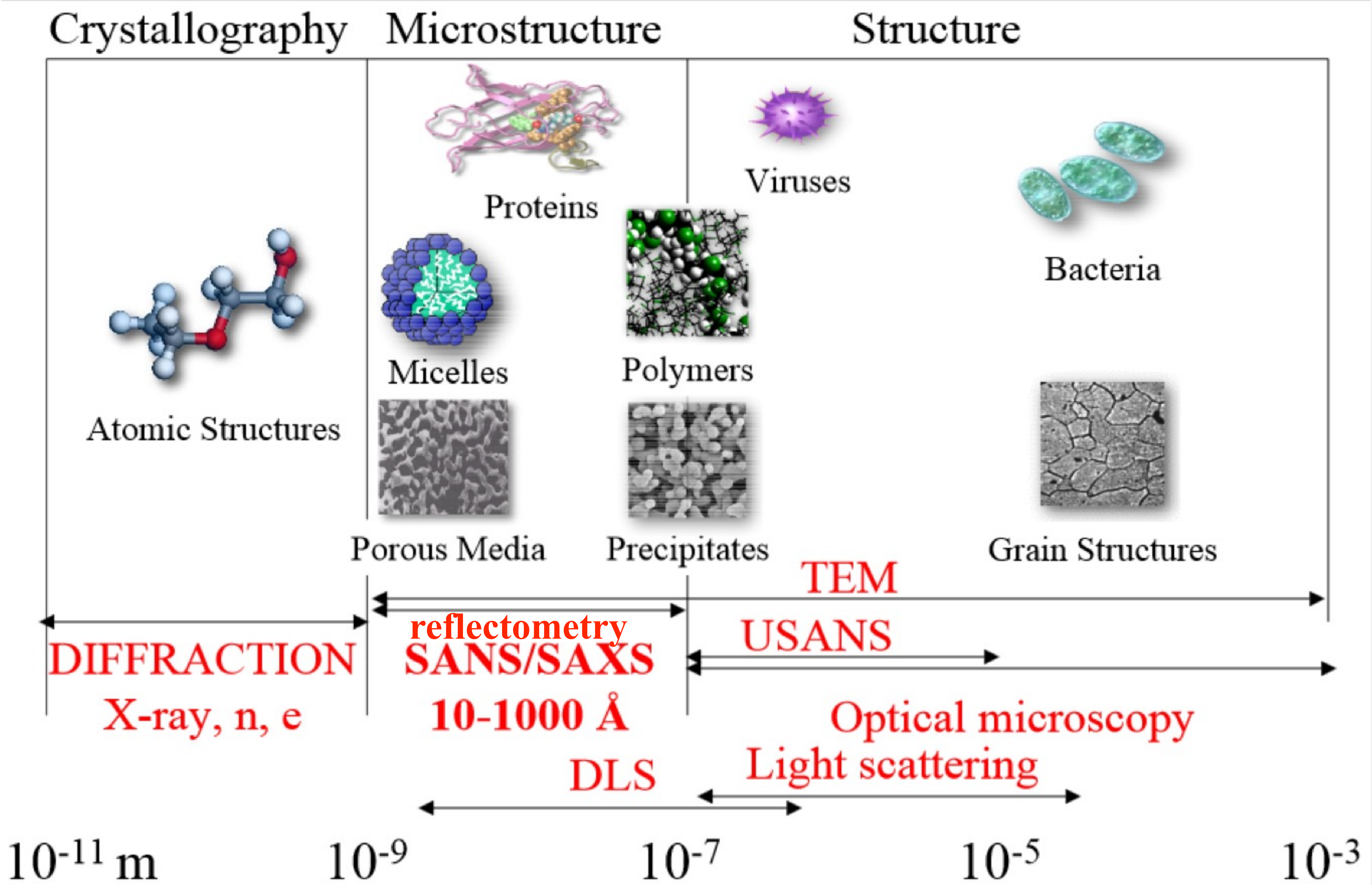
elastic or static

Conformation, structure, size

quasielastic, inelastic or dynamic

Local and global dynamics, diffusion, vibrations, rotation

STRUCTURE

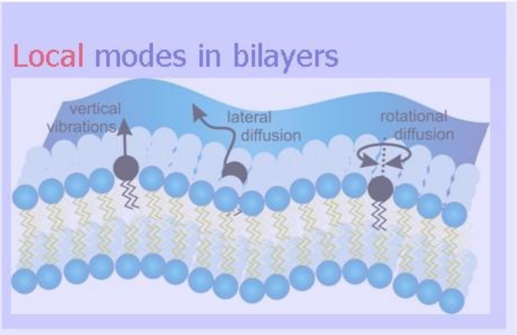

Crystallography
Microstructure
Structure
Proteins
Viruses
Bacteria
Micelles
Polymers
Atomic Structures
Porous Media
Precipitates
Grain Structures
TEM
reflectometry
USANS
DIFFRACTION
X-ray, n, e
SANS/SAXS
10-1000 Å
Optical microscopy
Light scattering
DLS
10^{-11} m
10^{-9}
10^{-7}
10^{-5}
10^{-3}

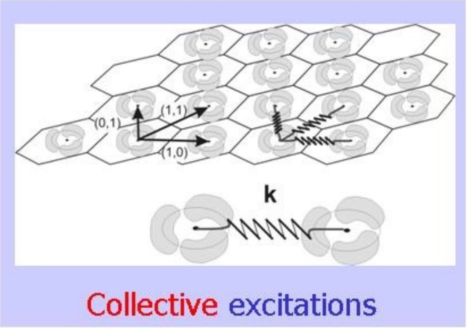
DYNAMICS

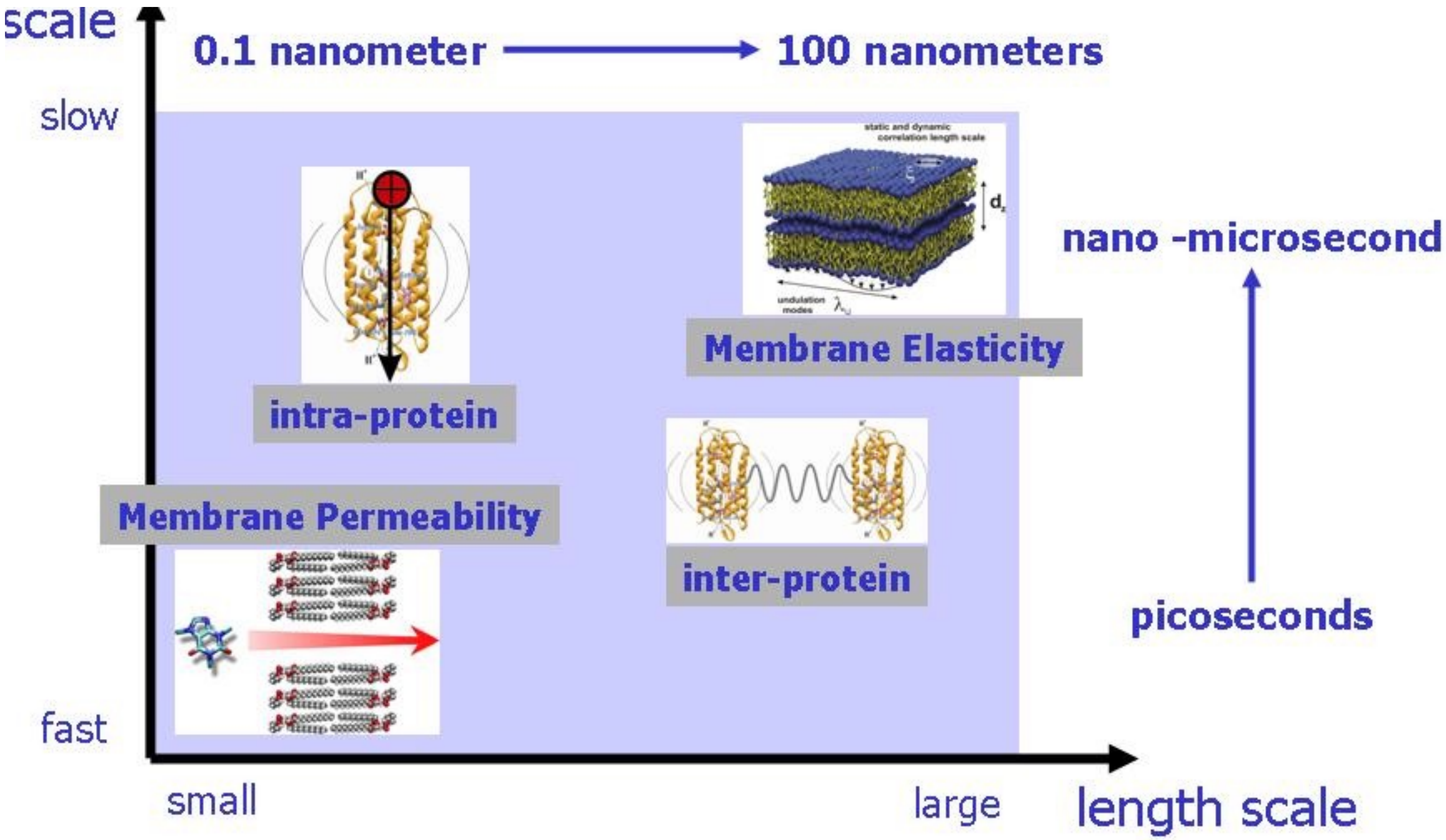
http://www.rheinstaedter.de/maikel/

time scales from about 0.1 ps
to almost 1 µs

Inelastic, Backscattering, Spin-Echo





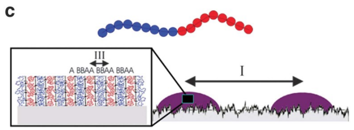


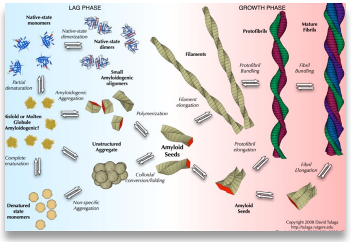
In the next days you will have a detailed overview of the use of scattering techniques for the study of biological systems including:

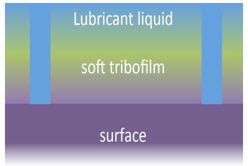
- High resolution structure of proteins (position of hydrogens, enzymatic mechanisms incolving protons, hydrogen bonds of drugs in proteins)
- Low resolution structure of proteins and complexes (protein-protein, protein-DNA, nanodiscs,…)
- Model biological membranes and interaction with peptides, proteins, drugs, …)
- Hydration water
- Movement of atoms inside proteins related to function
- ….

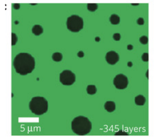
- Wide complementarity with x-rays but not only
- Need for information from other techniques often essential
- Deuteration is a fantastic tool to help research with neutrons in soft-bio related areas

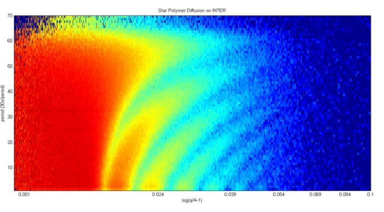
Huge Range of Science for deuteration

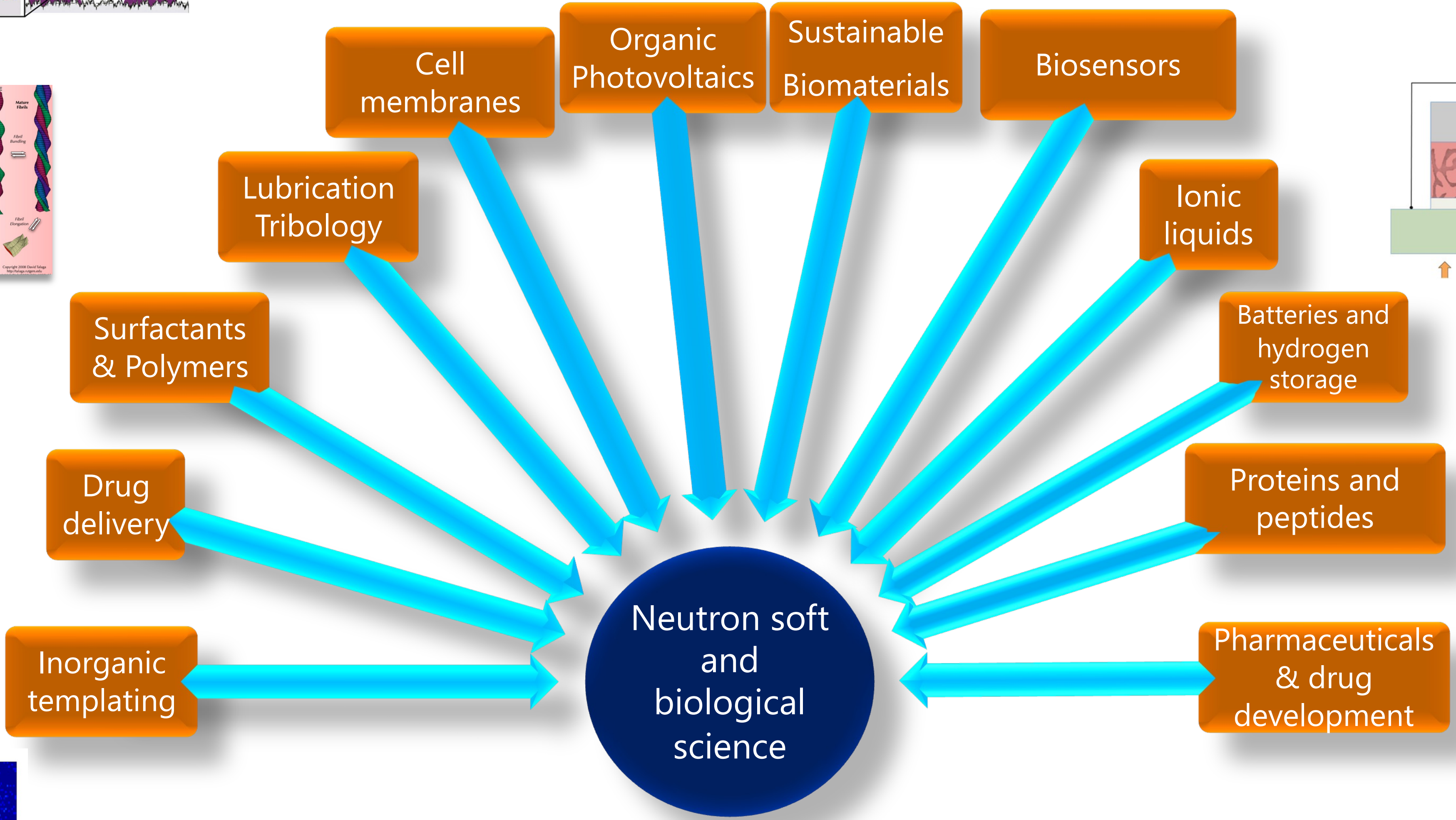












Cell membranes

Organic Photovoltaics

Sustainable Biomaterials

Biosensors

Lubrication Tribology

Ionic liquids

Surfactants & Polymers

Batteries and hydrogen storage

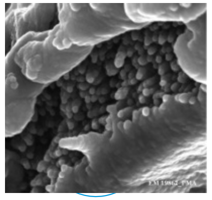
Drug delivery

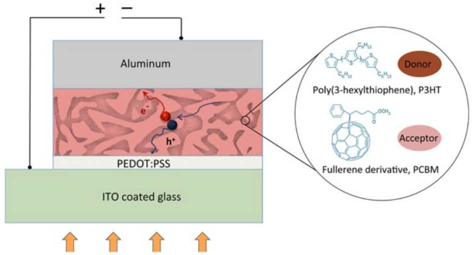
Proteins and peptides

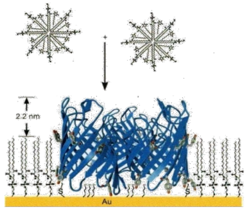
Inorganic templating

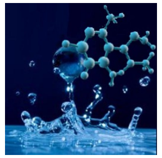
Pharmaceuticals & drug development

Neutron soft and biological science





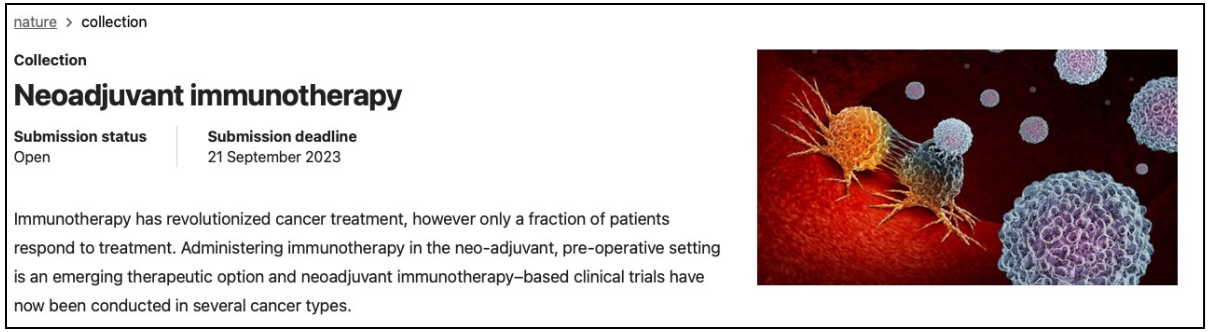




Deuteration/contrast variation/isotopic labelling are powerful methods to study structure and interactions: it is essential to foster development at neutron facilities in collaboration with the user base

What the field is doing

Current headlines in Life Science Research



nature > collection

Collection

Neoadjuvant immunotherapy

Submission status
Open

Submission deadline
21 September 2023

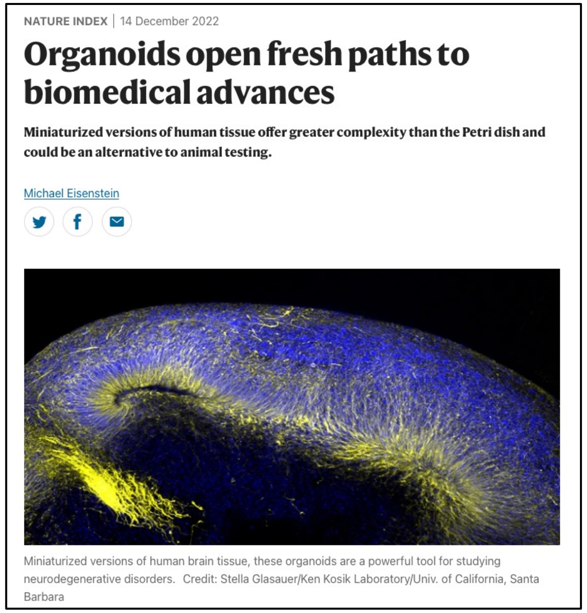
Immunotherapy has revolutionized cancer treatment, however only a fraction of patients respond to treatment. Administering immunotherapy in the neo-adjuvant, pre-operative setting is an emerging therapeutic option and neoadjuvant immunotherapy–based clinical trials have now been conducted in several cancer types.

nature > collection

Collection | **07 October 2022**

Methods for studying noncoding RNA

Research interest is growing in profiling noncoding RNAs and understanding their biological functions in health and disease contexts. The articles featured in this collection highlight recent method developments and key resources that enable researchers to further explore the noncoding RNA field.



NATURE INDEX | 14 December 2022

Organoids open fresh paths to biomedical advances

Miniaturized versions of human tissue offer greater complexity than the Petri dish and could be an alternative to animal testing.

Michael Eisenstein

Miniaturized versions of human brain tissue, these organoids are a powerful tool for studying neurodegenerative disorders. Credit: Stella Glasauer/Ken Kosik Laboratory/Univ. of California, Santa Barbara

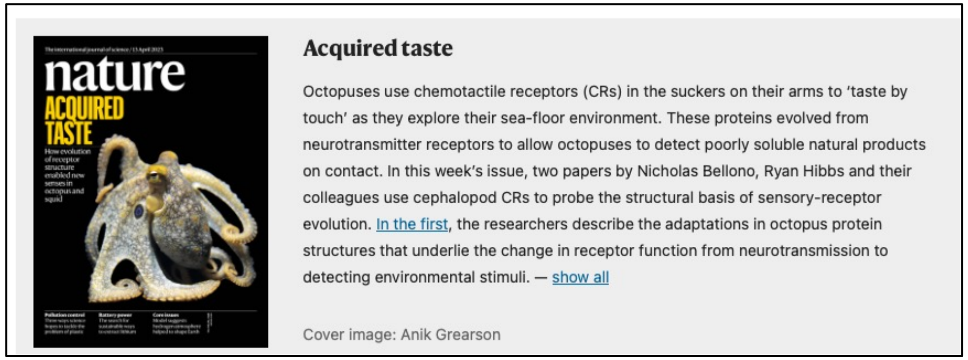
NEWS | 29 March 2023

'Astonishing' molecular syringe ferries proteins into human cells

Technique borrowed from nature, and honed using artificial intelligence, could spur the development of better drug-delivery systems.

Heidi Ledford

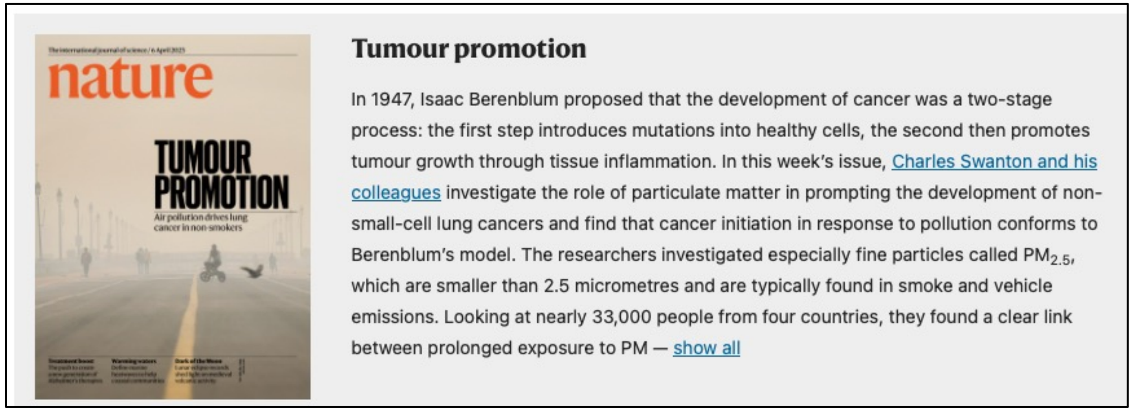
The bacterium *Photorhabdus asymbiotica* uses molecular spikes to pierce a hole in the membranes of host cells. Credit: F. Zhang *et al./Nature*



Acquired taste

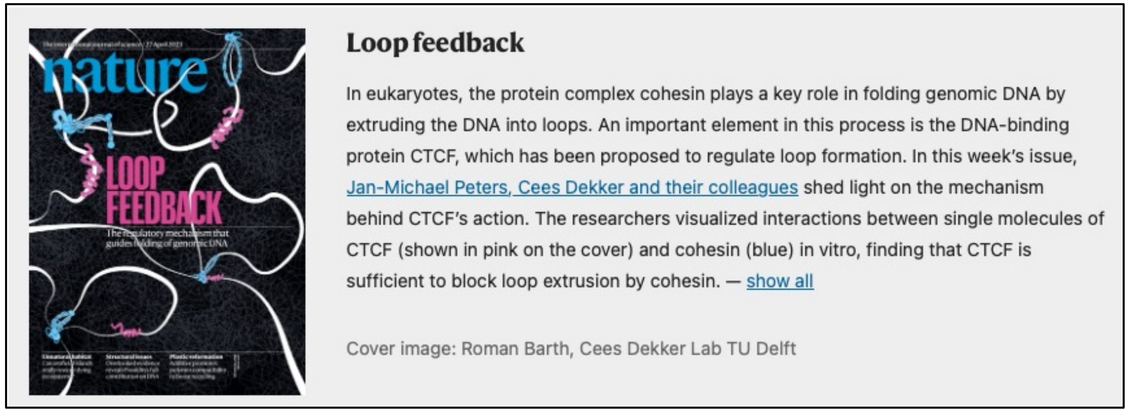
Octopuses use chemotactile receptors (CRs) in the suckers on their arms to 'taste by touch' as they explore their sea-floor environment. These proteins evolved from neurotransmitter receptors to allow octopuses to detect poorly soluble natural products on contact. In this week's issue, two papers by Nicholas Bellono, Ryan Hibbs and their colleagues use cephalopod CRs to probe the structural basis of sensory-receptor evolution. In the first, the researchers describe the adaptations in octopus protein structures that underlie the change in receptor function from neurotransmission to detecting environmental stimuli. — show all

Cover image: Anik Grearson



Tumour promotion

In 1947, Isaac Berenblum proposed that the development of cancer was a two-stage process: the first step introduces mutations into healthy cells, the second then promotes tumour growth through tissue inflammation. In this week's issue, Charles Swanton and his colleagues investigate the role of particulate matter in prompting the development of non-small-cell lung cancers and find that cancer initiation in response to pollution conforms to Berenblum's model. The researchers investigated especially fine particles called $PM_{2.5}$, which are smaller than 2.5 micrometres and are typically found in smoke and vehicle emissions. Looking at nearly 33,000 people from four countries, they found a clear link between prolonged exposure to PM — show all



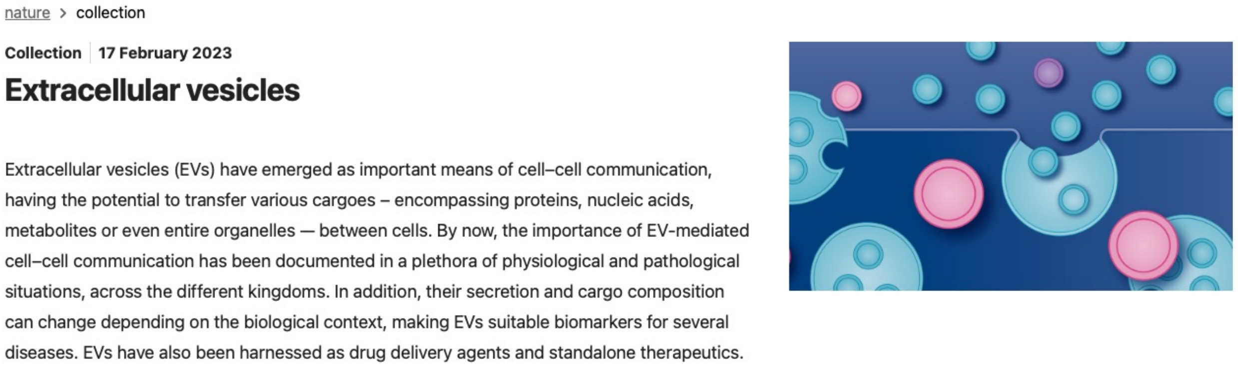
Loop feedback

In eukaryotes, the protein complex cohesin plays a key role in folding genomic DNA by extruding the DNA into loops. An important element in this process is the DNA-binding protein CTCF, which has been proposed to regulate loop formation. In this week's issue, Jan-Michael Peters, Cees Dekker and their colleagues shed light on the mechanism behind CTCF's action. The researchers visualized interactions between single molecules of CTCF (shown in pink on the cover) and cohesin (blue) in vitro, finding that CTCF is sufficient to block loop extrusion by cohesin. — show all

Cover image: Roman Barth, Cees Dekker Lab TU Delft

Areas that neutrons already contribute to:

Challenges for neutron science

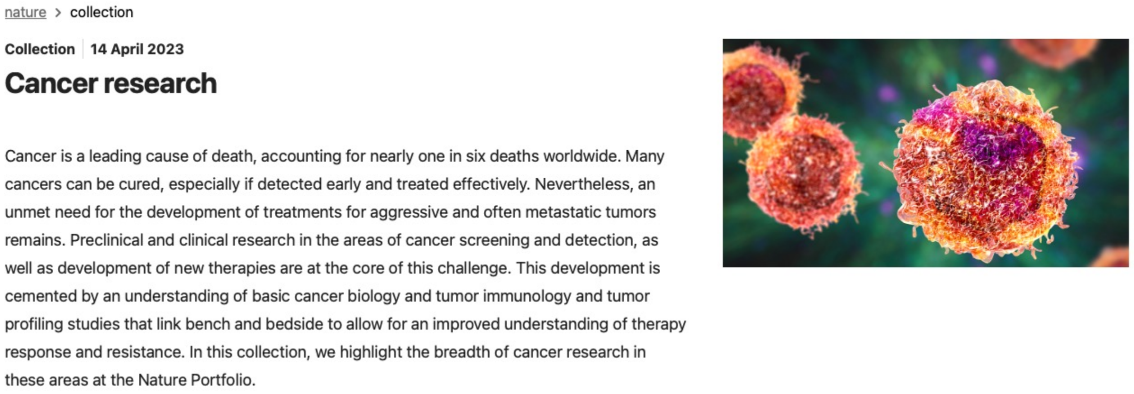


nature > collection

Collection | **17 February 2023**

Extracellular vesicles

Extracellular vesicles (EVs) have emerged as important means of cell–cell communication, having the potential to transfer various cargoes – encompassing proteins, nucleic acids, metabolites or even entire organelles — between cells. By now, the importance of EV-mediated cell–cell communication has been documented in a plethora of physiological and pathological situations, across the different kingdoms. In addition, their secretion and cargo composition can change depending on the biological context, making EVs suitable biomarkers for several diseases. EVs have also been harnessed as drug delivery agents and standalone therapeutics.



nature > collection

Collection | **14 April 2023**

Cancer research

Cancer is a leading cause of death, accounting for nearly one in six deaths worldwide. Many cancers can be cured, especially if detected early and treated effectively. Nevertheless, an unmet need for the development of treatments for aggressive and often metastatic tumors remains. Preclinical and clinical research in the areas of cancer screening and detection, as well as development of new therapies are at the core of this challenge. This development is cemented by an understanding of basic cancer biology and tumor immunology and tumor profiling studies that link bench and bedside to allow for an improved understanding of therapy response and resistance. In this collection, we highlight the breadth of cancer research in these areas at the Nature Portfolio.

Article | Open Access | Published: 14 April 2023

Temporal nanofluid environments induce prebiotic condensation in water

Andrea Greiner de Herrera, Thomas Markert & Frank Trixler

Communications Chemistry **6**, Article number: 69 (2023) | Cite this article

468 Accesses | **2** Altmetric | Metrics

COMMENT | 02 May 2023

Address the growing urgency of fungal disease in crops

More political and public awareness of the plight of the world's crops when it comes to fungal disease is crucial to stave off a major threat to global food security.

Bacterial cellulose comes out of the woodwork

Polymer scientists in Japan are harnessing the power of botany and bacteria to produce bioplastics that don't harm the environment.

NATURE INDEX | 14 December 2022

Three ways to combat antimicrobial resistance

With a dearth of new antibiotics coming to market, researchers are finding creative ways to keep bacteria at bay.

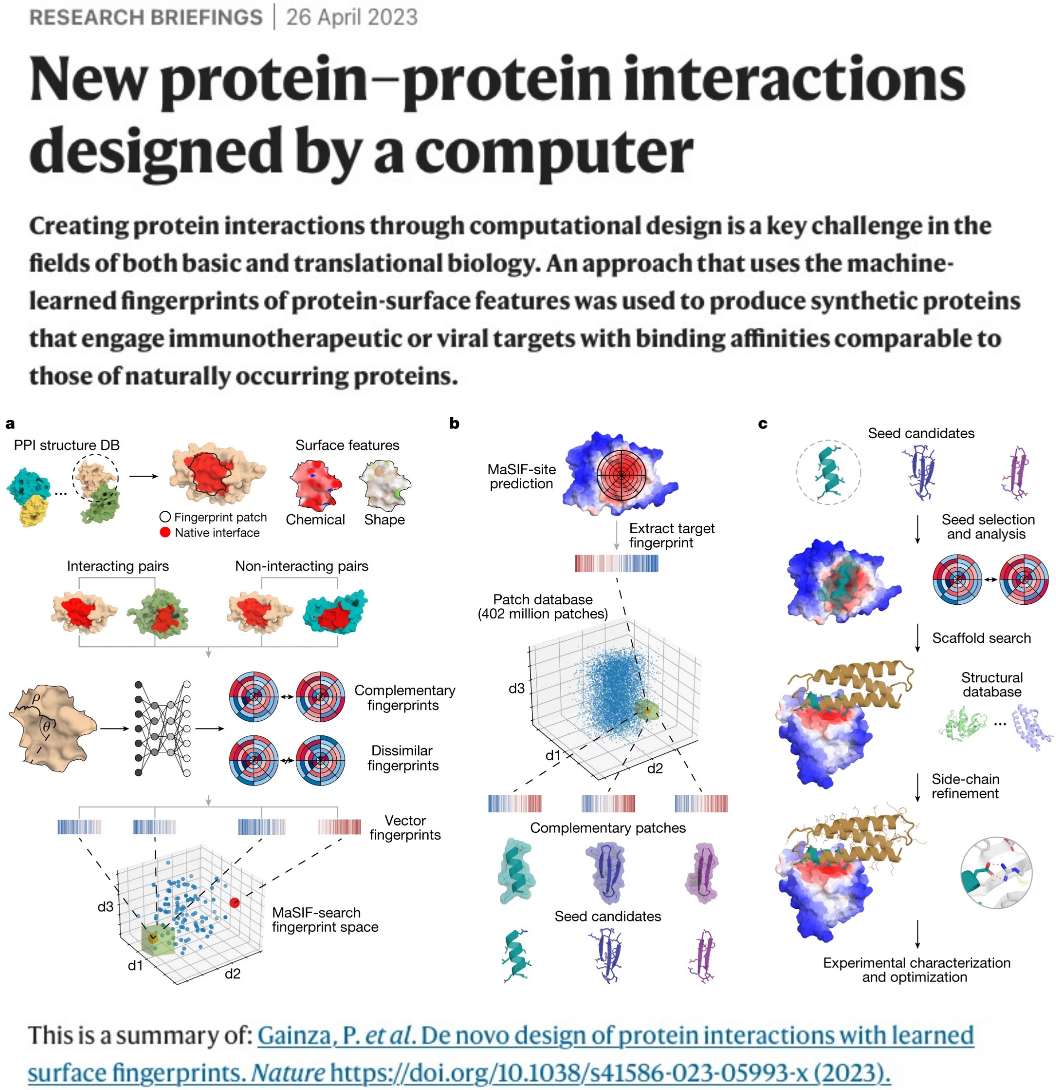
NEWS FEATURE | 04 April 2023

Conquering Alzheimer's: a look at the therapies of the future

Researchers are looking to drug combinations, vaccines and gene therapy as they forge the next generation of treatments for the condition.

E.g. what ESS could advance (with smaller samples/higher throughput/deuteration):

Challenges for neutron science



RESEARCH BRIEFINGS | 26 April 2023

New protein–protein interactions designed by a computer

Creating protein interactions through computational design is a key challenge in the fields of both basic and translational biology. An approach that uses the machine-learned fingerprints of protein-surface features was used to produce synthetic proteins that engage immunotherapeutic or viral targets with binding affinities comparable to those of naturally occurring proteins.

This is a summary of: Gainza, P. *et al.* De novo design of protein interactions with learned surface fingerprints. *Nature* https://doi.org/10.1038/s41586-023-05993-x (2023).

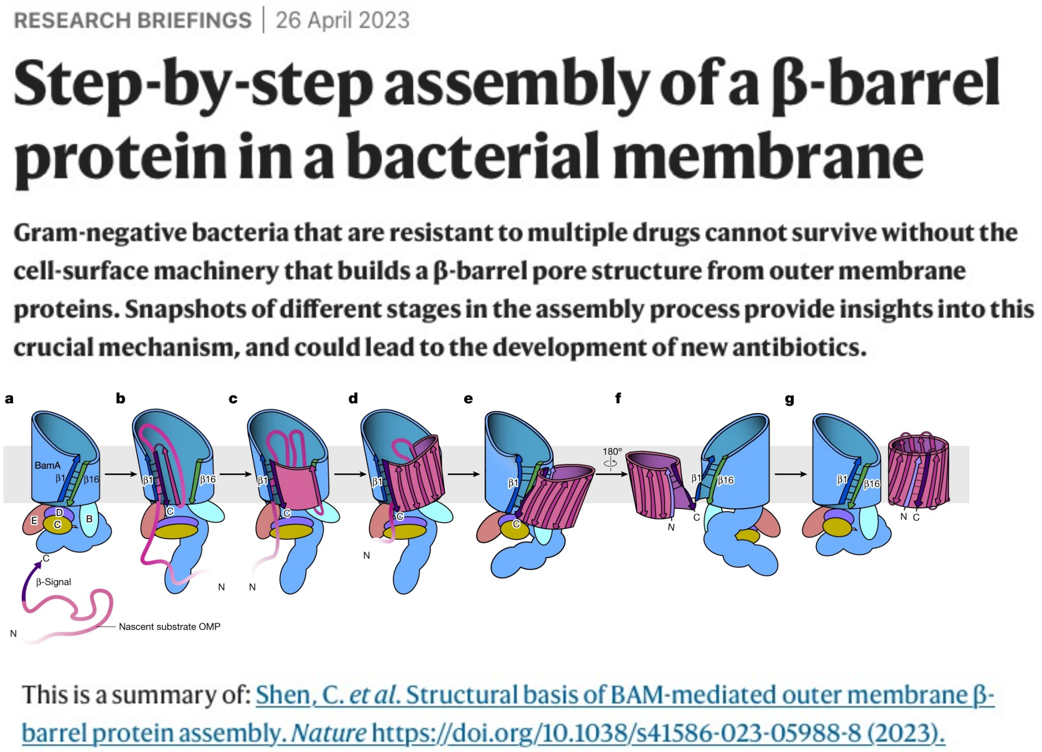
nature > articles > article

Article | Published: 05 April 2023

mRNA recognition and packaging by the human transcription–export complex

Belén Pacheco-Fiallos, Matthias K. Vorländer, Daria Riabov-Bassat, Laura Fin, Francis J. O'Reilly, Farja I. Ayala, Ulla Schellhaas, Juri Rappsilber & Clemens Plaschka

Nature **616**, 828–835 (2023) | Cite this article



RESEARCH BRIEFINGS | 26 April 2023

Step-by-step assembly of a β-barrel protein in a bacterial membrane

Gram-negative bacteria that are resistant to multiple drugs cannot survive without the cell-surface machinery that builds a β-barrel pore structure from outer membrane proteins. Snapshots of different stages in the assembly process provide insights into this crucial mechanism, and could lead to the development of new antibiotics.

This is a summary of: Shen, C. *et al.* Structural basis of BAM-mediated outer membrane β-barrel protein assembly. *Nature* https://doi.org/10.1038/s41586-023-05988-8 (2023).

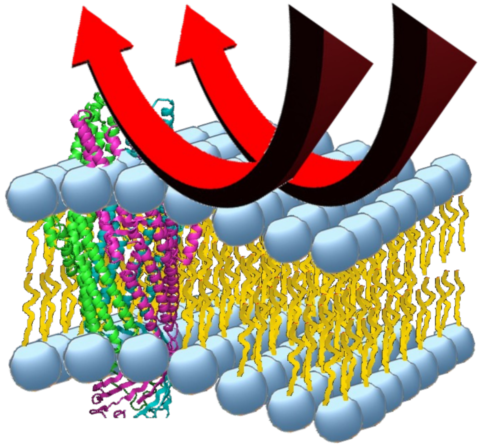
Conclusions

- Neutron scattering is an essential tool for the study of structure at the nanometer level of soft self-assembled systems.

- Complementary to x-ray and synchrotron radiation, advantages include high penetration, sensitivity to light elements (H, C, O, N, …) and isotopic labelling/contrast variation –disadvantages relate to the lower fluxes leading to lower resolution, slowest kinetics and bigger samples

- Possibility to work in real (physiological) conditions

- Possibility for in-situ studies of systems under deformation.



- Need optimised sample preparation

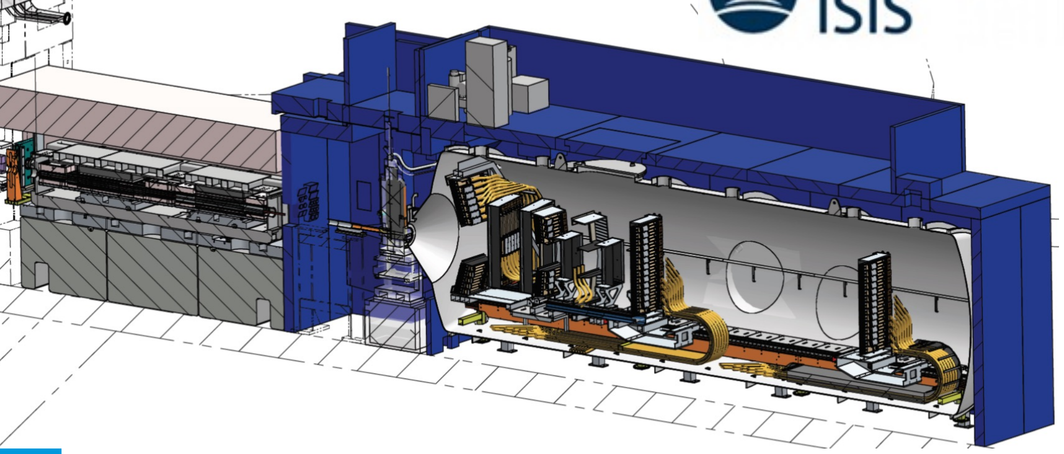
- Perspectives in biology are very numerous.

Additional slides

ESS instruments for soft-bio science

LoKI : Broad Band SANS

Science Case

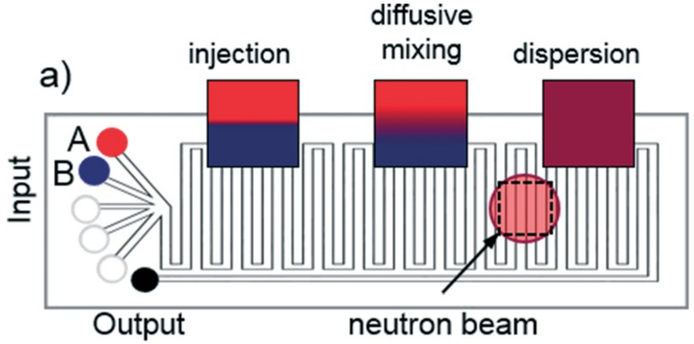


→ high flux, wide simultaneous size range, and a flexible sample area.

ABILITIES:

- Investigate **multiple length scale** systems (simultaneously 0.5-300 nm)
- Perform **“single-shot” kinetic measurements** on sub-second timescales.
- Perform experiments that use flow e.g. rheology & microfluidics **with small beam sizes**
- **High throughput** of regular SANS measurements

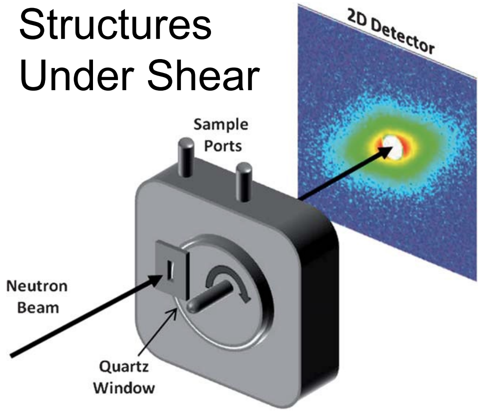
Microfluidic SANS:
High Throughput Mixing & Tailored Flow Geometry



Lab Chip, 2017, **17**, 1559

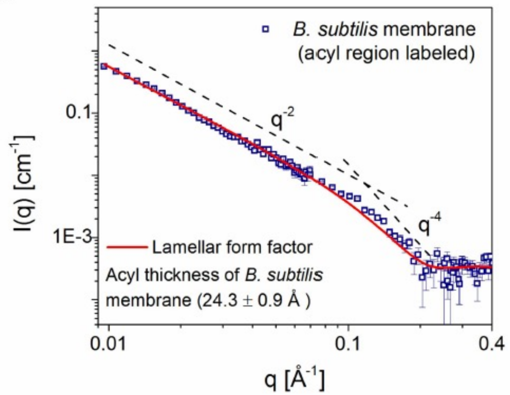
Rheo-SANS:

Structures Under Shear



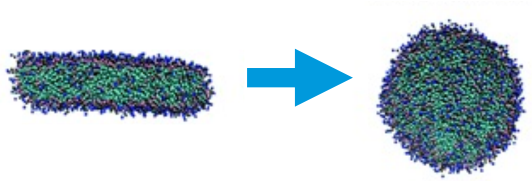
Soft Matter, 2011, **7**, 9992

Biological Samples:
Weak Scatterers & Dilute Solutions



PLoS Bio, 2017, **15**, e2002214

Non-Equilibrium Studies:
Self-Assembly & Kinetics

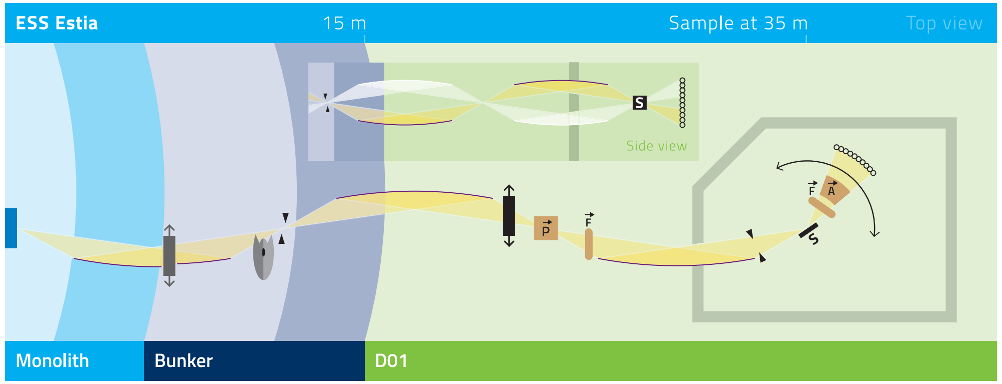


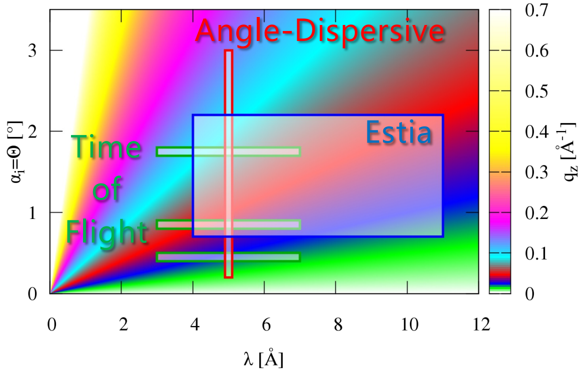
Colloid Polym Sci, 2010, **288**, 827

Courtesy J. Houston

Estia

Focussing Polarised Reflectometer for Tiny Samples

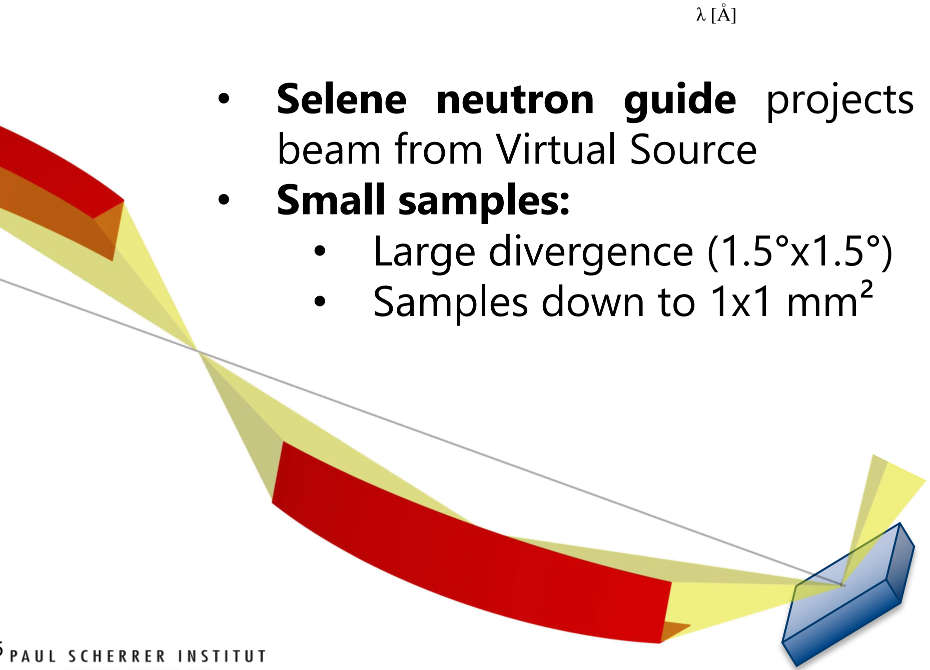




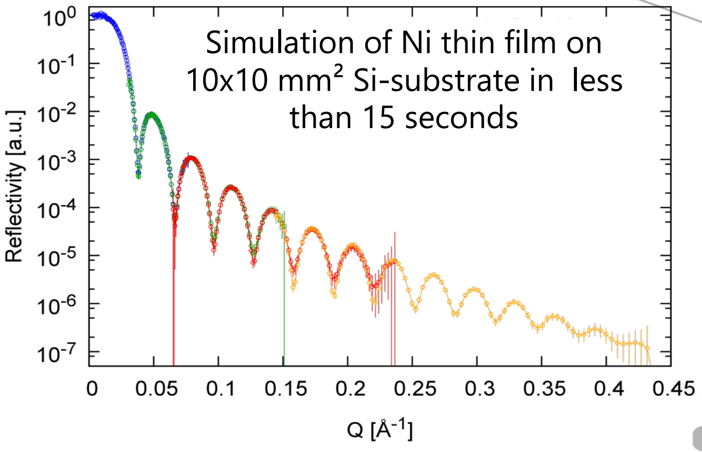
Estia Quick Facts.

Estia Quick Facts	
Instrument Class	Reflectometry
Moderator	Cold
Primary Flightpath	35 m
Secondary Flightpath	4 m
Wavelength Range	3.75–28 Å
Polarised Incident Beam	Optional
Polarisation Analysis	Optional
Sample Orientation	Vertical
Total Q-Range	0.001 to 3.15 Å^{-1}/–0.001 to –0.3 Å^{-1}
Standard Mode (14 Hz)	
Bandwidth	7 Å
Flux at Sample at 2 MW[a]	6×10^8 n s^{-1} cm^{-2}
Relative Q-Range	$Q_{max} = 2.85 \times Q_{min}$
Q-Resolution ΔQ/Q	7.8%–3.0% over Q-range
2-Pulse Skipping Mode (4.7 Hz)	
Bandwidth	21 Å
Flux at Sample at 2 MW[a]	2×10^8 n s^{-1} cm^{-2}
Relative Q-Range	$Q_{max} = 6.6 \times Q_{min}$
Q-Resolution ΔQ/Q	7.8%–1.3% over Q-range

[a] Full-divergence beam averaged over 5(H) × 10(V) mm².



- **Selene neutron guide** projects tiny beam from Virtual Source
- **Small samples:**
  - Large divergence (1.5°x1.5°)
  - Samples down to 1x1 mm²



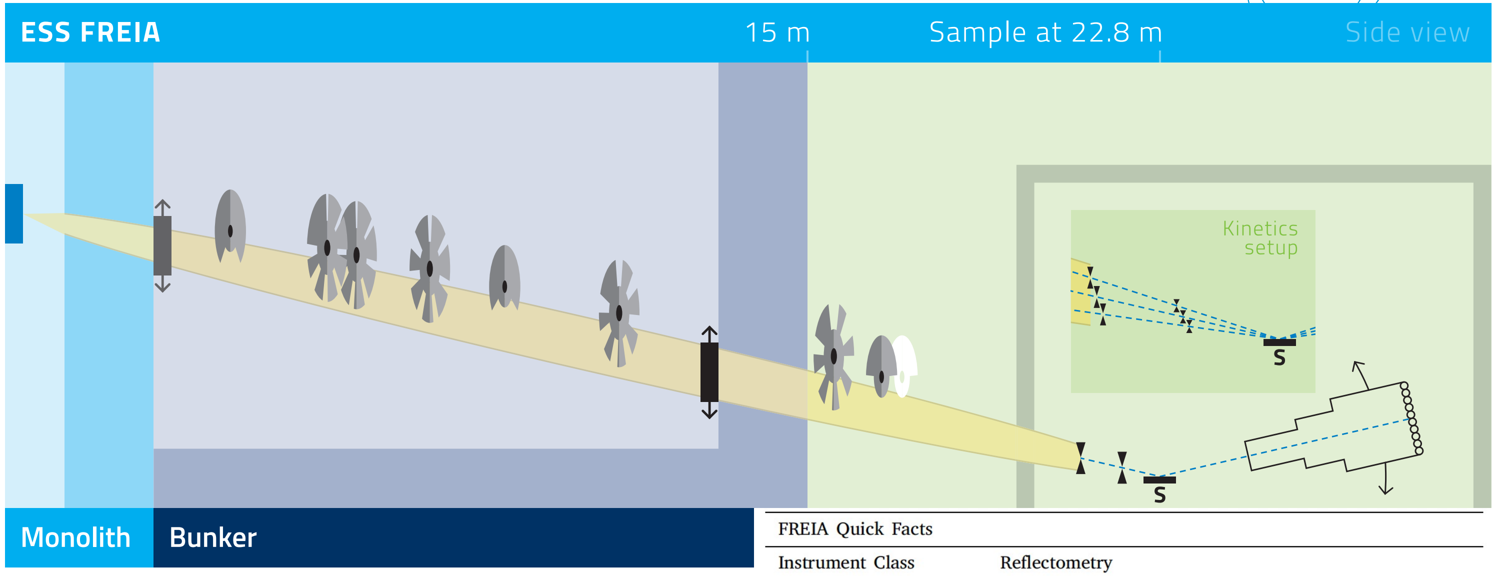
For the study of surfaces and interfaces including magnetic layers

FREIA Horizontal Reflectometer

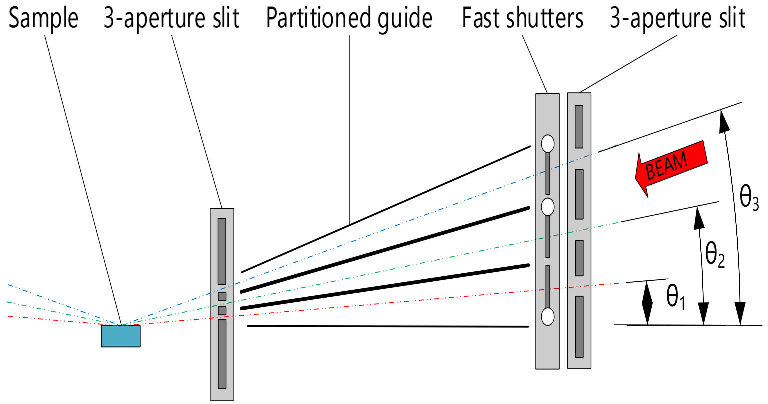
FREIA is a flexible instrument optimised for **time-resolved** and high throughput studies:

- Wide vertical divergence; **extended simultaneous Q range** & avoids slow sample movements
- Downward orientation for **liquid interfaces**
- **Flexible** Collimation options
- High flux (dλ/λ = 3-20 %) or high resolution (dλ/λ < 3%) modes

Wide ranging science case in **soft-matter and biosciences**



FREIA Quick Facts	
Instrument Class	Reflectometry
Moderator	Cold
Primary Flightpath	22.8 m
Secondary Flightpath	3.0 m
Polarised Incident Beam	Available as a foreseen upgrade
Sample Orientation	Horizontal
Representative Incident Beam Angles	0.45°, 0.9°, 3.4° (full range 0.2°–3.7° depending on angular resolution)
Standard Mode (14 Hz)	
Wavelength Range	2-10 Å
Flux at Sample at 2 MW	1×10^5, 5×10^5, 7×10^6 n s^{-1} cm^{-2} [high res (WFM) mode] 1×10^6, 4×10^6, 6×10^7 n s^{-1} cm^{-2} [high flux mode] 1×10^8 n s^{-1} cm^{-2} [full divergence mode]
Q-Range	0–1 $Å^{-1}$ (solid samples) 0.0045–0.38 $Å^{-1}$ (free liquids)
Q-resolution	3%–3.5% [high res (WFM) mode] 5%–23% (across free-liquid Q-range) [high flux mode] 2%–6% [full divergence (WFM) mode]
Pulse Skipping Mode (7 Hz)	
Wavelength Range	2–18 Å
Flux at Sample	5×10^5, 2×10^6, 3×10^7 n s^{-1} cm^{-2} [high flux mode]
Q-Range	0–1 $Å^{-1}$ (solid samples) 0.002–0.38 $Å^{-1}$ (free liquids)
Q-resolution	3%–23% (across free-liquid Q-range) [high flux mode]



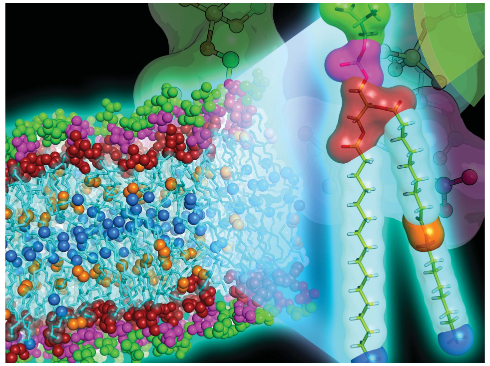
Fast Shutter development

Rapidly change angles without moving sample… allows full Q-range measurement with collimated beam with sub-second time resolution

FREIA

Science Case

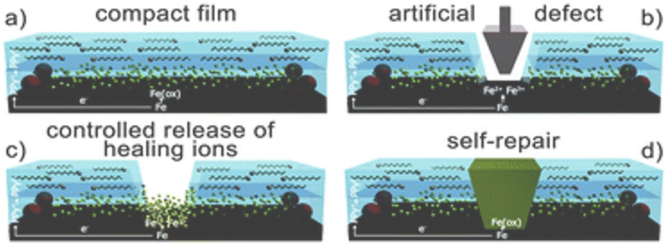
In-situ time-resolved reflectometry for soft condensed matter, life science and functional materials



Instrument characteristics to allow very fast measurements:

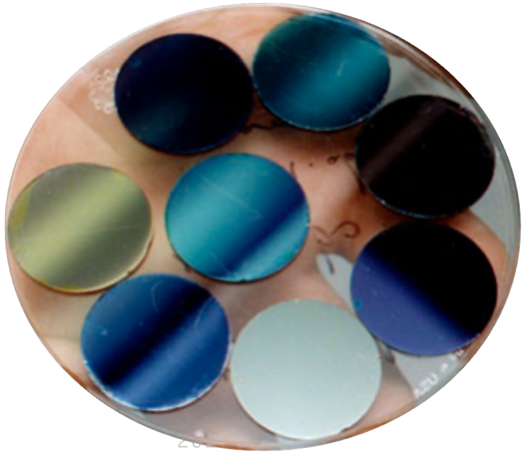
- Very high flux
- Horizontal sample geometry
- Flexible collimation
- Variable resolution
- Broad simultaneous Q
- No sample movement

Applications

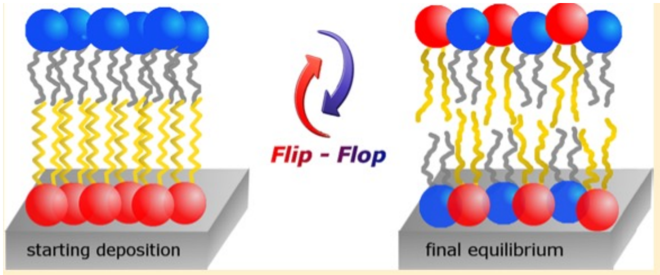


- response to external stimuli
- in situ and in operando
- complex sample environments

Design

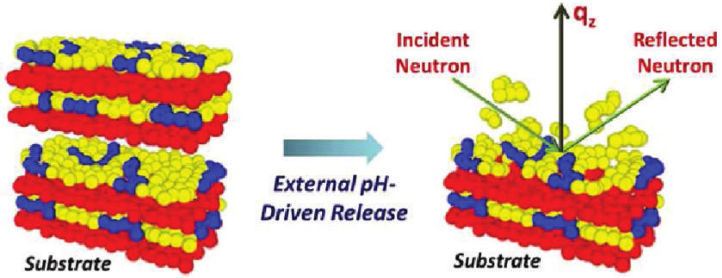


Dynamics



- deposition, structure and phase behavior
- adsorption, self-assembly and reactions
- gas/liquid/solid interfaces

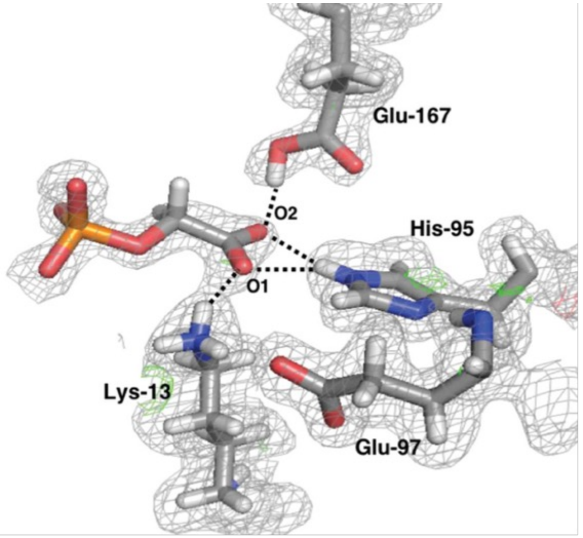
Function



NMX Macromolecular Diffractometer

Neutron macromolecular crystallography

Hydrogens are visible
No radiation damage



Kelpsas, V., Caldararu, O. et al. (2021) *IUCrJ* **8** 633-643

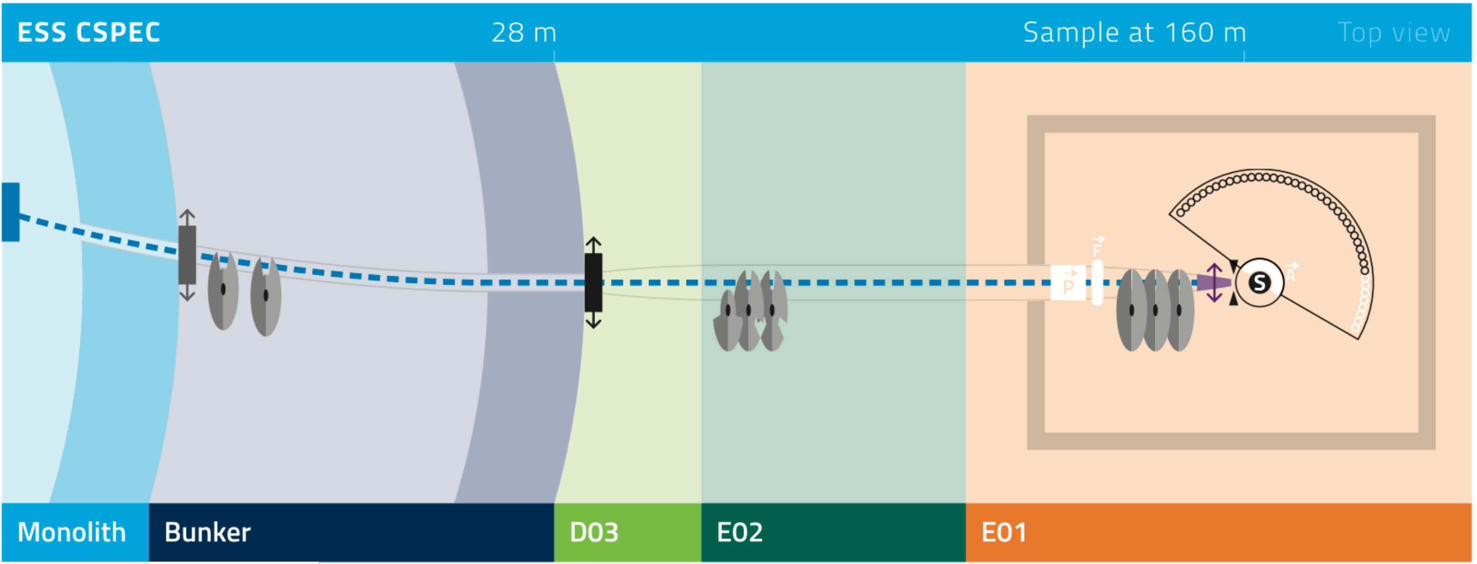
Where are hydrogens important?

Enzyme mechanisms
Protein-ligand interactions
Proton transport across membranes

Cold, TOF-Laue, Δλ<1.75 Å
158 m length
λ-range 1.8-10 Å
Robotic detector positioning
Gd-GEM detector

CSPEC: The cold chopper spectrometer of the ESS

Study of low lying excitations of materials with a focus on small samples, in-operando/kinetic behaviour
Need 10-50 x current day signal/noise to perform adequately



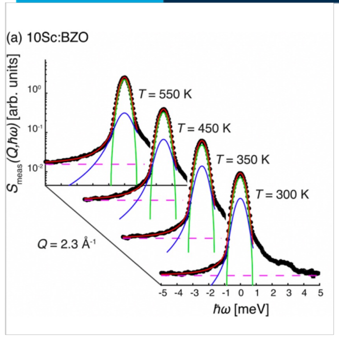
CSPEC: Scientific aims

Quasielastic scattering:

Translational dynamics

Diffusive dynamics

Rotational dynamics



Materials: Glass forming, liquid dynamics, crystal growth, hydrogen storage, fuel cells.

Soft matter: Polymer nanocomposites, organic photovoltaics, polymer electrolytes

Biology: hydration water, protein structure-dynamics-function, cell membrane-protein, drug delivery

Chemistry: ionic liquids, clays, complex fluids

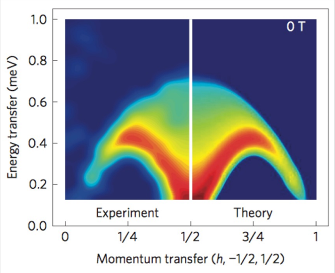
Low lying energy modes:

Spin dynamics

Critical scattering

Collective excitations

Quasiparticles



Nature Physics 9, 435–441 (2013)

Magnons, phonons, polarons

Topological states of matter: Majorana fermions.

RVB states, Quantum spin liquids, emergent behaviour.

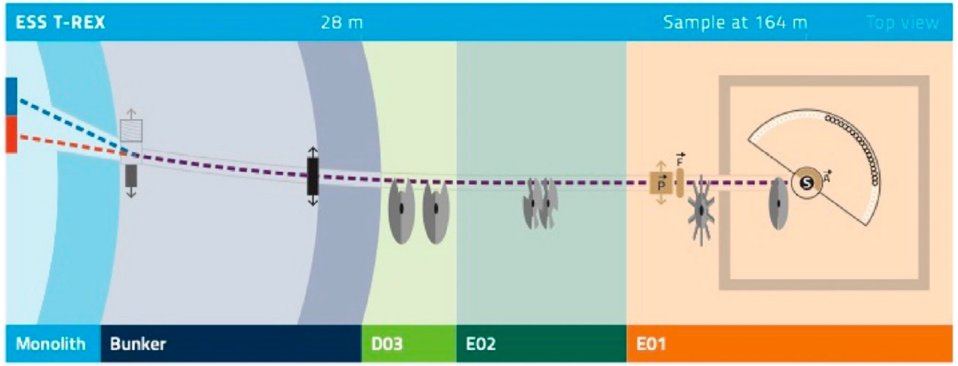
CSPEC quick facts

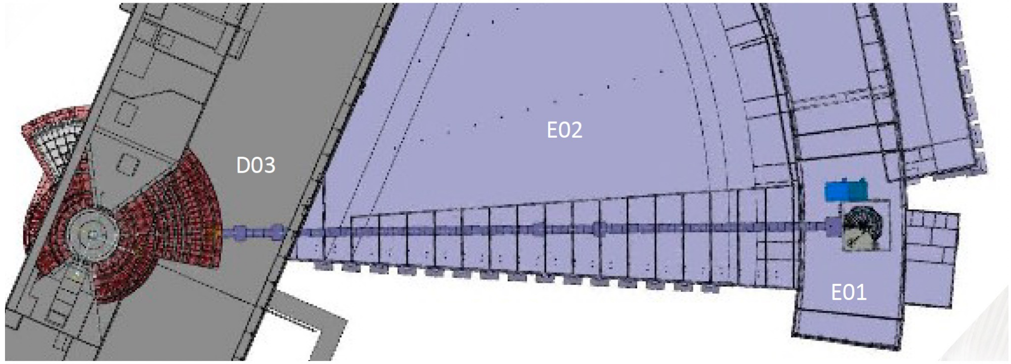
Primary flight path	160 m
Secondary flight path	3.5 m
Moderator	Cold
Wavelength range	2-20 Å
Bandwidth	1.72 Å
Flux at sample (2 MW, λ = 5 Å, $\Delta E/E_i$ = 3%, no RRM)	$9\ 10^5$ n s^{-1} cm^{-2} (4 x 2 cm^2 standard beam) $4\ 10^6$ n s^{-1} cm^{-2} (1 x 1 cm^2 focussed beam)
Full detector coverage	5° – 140° [H] ± 26° [V]
Energy resolution	1% - 5% E_i
Polarisation analysis	Foreseen upgrade

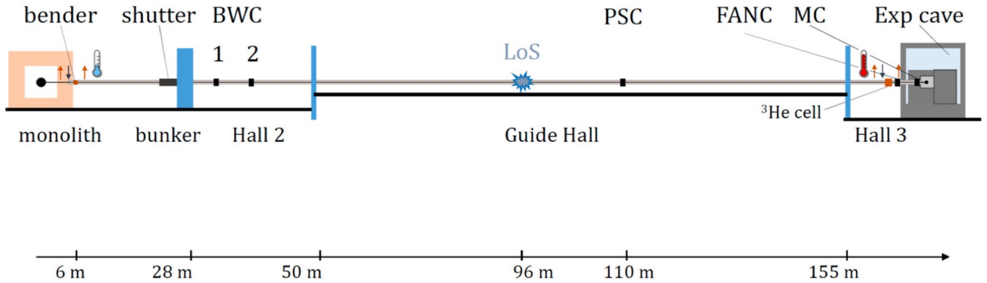
T-REX

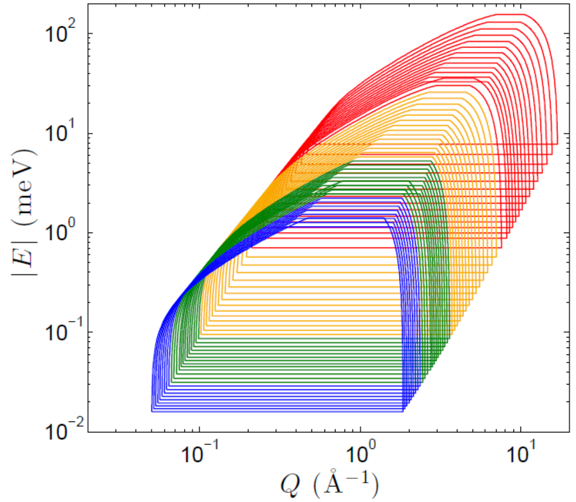
Time-of-Flight Recoprocal Space Explorer

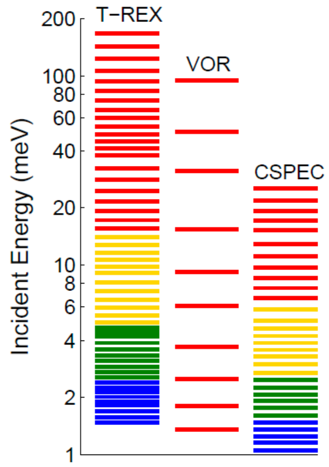
A neutron spectrometer for magnetism material science and soft matter







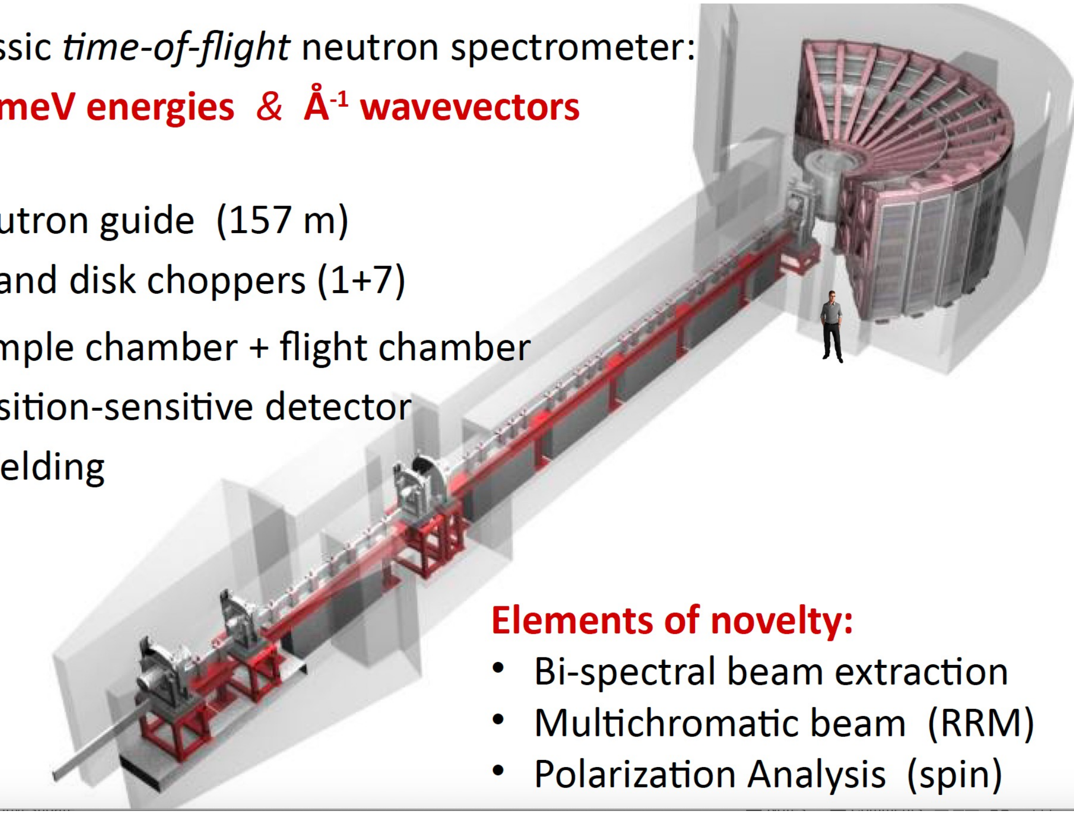




A classic *time-of-flight* neutron spectrometer:

meV energies & Å^{-1} wavevectors

- neutron guide (157 m)
- T_0 and disk choppers (1+7)
- sample chamber + flight chamber
- position-sensitive detector
- shielding



Elements of novelty:

- Bi-spectral beam extraction
- Multichromatic beam (RRM)
- Polarization Analysis (spin)