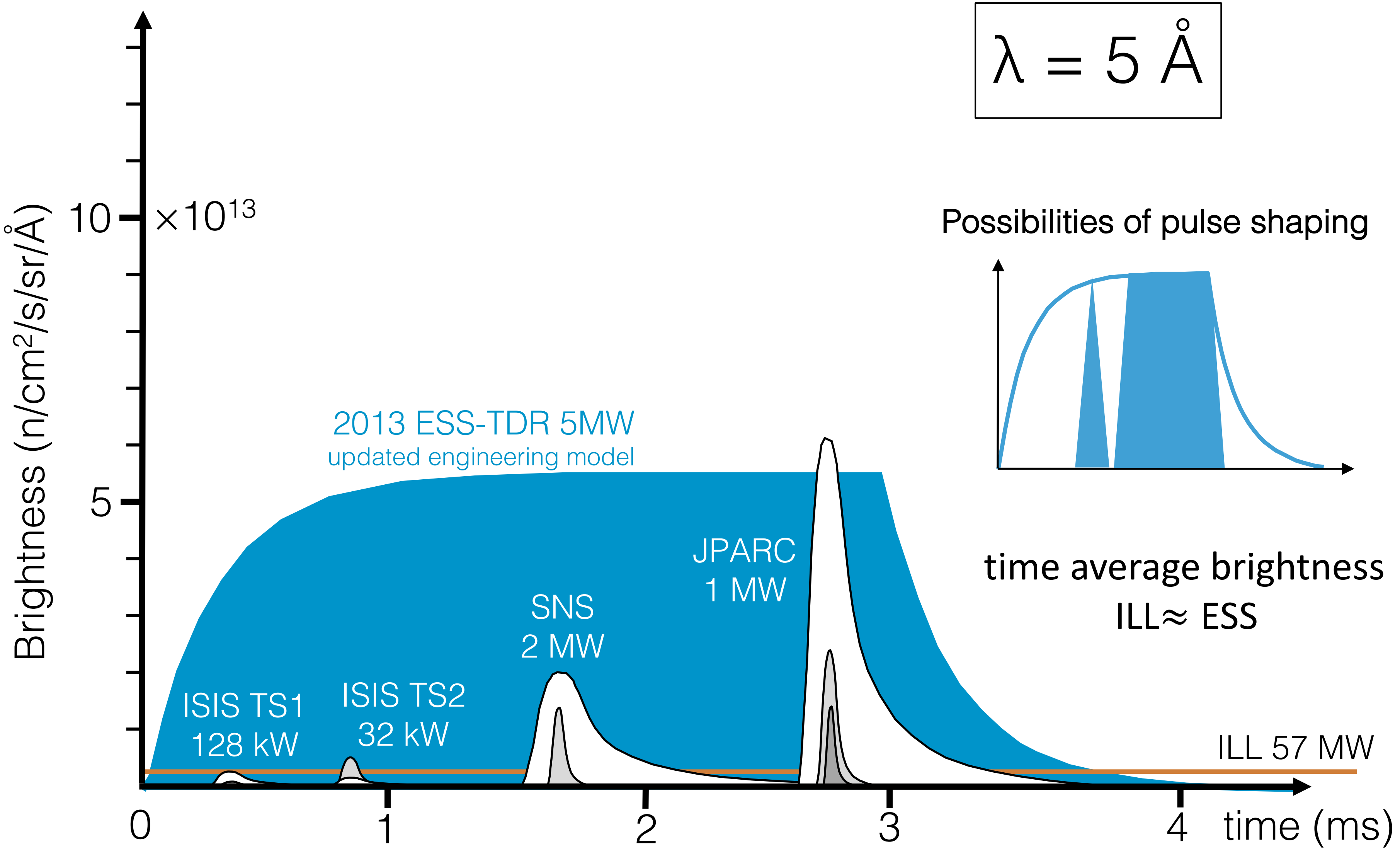
Overview of ESS Instruments

PRESENTED BY ANDREW JACKSON
// GROUP LEADER INSTRUMENT SCIENTISTS
// ACTING HEAD NEUTRON INSTRUMENTS DIVISION

2022-10-10

ESS is designed to be world leading

$\lambda = 5$ Å



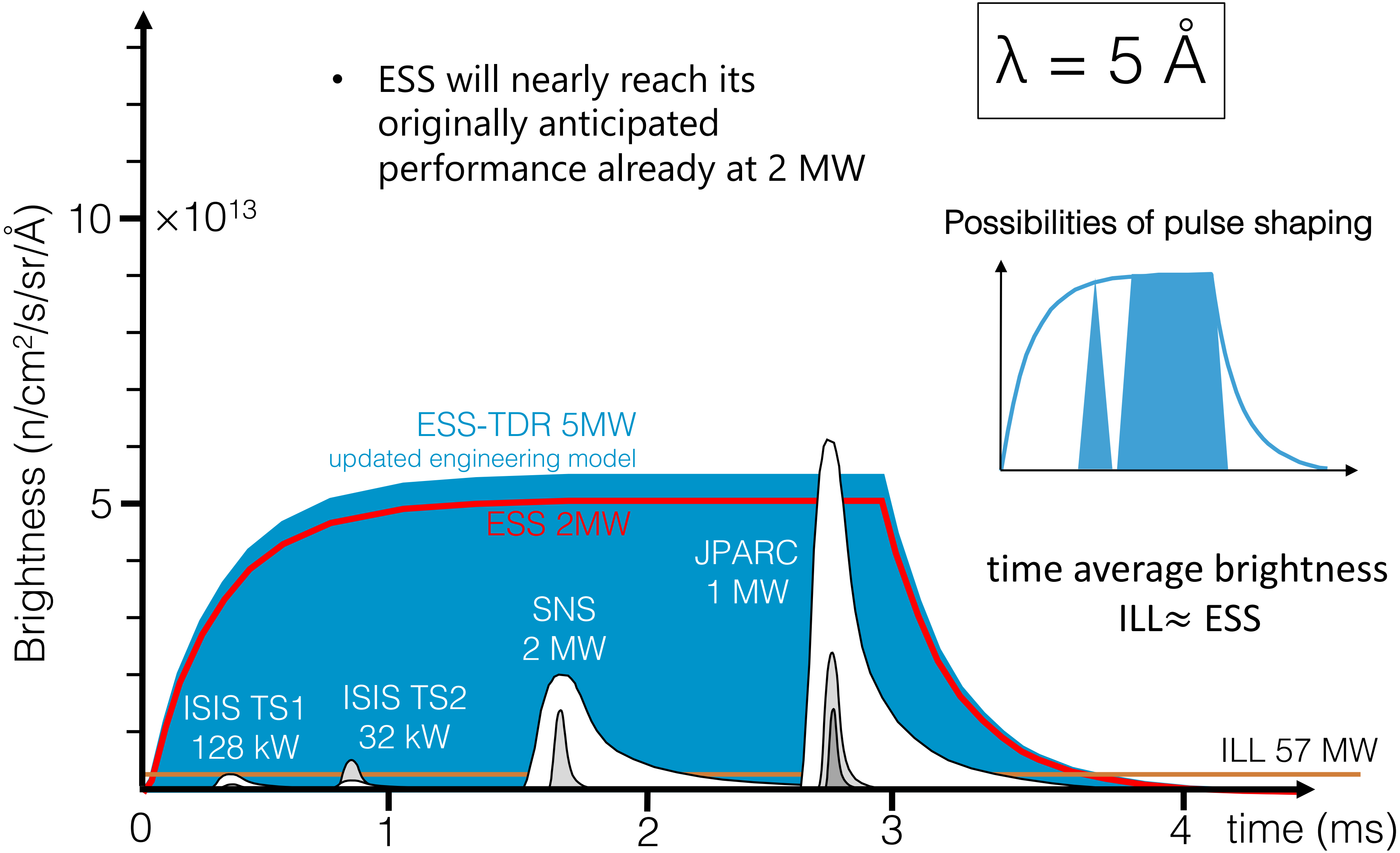
Possibilities of pulse shaping

time average brightness
ILL≈ ESS

ESS is designed to be world leading

Impressive improvement during design phase

- ESS will nearly reach its originally anticipated performance already at 2 MW



$\lambda = 5$ Å

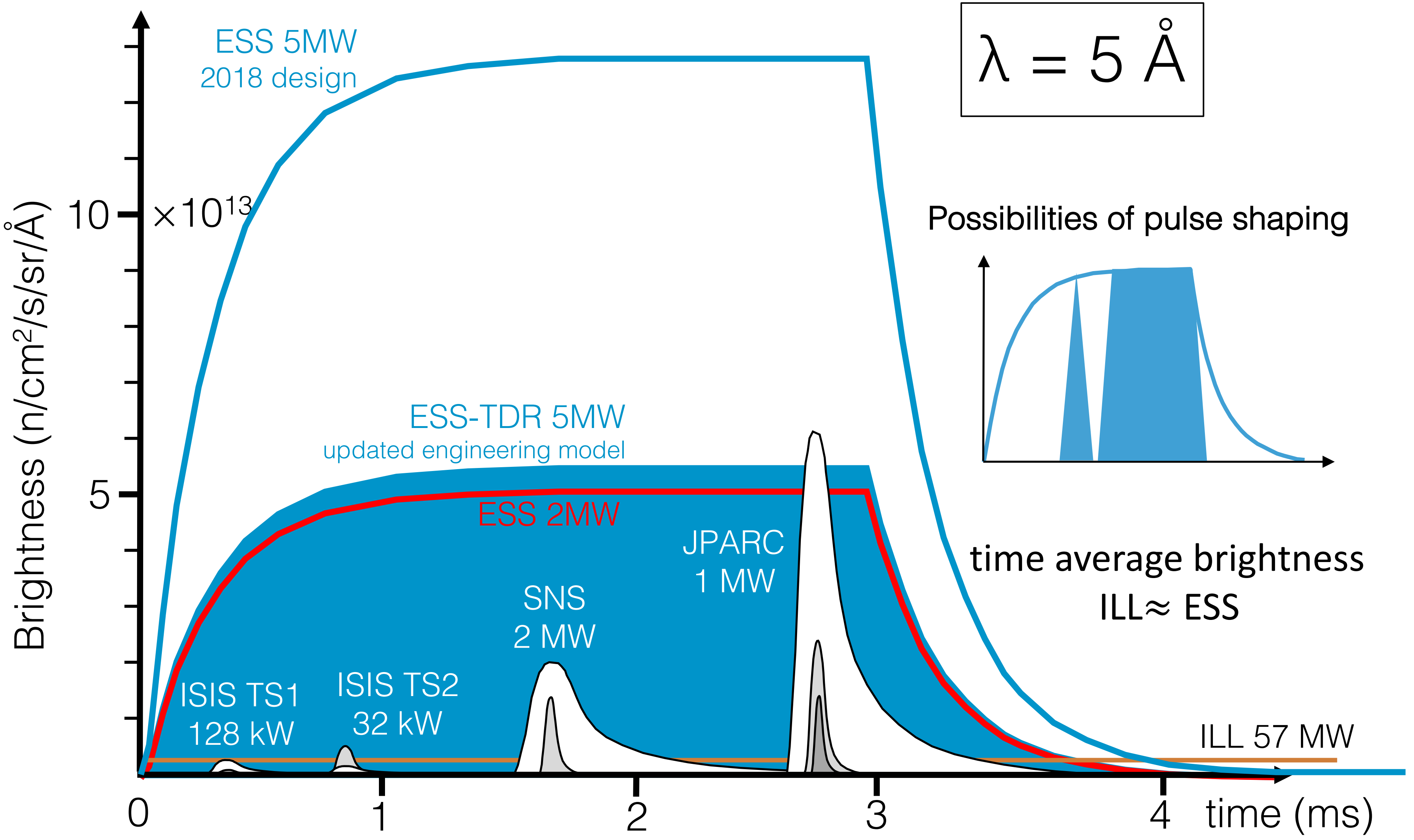
Possibilities of pulse shaping

time average brightness

ILL≈ ESS

ESS is designed to be world leading

Upgrade to 5MW will provide flux advantage to current and future instruments



Neutron Instruments

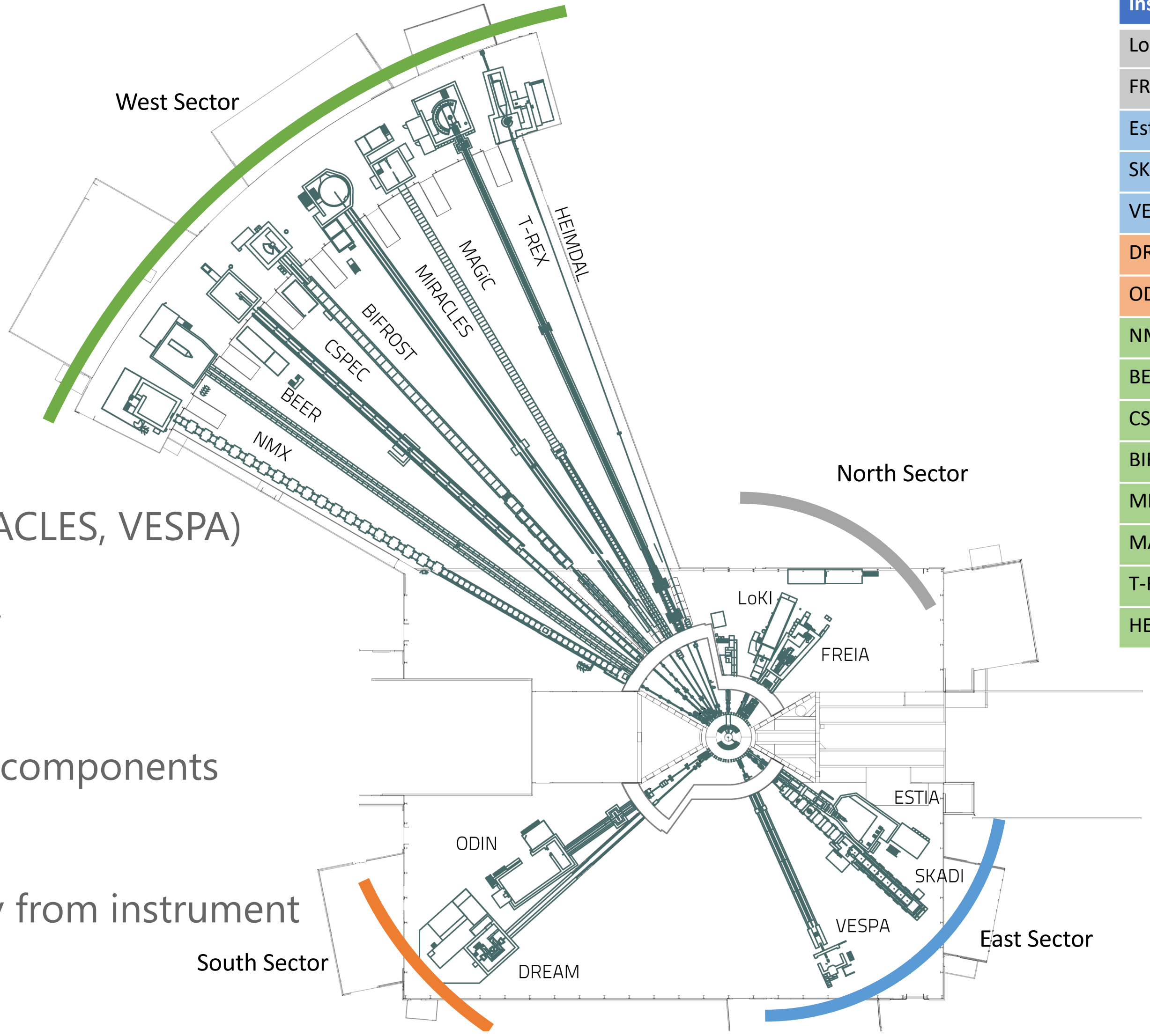
Andersen, K. H.; Argyriou, D. N.; Jackson, A. J. et al. The Instrument Suite of the European Spallation Source. *Nuclear Instruments and Methods in Physics Research Section A:* **2020**, *957*, 163402. https://doi.org/10.1016/j.nima.2020.163402.

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

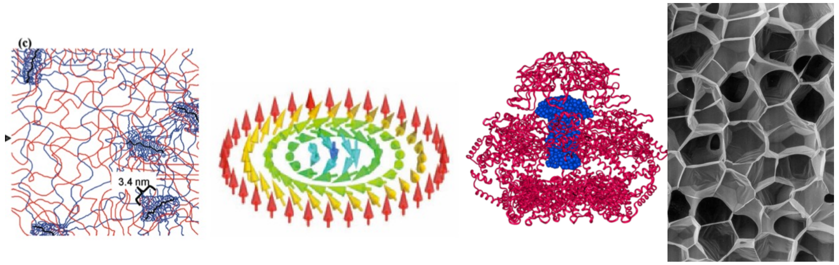
Large Scale Structures

5 Instruments

Instrument class coordinator: Tom Arnold

Small Angle Neutron Scattering (SANS)

Accessing length-scales up to μm

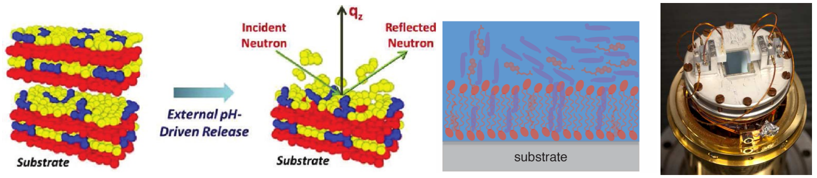


LoKI: Broad-band SANS for soft matter, materials and bio-science
Lead scientists: Judith Houston (ESS)
IK partners: ISIS (100%)

SKADI: High-resolution versatile SANS
Lead scientist: Sebastian Jaksch (FZJ)
IK partners: FZJ (50%), LLB (50%)

Reflectometry

Surfaces, thin films and interfaces

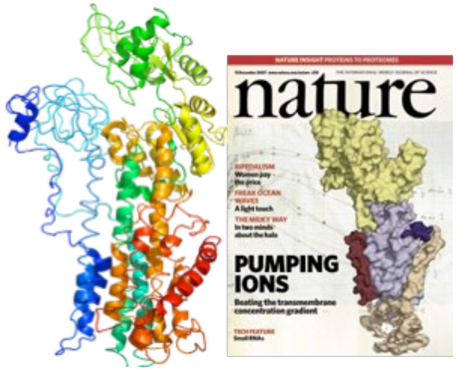


ESTIA: Small-sample reflectometer for magnetism and soft matter
Lead scientist: *Open Position* (PSI/ESS)
IK partners: PSI (100%)

FREIA: Kinetics reflectometer for liquid surfaces and soft matter
Lead scientist: Tom Arnold (ESS)
IK partners: ISIS (100%)

Macromolecular Crystallography

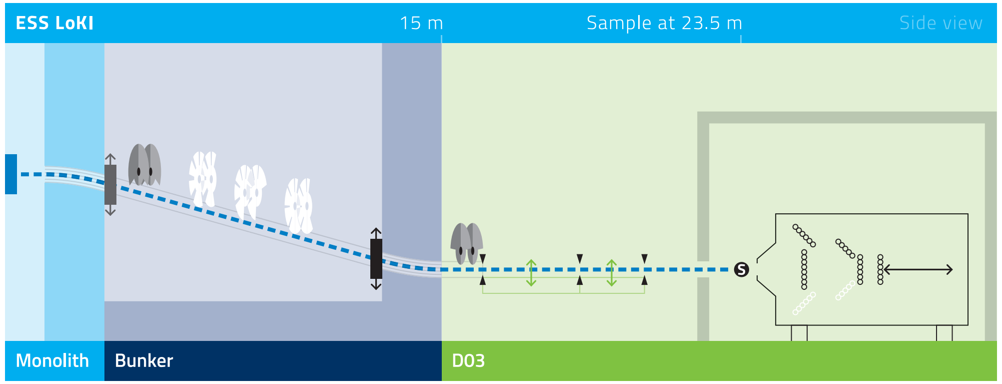
Biomolecule Crystal Structure



NMX: Macromolecular crystallography
Lead scientist: Esko Oksanen (ESS)
IK partners: Wigner/EK/BRC (38%), LLB/IBS (8%), UiBergen (19%)

LoKI

SANS for Soft Matter, Materials and Bio-science

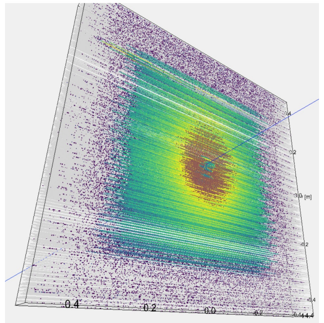


Detector mechanics and modules awaiting delivery

Detector tank installed
Shielding walls under installation

Detector Tests

We collected calibration data on the LoKI rear detector panel using the full ESS software stack at ISIS. Excellent test for hot commissioning.



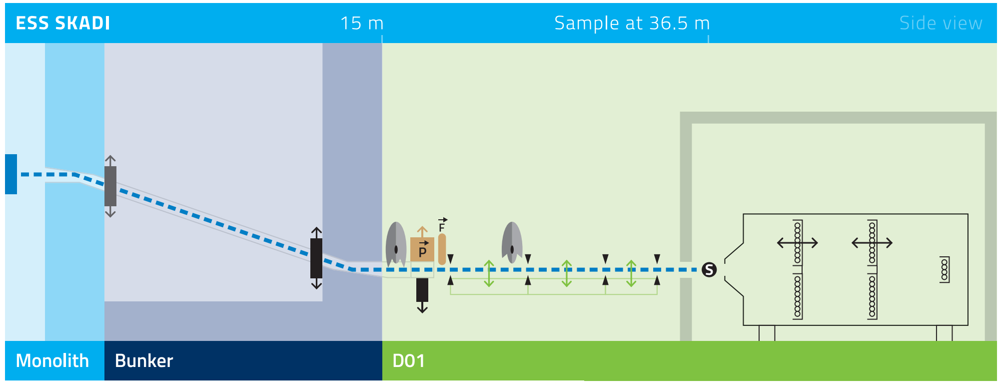
NeXus file displayed in scipp
From the latest measurements in March 2022

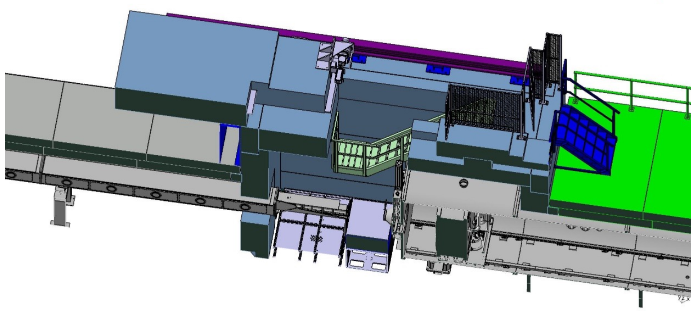
LoKI Quick Facts	
Instrument Class	SANS
Moderator	Cold
Primary Flightpath	23.5 m, L_1 = 3, 5, 8 m
Secondary Flightpath	L_2 = 1.5 m, 3 m, 5–10 m
Wavelength Range	2–22 Å
Standard Mode (14 Hz)	
Bandwidth	7.5 Å [L_2 = 10 m] 10 Å [L_2 = 5 m]
Flux at Sample at 2 MW	4×10^8 n s^{-1} cm^{-2} [L_1 = 3 m] 5.6×10^7 n s^{-1} cm^{-2} [L_1 = 8 m]
Q-Range	0.01–2 $Å^{-1}$ [L_1 = 3 m, L_2 = 1.5, 5 m] 0.005–2 $Å^{-1}$ [L_1 = 8 m, L_2 = 1.5, 10 m]
Pulse Skipping Mode (7 Hz)	
Bandwidth	15 Å [L_2 = 10 m] 20 Å [L_2 = 5 m]
Flux at Sample at 2 MW	2×10^8 n s^{-1} cm^{-2} [L_1 = 3 m] 2.8×10^7 n s^{-1} cm^{-2} [L_1 = 8 m]
Q-Range	0.005–2 $Å^{-1}$ [L_1 = 3 m, L_2 = 1.5, 5 m] 0.002–2 $Å^{-1}$ [L_1 = 8 m, L_2 = 1.5, 10 m]

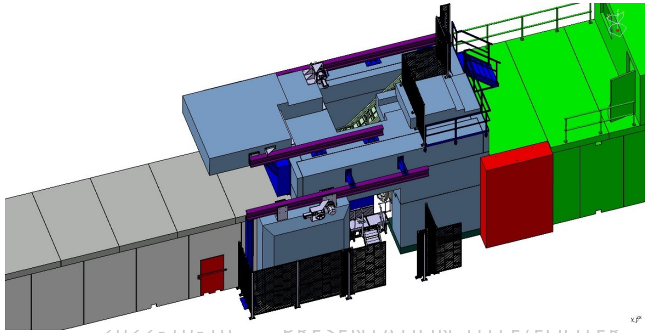
Science and Technology Facilities Council

SKADI

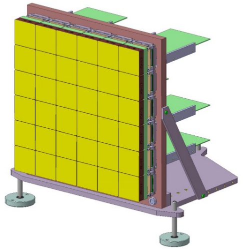
Small-K Advance Diffractometer – Polarised SANS for Materials Science

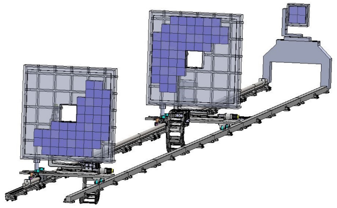






SoNDe
Solid-State Neutron Detector





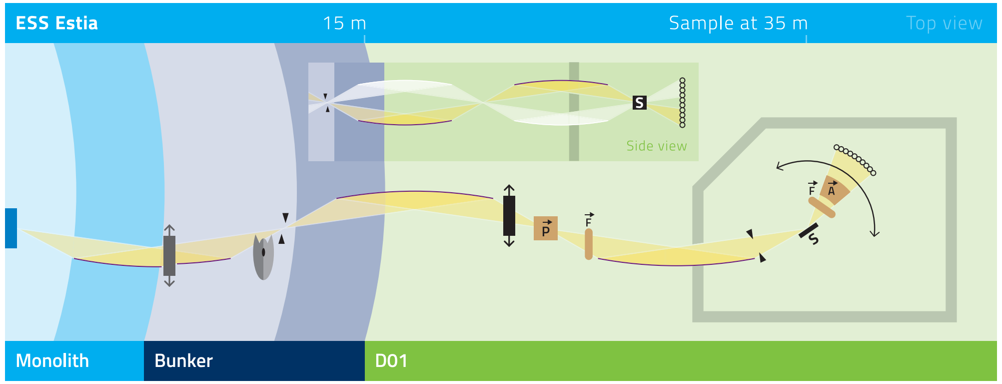
Quick Facts	
Sector	East
Beam Port	E03
Class	Polarized SANS
Moderator	Cold
Length	58 m
Q-Range	10^{-4} – 1 $Å^{-1}$
Flux at sample position	7.7×10^{8} n s^{-1} cm^{-2}
Start of operation	Close to BOT
Standard Mode (14 Hz)	
Wavelength Band	5 Å
Wavelength Range	3 – 21 Å
Momentum Resolution	ΔQ/Q= 2-7 %
Pulse Skipping Mode (7 Hz)	
Wavelength Band	10 Å
Wavelength Range	3 – 21 Å
Momentum Resolution	ΔQ/Q = 1-7 %

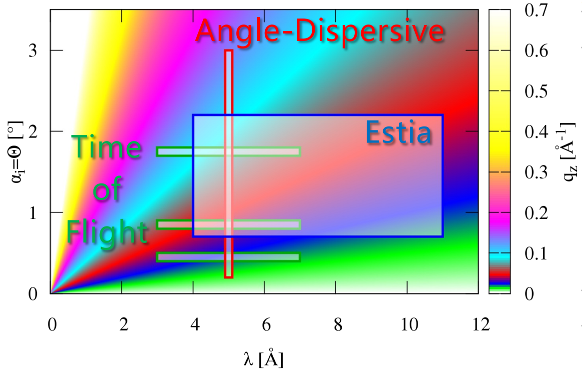
Orphée Laboratoire Léon Brillouin

JÜLICH FORSCHUNGSZENTRUM

Estia

Focussing Polarised Reflectometer for Tiny Samples

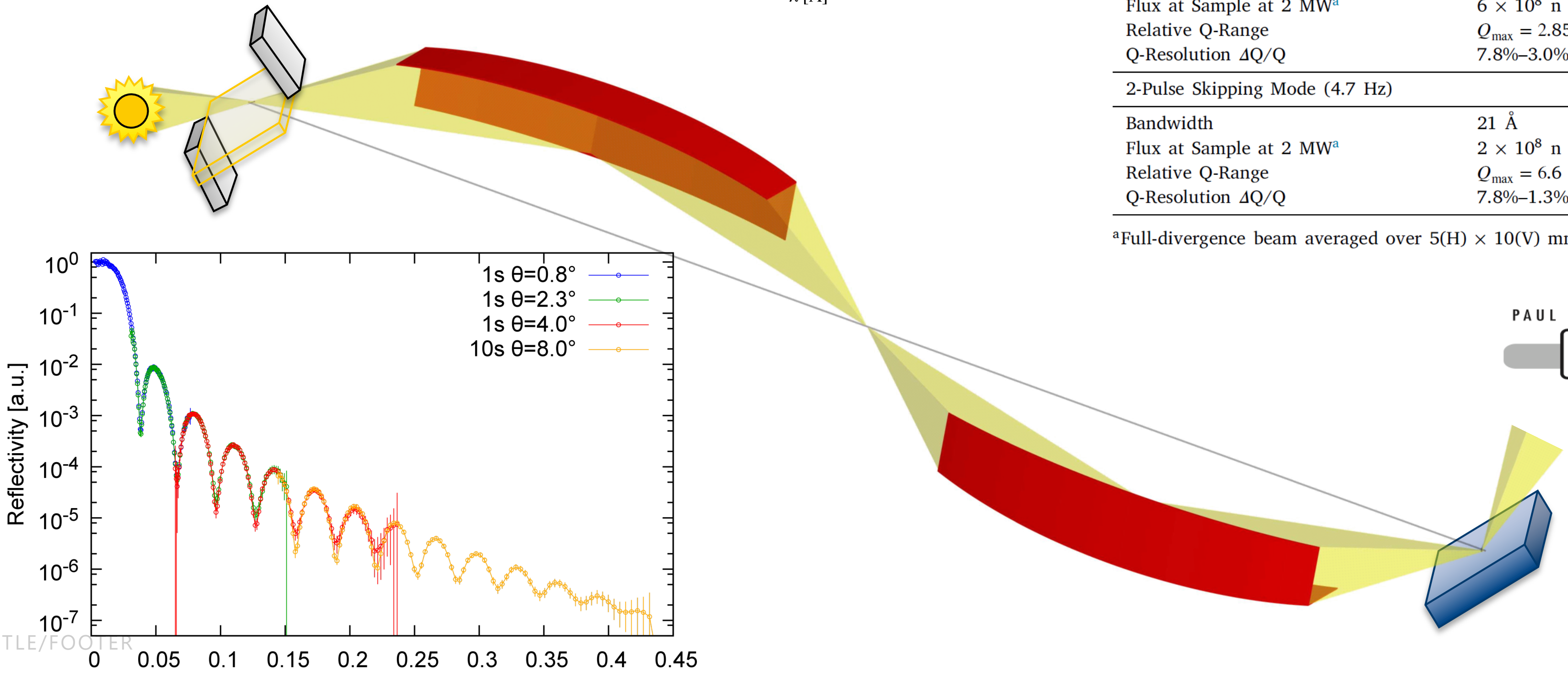




Estia Quick Facts.

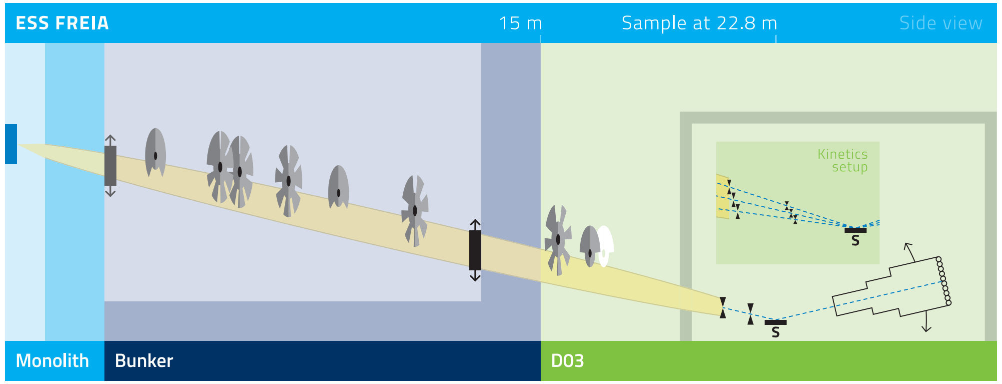
Estia Quick Facts	
Instrument Class	Reflectometry
Moderator	Cold
Primary Flightpath	35 m
Secondary Flightpath	4 m
Wavelength Range	3.75–28 Å
Polarised Incident Beam	Optional
Polarisation Analysis	Optional
Sample Orientation	Vertical
Total Q-Range	0.001 to 3.15 Å^{-1}/–0.001 to –0.3 Å^{-1}
Standard Mode (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.

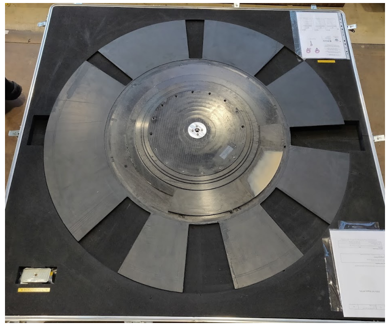


FREIA

A neutron reflectometer optimised for soft matter and life sciences.



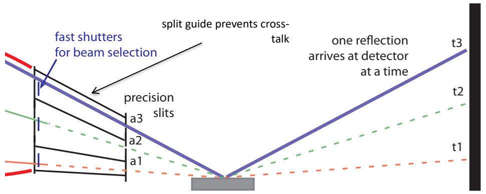
Carbon fibre, 1.3m chopper discs delivered (Airbus)



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 2MW*	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]
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]
Pulse Skipping Mode (7 Hz)	
Wavelength Range	2-18 Å
Flux at Sample at 2MW*	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]

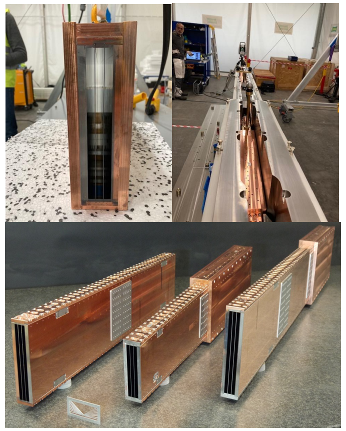
Fast-shutter project

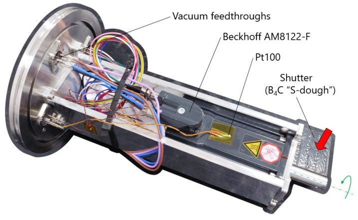
Collaboration with Marek Jacewicz, Niklas Johansson & Tord Ekelöf (FREIA lab, Uppsala University), James Doutch (ISIS, STFC) and Tommy Nylander & Ben Humphries (Lund University)

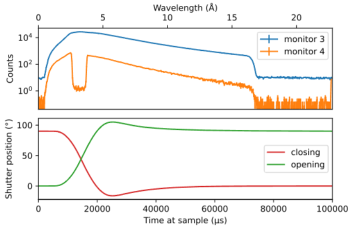


- used to rapidly change angles in between source pulses
- prototype tested with beam at ISIS (ZOOM)

In-monolith optics delivered (SD-H & Jülich)







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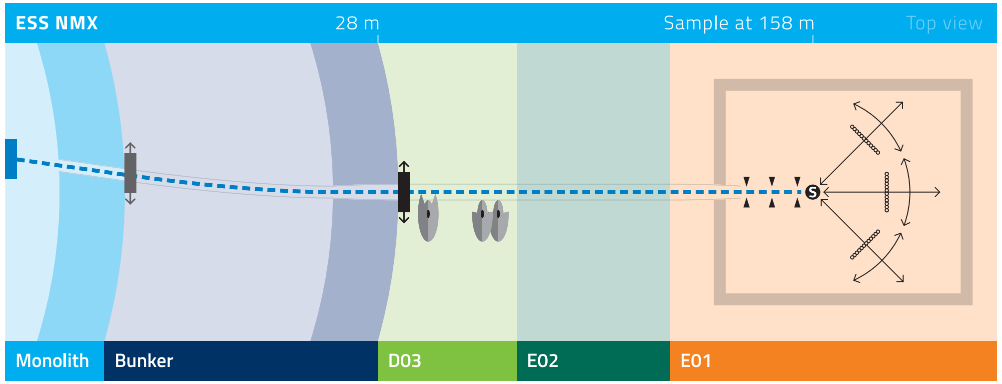
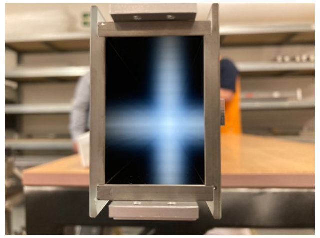
*All values quoted for the high resolution and high flux modes assume the incident angles stated, an angular resolution of 2.5% $\Delta\theta/\theta$ (this resolution could be improved for the high-resolution mode or relaxed for the high-flux mode) and a beam footprint of 8cm x 3cm .

Science and Technology Facilities Council

NMX

Macromolecular Diffractometer

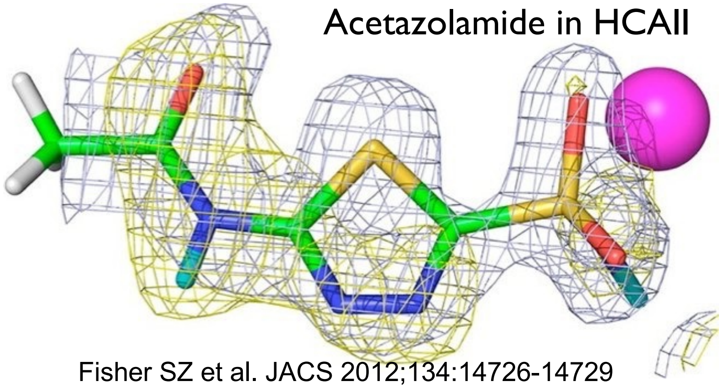




NMX Quick Facts.

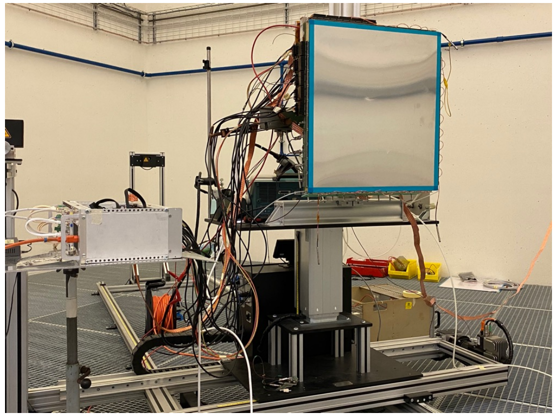
NMX Quick Facts	
Instrument Class	Large-Scale Structures
Moderator	Cold
Primary Flightpath	157 m
Secondary Flightpath	0.2–1.0 m
Wavelength Range	1.8–10 Å
Bandwidth	1.74 Å
Flux at Sample at 2 MW	1×10^9 n s^{-1} cm^{-2} (1.8–3.5 Å)
Wavelength Resolution $\Delta\lambda/\lambda$	2%–4% (over wavelength range)
Beam Divergence	Adjustable up to $\pm 0.2°$
Beam Size	0.2–5 mm

- Enzyme mechanisms
- Protein-ligand interactions
- Proton transport across membranes



Acetazolamide in HCAII

Fisher SZ et al. JACS 2012;134:14726-14729



Imaging & Engineering

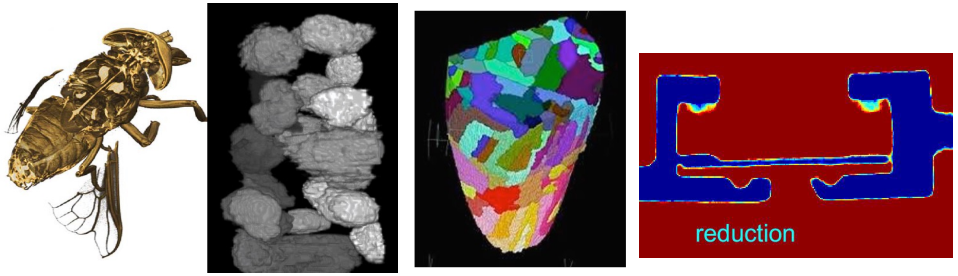
2 Instruments

Instrument class coordinator: Robin Woracek

Imaging: rapidly developing real-space technique, resolution down to few μm

ODIN: Multi-purpose imaging beamline
Lead scientists: Aureliano Tartaglione (TUM), Manuel Morgano (ESS)

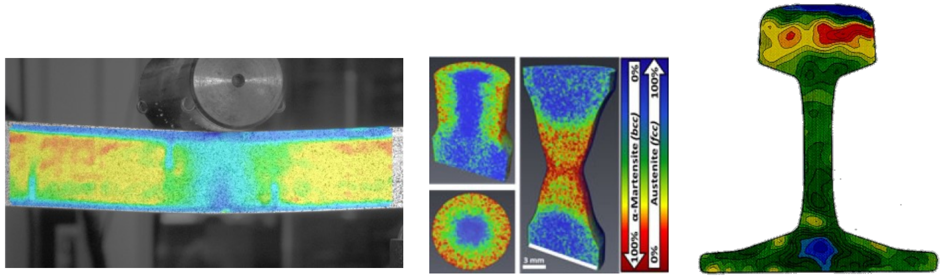
IK partners: TUM (55%), PSI (35%), ESS (10%)



Engineering: strains and structure of engineering components, in-situ materials processing

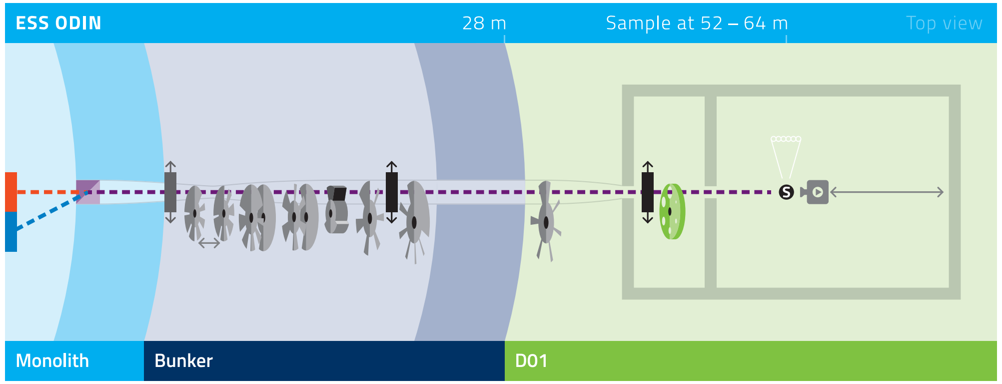
BEER: Engineering materials diffractometer
Lead scientists: Premek Beran (ESS), Gregor Nowak (Hereon)

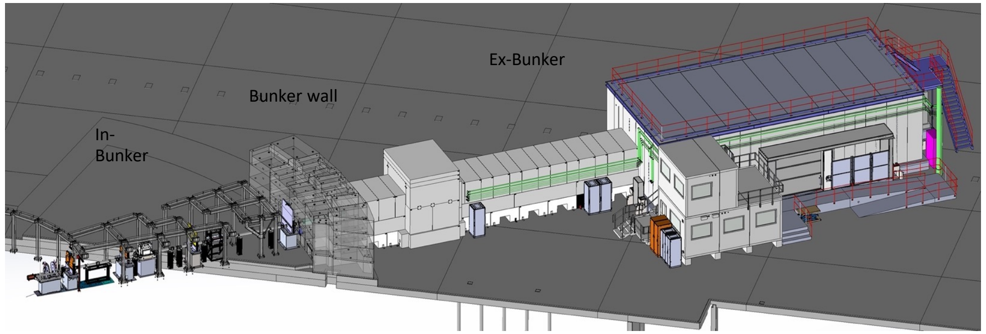
IK partners: NPI (50%), Hereon (50%)

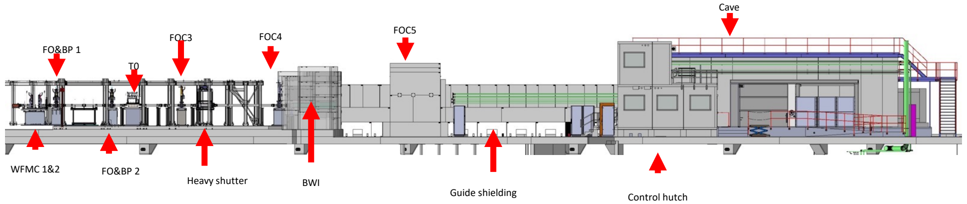


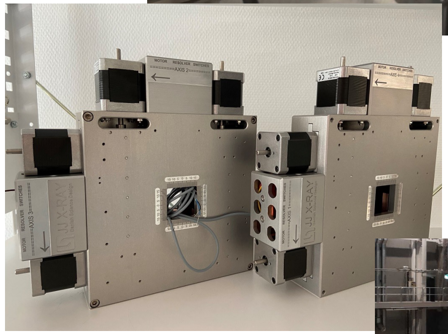
ODIN

Optical and Diffraction Imaging with Neutrons









ODIN Quick Facts	
Instrument Class	Imaging
Moderator	Bispectral
Primary Flightpath	50 m (to pinhole)
Secondary Flightpath	2 – 14 m (pinhole to detector)
Wavelength Range	1 – 10 Å
Field of View	20 x 20 cm^2
L/D Ratio	Tunable 300 – 10000
Incident Beam Polarisation	Optional
Polarisation Analysis	Optional
Bandwidth at 14 Hz	4.5 Å
White Beam Mode	
Flux at Sample at 2 MW	1.2 x 10^9 n s^{-1} at 10 m, L/D = 300
Spatial Resolution	< 10 µm
TOF Mode without Pulse-Shaping	
Flux at Sample at 2 MW	9 x 10^8 n s^{-1} at 10 m, L/D = 300
Spatial Resolution	< 10 µm
Wavelength Resolution	Δλ/λ = 10% at λ = 2 Å
TOF Mode width Pulse-Shaping	
Flux at Sample at 2 MW	1 x 10^8 n s^{-1} at 10 m, L/D = 300
Spatial Resolution	< 10 µm
Wavelength Resolution	Adjustable <0.5% - 1% (constant for all λ)

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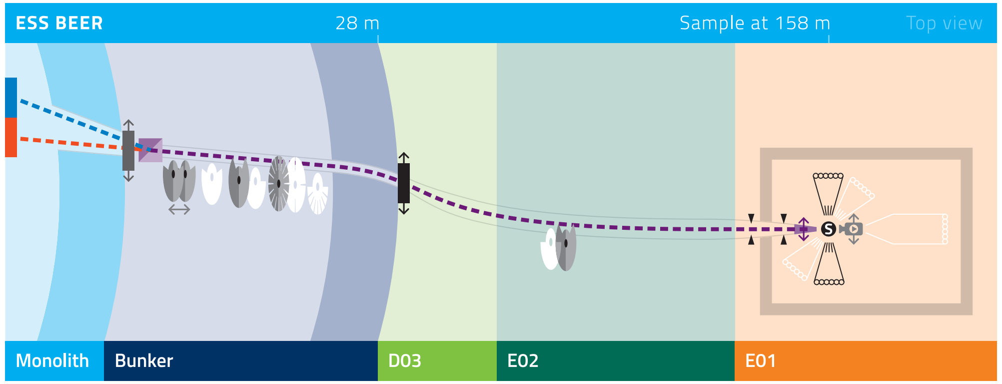
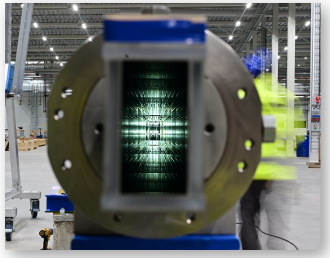
PAUL SCHERRER INSTITUT

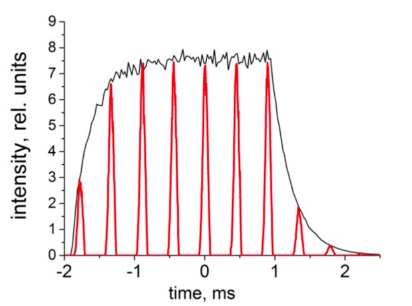
BEER

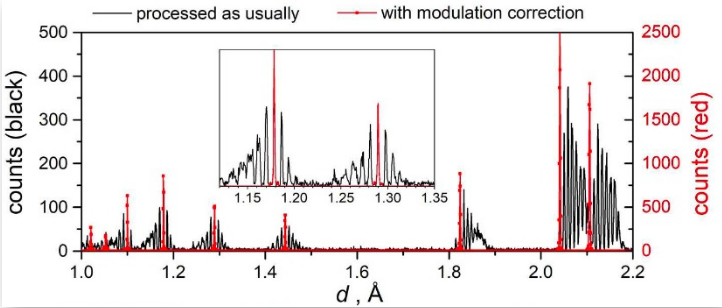
Engineering & Material Science Diffraction



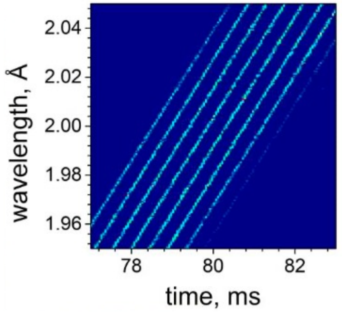


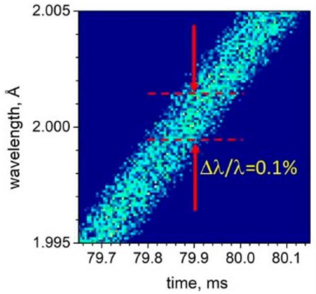
BEER Quick Facts	
Instrument Class	Engineering Diffraction
Moderator	Bispectral
Primary Flightpath	158 m
Secondary Flightpath	2 m
Wavelength Range	0.8 – 6 Å
Bandwidth	1.7 Å
d-spacing Range	0.6 – 7 Å
Pulse-Shaping Mode	
Resolution Δd/d	0.15 – 0.6 %
Flux at Sample at 2MW	0.18 – 1.4·10^8 n s^{-1} cm^{-2}
Modulation Mode	
Resolution Δd/d	0.1 – 0.3 %
Flux at Sample at 2MW	0.18 – 0.87·10^8 n s^{-1} cm^{-2}

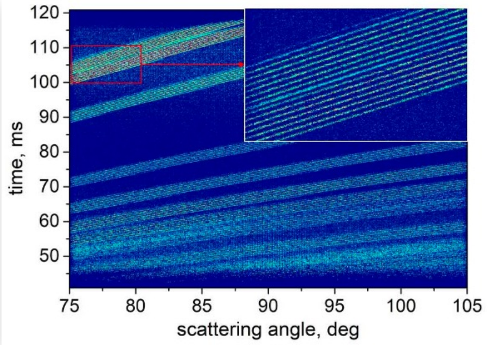




- In-situ and in-operando experiments close to the real conditions
- Fast strain scanning
- Phase analysis of multi-phase and composite materials
- In-situ texture or grain growth evolution
- Long term experiments







Helmholtz-Zentrum hereon

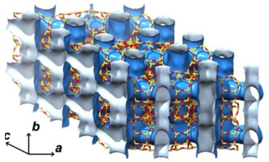
Diffraction

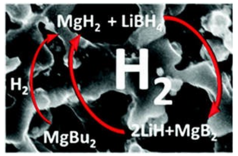
3 Instruments

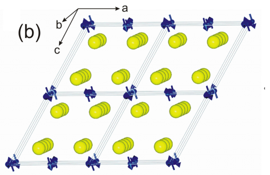
Instrument class coordinator: Werner Schweika

Powder Diffraction

Structural characterisation of materials





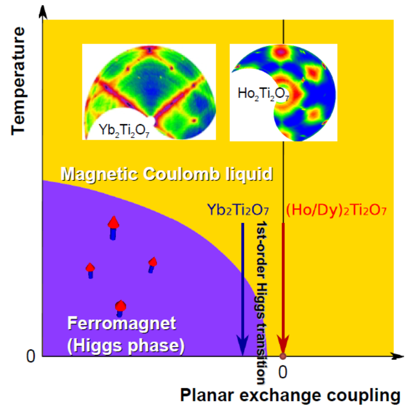


DREAM: General-purpose powder diffractometer
Lead scientist: Mikhail Feygenson (ESS)
IK partners: FZJ (76%), LLB (24%)

HEIMDAL: Thermal powder diffractometer
Lead scientist: Dan Mannix (ESS)
IK partners: ÅU (30%), PSI (35%), IFE (35%)

Single-Crystal Diffraction

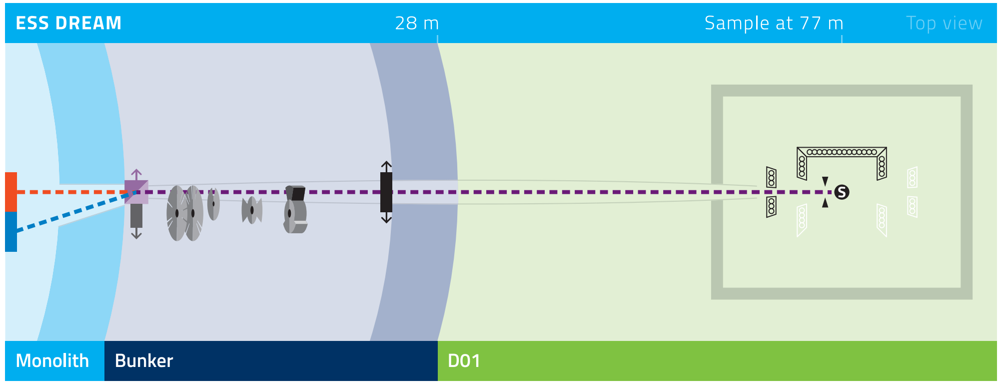
Determination of complex structures



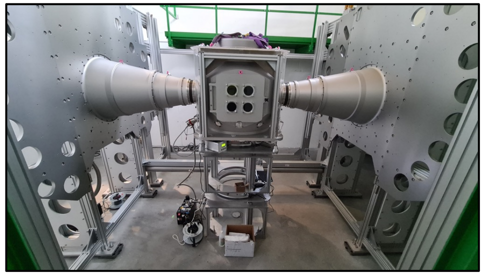
MAGiC: Magnetism diffractometer
Lead scientist: Xavier Fabrèges (LLB)
IK partners: LLB (61%), FZJ (23%), PSI (16%)

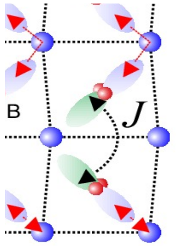
DREAM

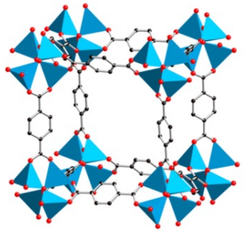
Diffraction Resolved by Energy and Angle Measurements



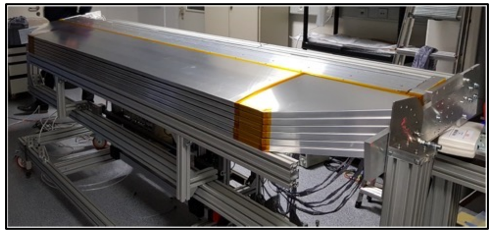
Sample vessel







Mantle & Endcap detectors



Experimental caves & Control hutches

Magnetism
superconductors
multiferroics
weak moments
orbital ordering
charge ordering

Energy Materials
Li, H -materials
in-situ measurements
multiphase
small coin cells

Nanostructures
magnetic nanoparticles
core-shell structures
real-time synthesis

Large Unit Cells
MOFs
catalysis
thermoelectrics
molecular sieves
H2- storage

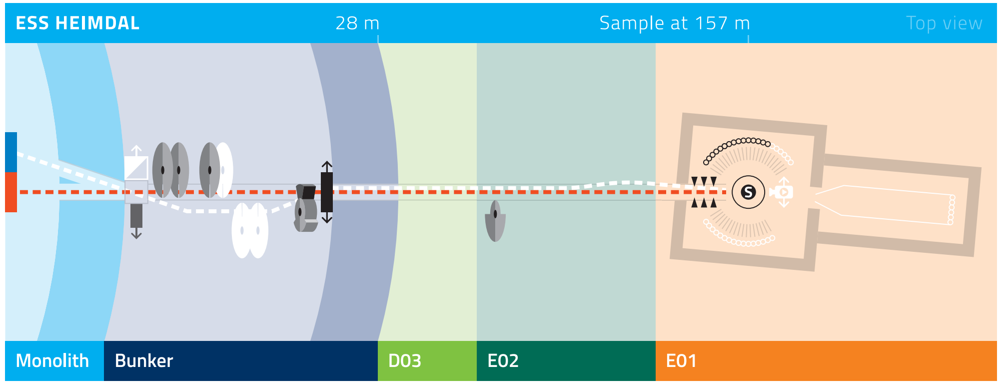
Moderator	Bi-spectral
Primary Flightpath	76.5 m
Secondary Flightpath	1.1 m (end-cap and mantle detectors) 2.5 m (high-resolution and low-angle detectors)
Wavelength Range	0.5–4.1 Å
Flux at sample at 2MW	1.4×10^{7}ns^{-1}cm^{-2} (Δd = 3×10^{-4} Å) 1.0×10^{9}ns^{-1}cm^{-2}(Δd = 2.5×10^{-2} Å)
Q-Range	0.01 – 25 Å^{-1}
Detector Coverage	1.82 sr first day operations 5.12 sr full scope
d-spacing Resolution Δd	Adjustable 3×10^{-4} – 2.5×10^{-2} Å

Orphée Laboratoire Léon Brillouin

JÜLICH FORSCHUNGSZENTRUM

HEIMDAL

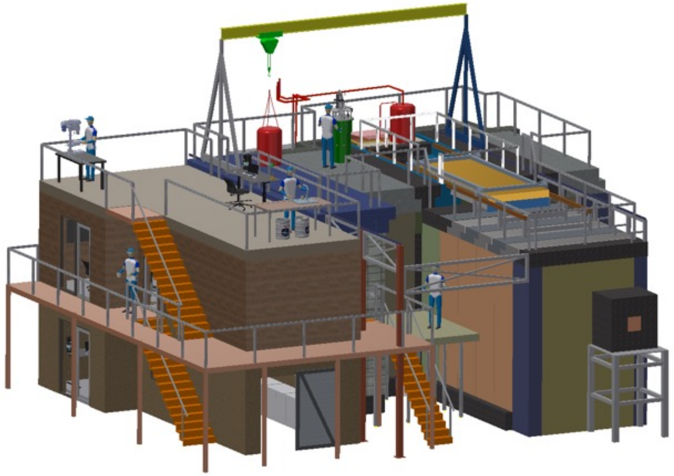
Hybrid Diffractometer: Combined Diffraction and SANS and Imaging



HEIMDAL Quick Facts.

HEIMDAL Quick Facts	
Instrument Class	Diffraction
Moderator	Thermal (Bispectral and Cold[a])
Primary Flightpath	157 m
Secondary Flightpath	Diffraction: 0.8 m (SANS: 10 m, Imaging: 4 m[a])
Wavelength Range	0.5–4 Å
Bandwidth	1.7 Å
Flux at Sample at 2 MW	10^6–10^8–10^9 n s^{-1} cm^{-2} (High-resolution – Medium-res. – High-flux)
Q-Range	0.5–25 $Å^{-1}$
d-spacing Resolution $\Delta d/d$	Adjustable 0.04%–1%
SANS and Imaging modes[a]	
Moderator	Cold
Wavelength Range	3–20 Å
Q-Range (SANS)	10^{-3}–4 $Å^{-1}$
Wavelength Resolution $\Delta\lambda/\lambda$ (SANS)	1.5% at $\lambda = 4$ Å 0.6% at $\lambda = 11$ Å
Field of View (Imaging)	50 × 50 mm^2
Spatial Resolution (Imaging)	50 μm

- Real time chemical synthesis
- Fast chemical reactions and kinetics
- 2D Rietveld Neutron Powder Diffraction
- In operando fuel cells and batteries
- Texture studies
- Magnetic Materials
- Superconductor Materials
- In situ catalysis
- Single crystal diffraction of small samples
- Nano-particles and core-shell structures



Full Technical Scope

- Bispectral Instrument
- Thermal + Cold Neutron Guides
- Optimised Diffraction & SANS
- 3D Neutron Imaging

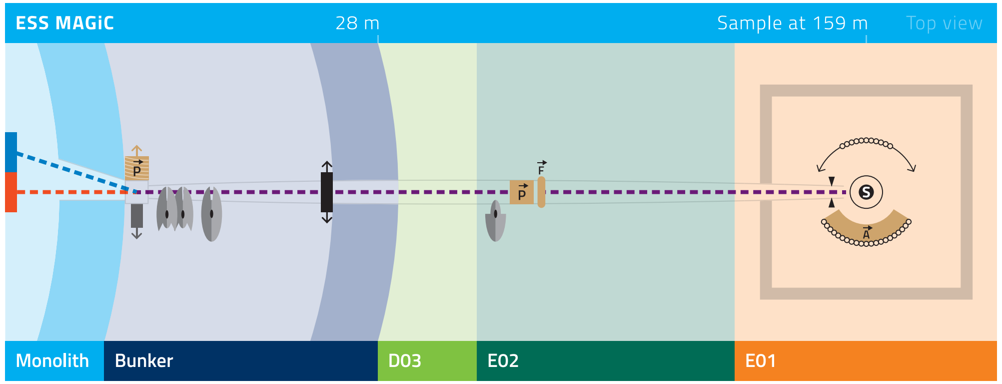
Aarhus University (AU)

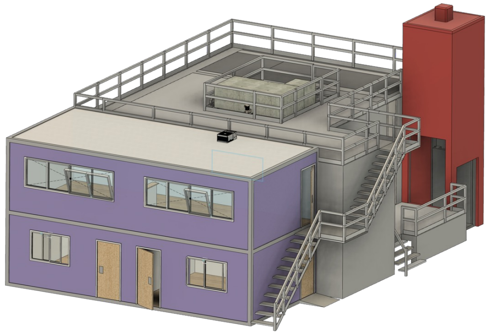
Institute for Energy Technology (IFE)

Paul Scherrer Institute (PSI)

MAGiC

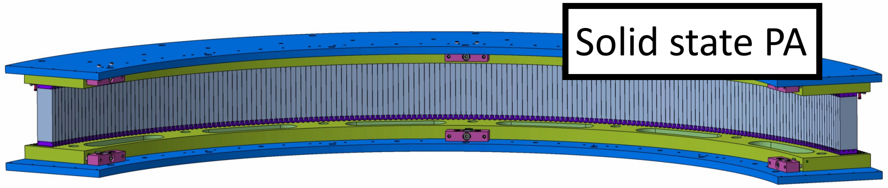
Polarised Diffractometer for Magnetism

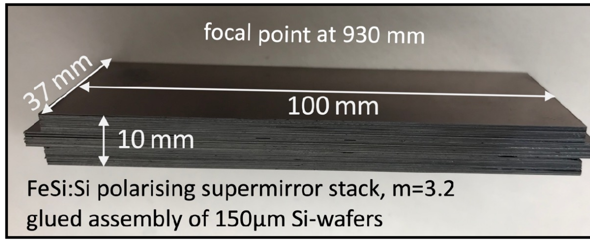




MAGiC Quick Facts	
Instrument Class	Diffraction
Moderator	Bispectral
Primary Flightpath	159 m
Secondary Flightpath	1 m
Wavelength Range	0.6 – 6 Å
Bandwidth	1.7 Å
Flux at Sample at 2MW	$8.0x10^{8}$ $n/s/cm^{2}$ (0.6 – 2.3 Å) 1.5 $x10^{9}$ $n/s/cm^{2}$ (2.0 – 3.7 Å)
Polarised Incident Beam	Permanent
Flipping Ratios Detector Bank	
Q-Range	0.2 – 21 $Å^{-1}$
Q-Resolution Δd/d	Adjustable 1 – 12 %
Detector Coverage	60°(H) × 48°(V)
Polarization Analysis Detector Bank	
Q-Range	0.2 – 6 $Å^{-1}$ (2.0 – 6.0 Å)
Q-Resolution Δd/d	Adjustable 0.2 – 4 %
Detector Coverage	120°(H) × 6°(V)

- Local susceptibility and spin densities;
- Exotic magnetic structure (long range, non-collinear, anisotropic Hamiltonian);
- Multifunctional materials;
- Superconductivity;
- Frustrated magnets and quantum spin liquids;
- Magnetism in thin films and at interfaces;





Spectroscopy

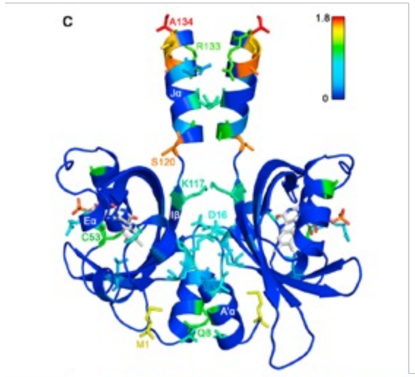
5 Instruments

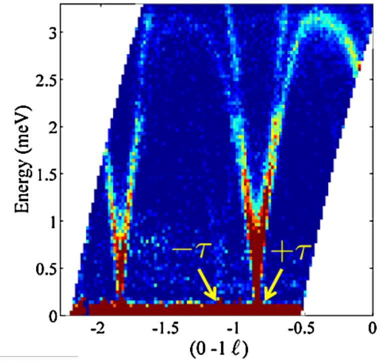
Direct-Geometry Spectroscopy
Coordinator: Pascale Deen

General-purpose chopper spectrometers

CSPEC: Cold chopper spectrometer
Lead scientist: Pascale Deen (ESS)
IK partners: TUM (50%), LLB (50%)

T-REX: Bispectral chopper spectrometer
Lead scientist: Christian Franz (FZJ)
IK partners: FZJ (75%), CNR (25%)





Biophysical Journal Volume 110 March 2016 1064–1074

Indirect-Geometry Spectroscopy
Coordinator: Pascale Deen

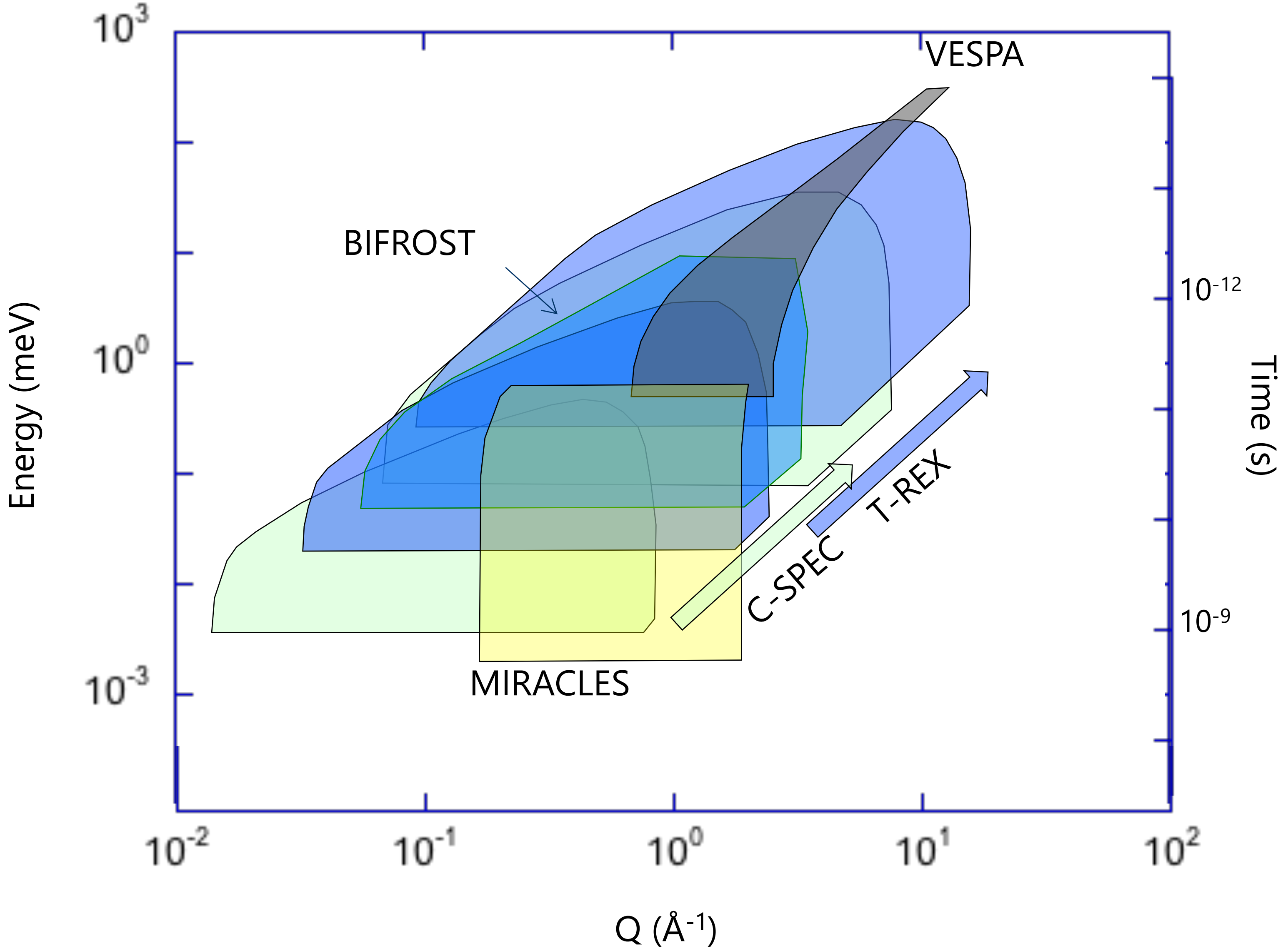
Crystal-analyser instruments

BIFROST: Single-crystal spectroscopy
Lead scientist: Rasmus Toft-Petersen (DTU)
IK partners: DK (24%), PSI (28%), LLB (21%), IFE (24%), Wigner (3%)

VESPA: Vibrational spectroscopy
Lead scientist: Daniele Colognesi (CNR)
IK partners: CNR (75%), ISIS (25%)

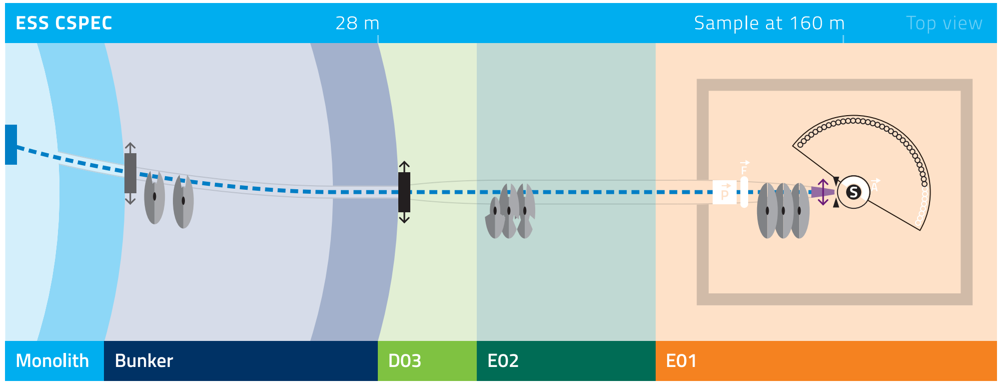
MIRACLES: Backscattering spectroscopy
Lead scientist: Felix Villacorta (ESS-Bilbao)
IK partners: ESS-Bilbao, KU

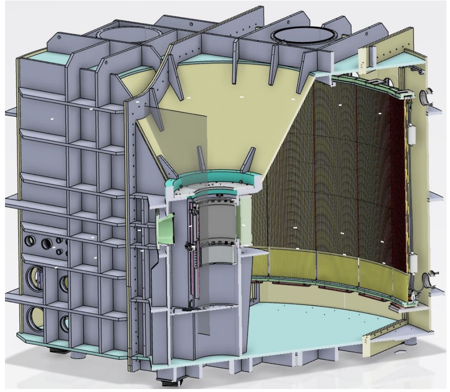
Spectroscopy Kinematic Range



CSPEC

Cold Chopper Spectrometer

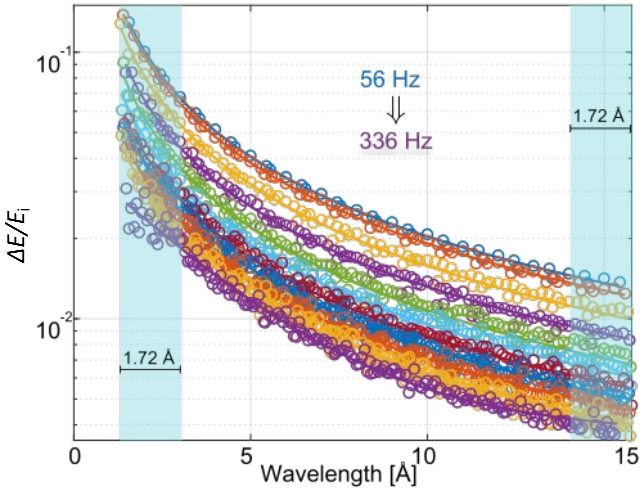




CSPEC quick facts

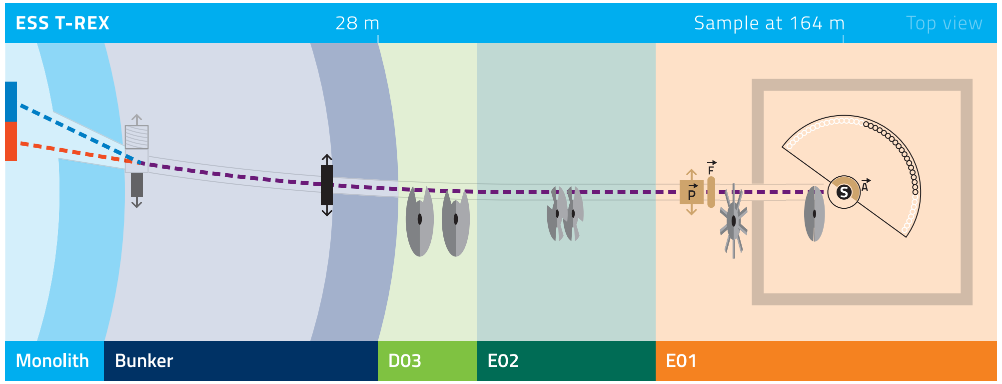
Primary flight path	160 m
Secondary flight path	3.5 m
Moderator	Cold
Wavelength range	2-20 Å
Bandwidth	1.72 Å
Flux at sample (2 MW, λ = 5 Å, $\Delta E/E_i$ = 3%, no RRM, with RRM ~ x6)	9 10^5 n s^{-1} cm^{-2} (4 x 2 cm^2 standard beam) 4 10^6 n s^{-1} cm^{-2} (1 x 1 cm^2 focussed beam)
Full detector coverage	5^o – 140^o [H] ± 26^o [V]
Energy resolution	1% - 5% E_i
Polarisation analysis	Foreseen upgrade

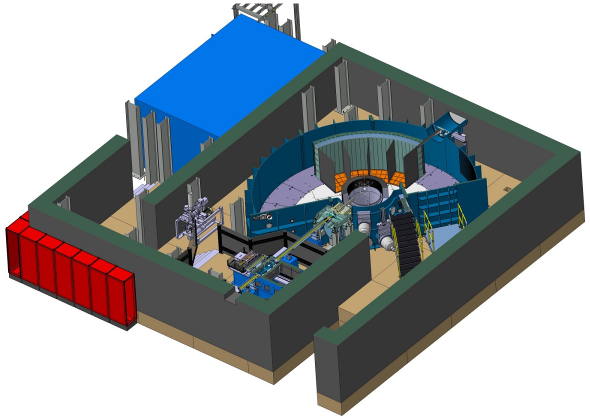
- Collective and quasiparticle excitations in frustrated compounds.
- Low lying excitations of quasiparticles in quantum materials.
- Magnon -phonon hybrid excitations in multiferroic materials.
- Time dependence of the rotational and translational diffusive processes in enzyme catalysis.
- Dynamics of hydration processes and the structural relaxation of the glassy water.
- Time dependent phenomena of hydrogen storage in clathrates.
- Proton diffusion in metal organic frameworks.
- Operando studies of proteins such as those involved in photosynthesis.



T-REX

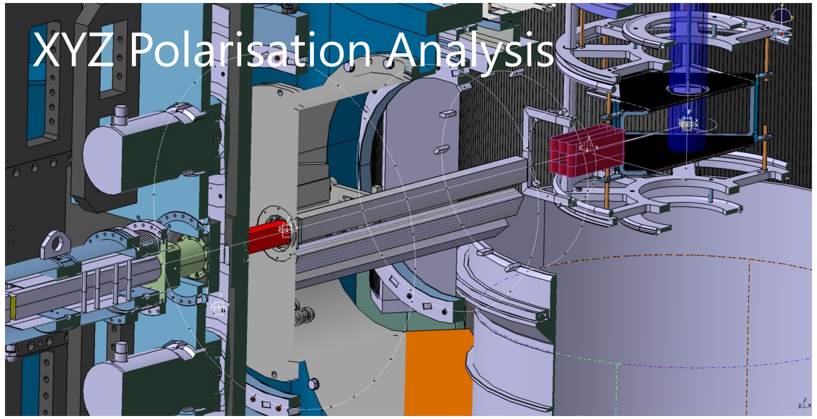
Polarised Bispectral Chopper Spectrometer





T-REX Quick Facts	
Instrument Class	Spectroscopy
Secondary Flightpath	3 m
Moderator	Bispectral
Primary Flightpath	164 m
Wavelength Range	0.7–6.5 Å
Bandwidth	1.7 Å
Incident Beam Polarisation	Optional
Polarisation Analysis	Optional
Flux at Sample at 2 MW (E_i = 8 meV)	0.8–5 × 10^6 $ns^{-1}cm^{-2}$
Flux at Sample at 2 MW (E_i = 50 meV)	0.3–2 × 10^6 $ns^{-1}cm^{-2}$
Detector Coverage	1°– 72° [H] × −25°–15° [V] (−36°–144° [H] × −25°–15° [V][a])
Energy Resolution (E_i = 2 meV)	Adjustable 1%–2.5% of E_i
Energy Resolution (E_i = 100 meV)	Adjustable 4%–7% of E_i
[a]) Available as a foreseen upgrade.	

- Understanding the effect of spin–orbit coupling in the classification of quantum spin liquids
- Magnetic excitations of emergent phenomena in magnetically frustrated materials
- Time dependence of the rotational or translational diffusive processes in enzyme catalysis.
- Time dependent phenomena of hydrogen storage in clathrates.
- Proton diffusion in metal organic frameworks.
- Diffusion dynamics and the relation to the ordering mechanism of solidification.
- Understanding light induced dynamics of antenna pigment/protein complexes.



ess

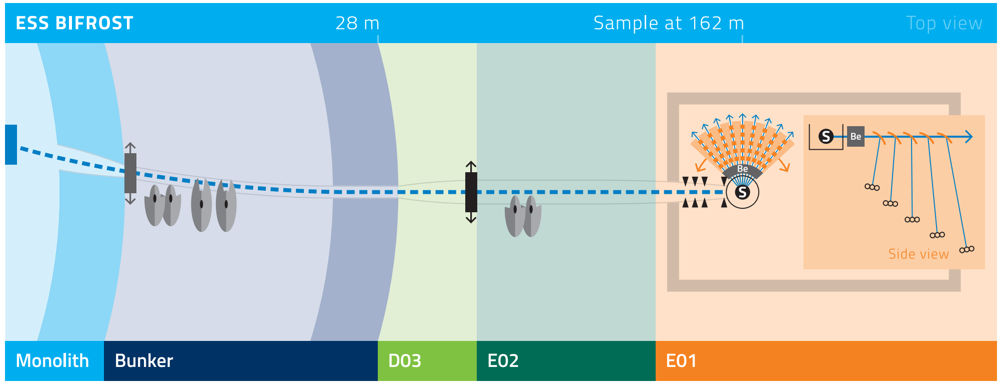
JÜLICH Forschungszentrum

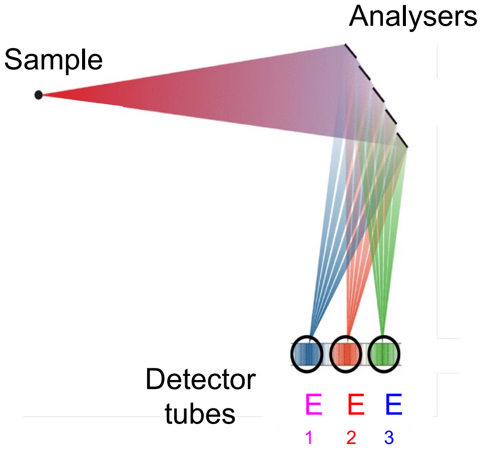
UNIVERSITÀ DEGLI STUDI DI PERUGIA

Consiglio Nazionale delle Ricerche

BIFROST

Multiplexing Indirect Spectrometer for Extreme Environments

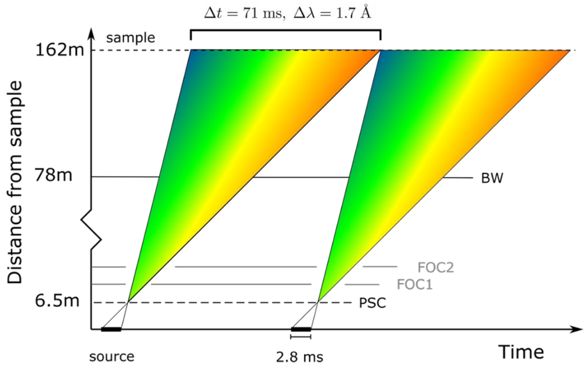




BIFROST Quick Facts.

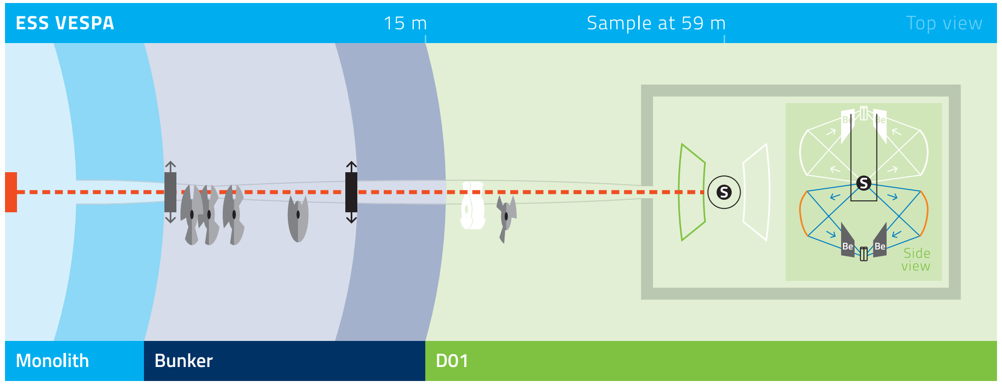
BIFROST Quick Facts	
Instrument Class	Spectroscopy
Moderator	Cold
Primary Flightpath	162 m
Sample-Analyser Flightpath	1.1–1.7 m
Wavelength Range	1.5–6 Å
Bandwidth	1.7 Å
2θ Range	7°–135°
2θ Coverage	90° in 2 settings
2θ Resolution	0.7°–1.2°
Analyser Energies	2.7, 3.2, 3.8, 4.4, 5.0 meV
Energy Transfer Range	−3 to +55 meV
High Flux Mode [2.3–4.0 Å]	
Flux at Sample at 2 MW	6×10^9 n s^{-1} cm^{-2}
Resolution ($E_f = 5$ meV, $\hbar\omega = 0$)	190 μeV
Resolution ($E_f = 5$ meV, $\hbar\omega = 5$ meV)	450 μeV
High Resolution Mode [2.3–4.0 Å]	
Flux at Sample at 2 MW	9×10^8 n s^{-1} cm^{-2}
Resolution ($E_f = 5$ meV, $\hbar\omega = 0$)	50 μeV (prismatic)
Resolution ($E_f = 5$ meV, $\hbar\omega = 5$ meV)	50 μeV (prismatic)

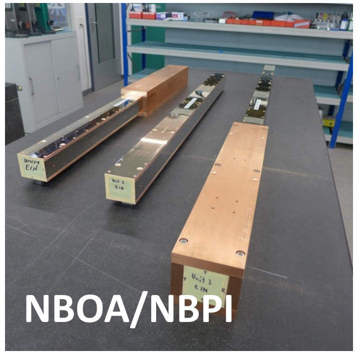
- Low-D magnets
- High-Tc superconductivity
- Functional magnetic materials
- Geoscience
- Parametric studies
- Weak signals & small samples



VESPA

Vibrational Excitation Spectrometer with Pyrolytic graphite Analysers



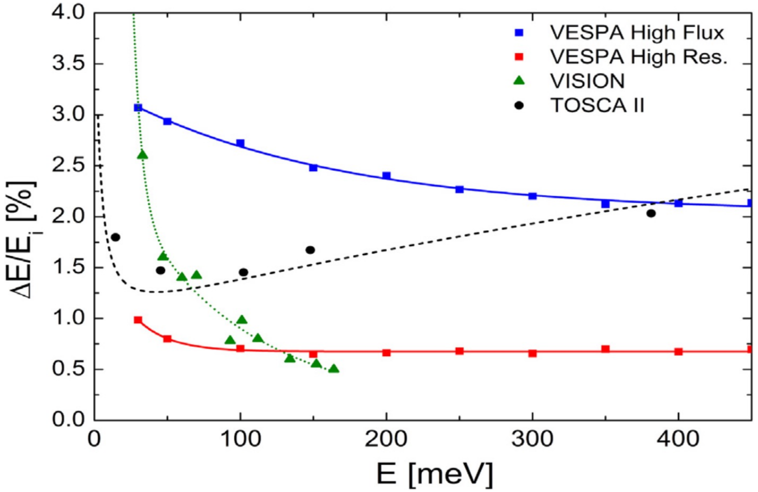


VESPA Quick Facts	
Instrument Class	Spectroscopy
Moderator	Thermal
Primary Flightpath	59 m
Sample-Analyser Flightpath	0.61–0.69 m
Wavelength Range	0.4–4.7 Å
Bandwidth	4.3 Å
Analyser Coverage	0.75 (5.25[a]) sr
Analyser Energies	3.7–4.8 meV
Energy Transfer Range	−1 to +500 meV
High Flux Mode	
Flux at Sample at 2 MW	2.3×10^8 n s^{-1} cm^{-2}
Energy Resolution	$\Delta E/\hbar\omega \approx 2.6\%$
High Resolution Mode	
Flux at Sample at 2 MW	6.5×10^7 n s^{-1} cm^{-2}
Energy Resolution	$\Delta E/\hbar\omega \approx 1.0\%$

[a]Available as a foreseen upgrade.

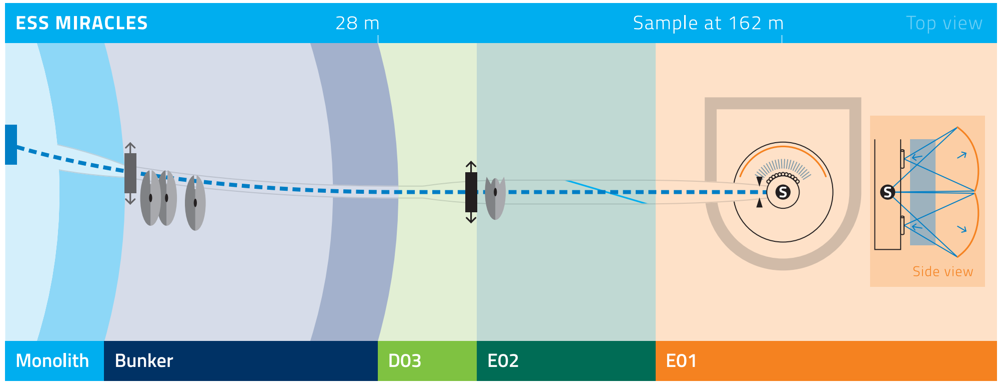
- NVS is used to investigate solids and liquids, soft matter, complex fluids, and bio-materials, permitting the identification of bonds and functional groups.

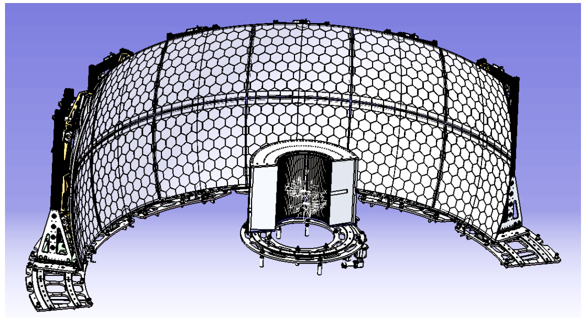
- NVS exploits the large incoherent scattering cross section of the hydrogen nucleus. Proton dynamics or vibrations connected to the movement of H atoms can be easily detected spectroscopically, even if hydrogen is dissolved at very low concentrations in materials composed mostly of heavier atoms.

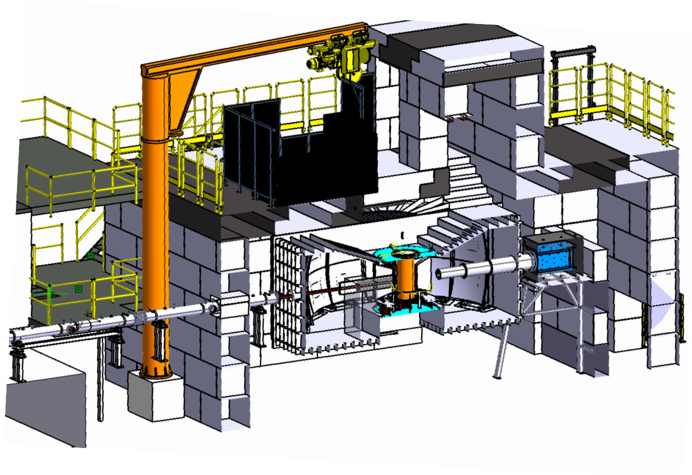


MIRACLES

Backscattering Spectrometer







- Life sciences: degenerative diseases, protein dynamics and enzyme catalysis
- Pharmaceutical studies, drug delivery.
- Energy sciences: catalysis, fuel cells and H2 storage, CO2 capture, proton diffusion.
- Polymer sciences: organic electronic devices, viscoelasticity.
- Climate change: waste containment, ice formation, Portland-alternative cements.
- Next-generation magnetic materials: molecular nanomagnets.

MIRACLES Quick Facts	
Instrument Class	Spectroscopy
Moderator	Cold
Primary Flightpath	162.5 m
Sample-Analyser Flightpath	2.5 m
Wavelength Range	2–20 Å
Bandwidth	1.5 Å, ±0.5 meV[a]
Energy Transfer Range	−2 to +20 meV
Q Range	0.2–2 $Å^{-1}$[a]
High Flux Mode	
Flux at Sample at 2 MW	1.5×10^9 n s^{-1} cm^{-2}[a]
Elastic Energy Resolution	45 μeV
High Resolution Mode	
Flux at Sample at 2 MW	4×10^7 n s^{-1} cm^{-2}[a]
Elastic Energy Resolution	2 μeV

[a]When centred on $\lambda = 6.27$ Å.

Instrument Project Lifecycle

Proposal and Planning

Instrument Proposal

Deliverables

- Science case covering scientific relevance, impact and usage
- Conceptual design with credible estimates of performance
- Preliminary costing.

Phase 0 – Preparation for Design

Deliverables

- Conceptual design updates
- Prototyping
- Definition of facility requirements and interfaces
- Clarification of institutional responsibilities
- Resource planning

Phase 1 – Preliminary Design

Deliverables

- Scientific and technical requirements
- Technical design concept
- Delivery plan for all phases (including hot commissioning)
- Delivery Schedule covering all phases
- Resource plan
- Staging plan for later enhancements
- Budget with contingency at 10% of cost to complete

Design and Construction

Phase 2 – Detailed Design

Deliverables

- Complete definition of all major technical components
- Completion of detailed plan for Phase 3
- Refined plan for phase 4
- Refined Resource plan
- Refined delivery schedule, with critical path items and dependencies
- Refined budget with contingency at 10% of cost to complete

Phase 3 – Manufacturing and Procurement

Deliverables

- Procurement and manufacture of all major technical components
- Completion of detailed plan for phase 4
- Site preparation
- Refined plans for phase 5 and for staging
- Refined Resource plan
- Refine instrument delivery schedule
- Maintain budget with contingency at 10% of cost to complete

Installation and Commissioning

Phase 4 – Installation and Integration

Deliverables

- Construction of physical infrastructure on site.
- Assembly and installation of technical components
- Integration and testing of technical components
- Installation, integration and testing of Personnel Safety System
- Submission of application for approval to hot commission
- Formal project completion

Phase 5 – Hot Commissioning

Deliverables

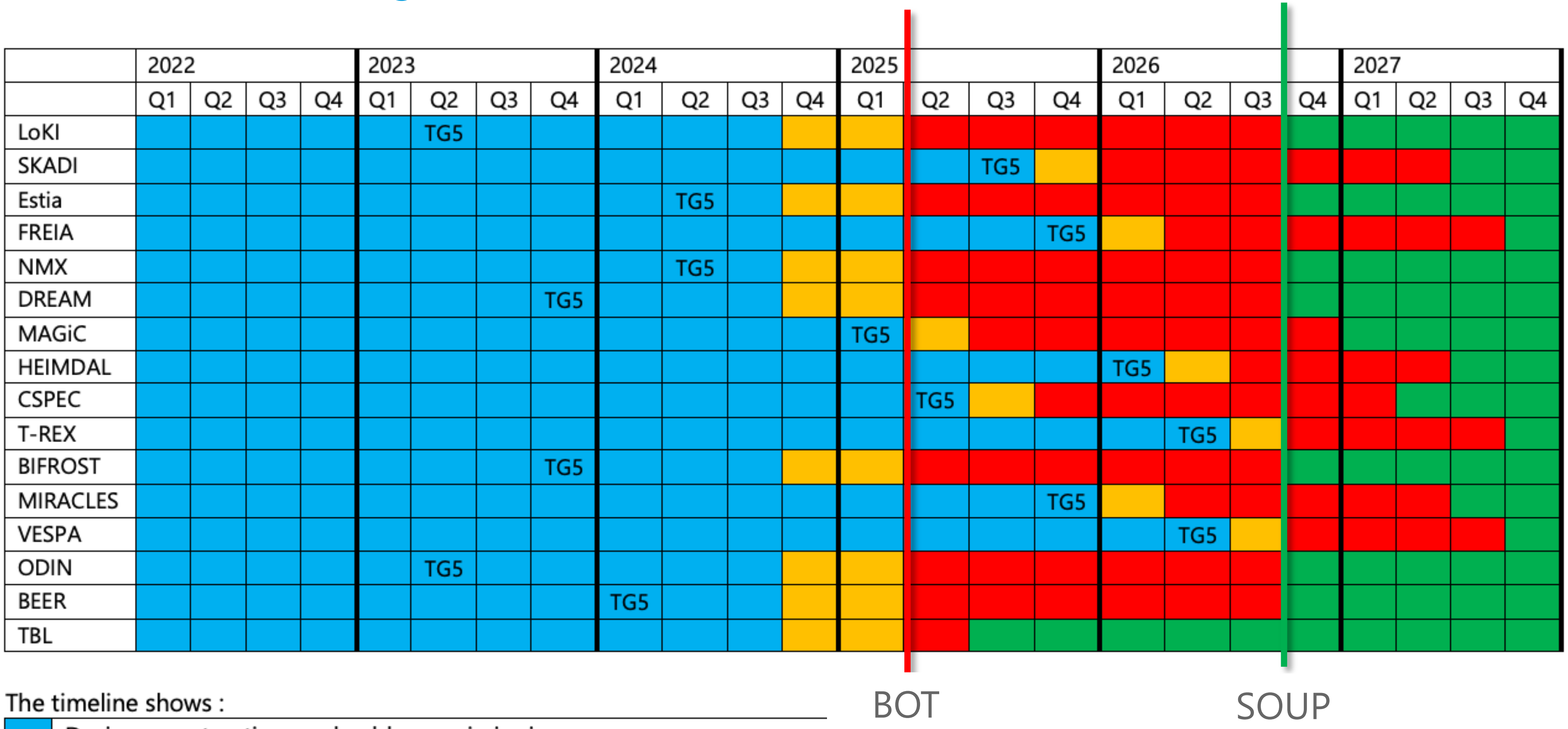
- Verification of performance of Personnel Safety System
- Proof of compliance with radiation dose limits
- Critical performance demonstration of basic functionality
- Scientific performance demonstration
- Friendly user experiments
- Completion of technical and user manuals

Tollgates and reviews

- **Tollgate 1** – Proposal Approval
- **Tollgate 2 (PDR)** – Preliminary Design Review
- **Tollgate 3 (CDR)** – Critical Design Reviews
- **Tollgate 4** – Installation Readiness Reviews
- **Tollgate 5** – Instrument handover to NSS
- **TRR SRR SAR**
- **TRR**
- **Operations Readiness Review**

Overall Instrument Timeline

Estimates as of August 2022 – with BOT in Q2 2025

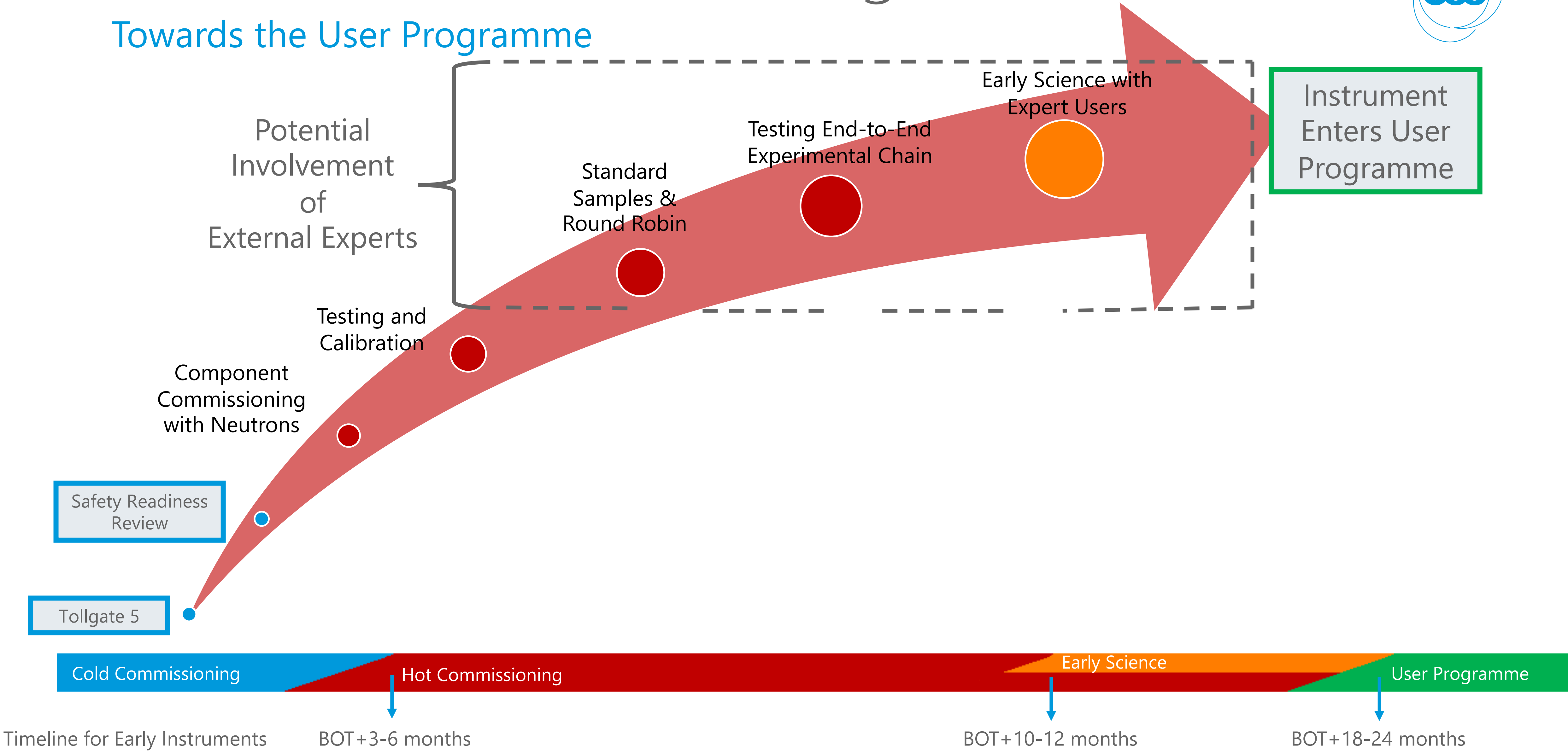


The timeline shows :

(blue)	Design, construction, and cold commissioning
(yellow)	Safety readiness checks and approvals
(red)	Hot commissioning (testing and validation with neutrons) and Early Science
(green)	User programme

Instrument Commissioning

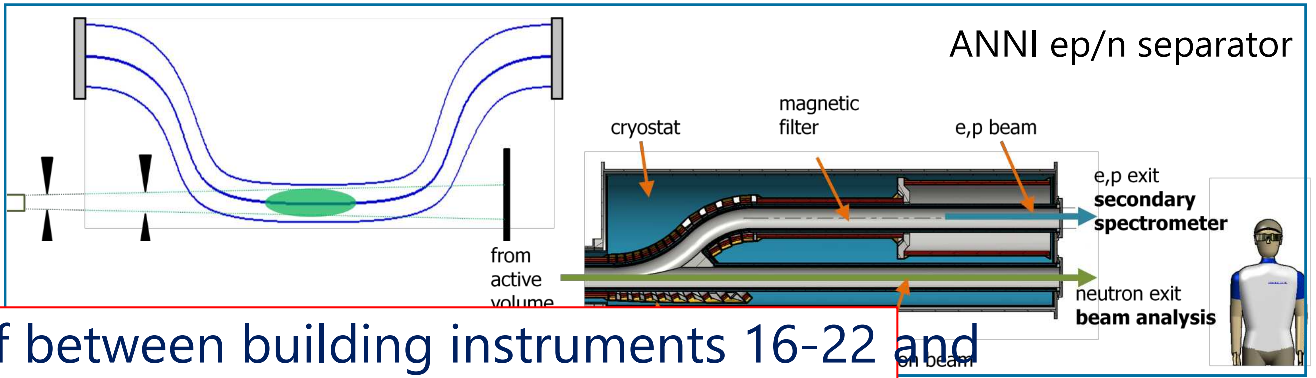
Towards the User Programme



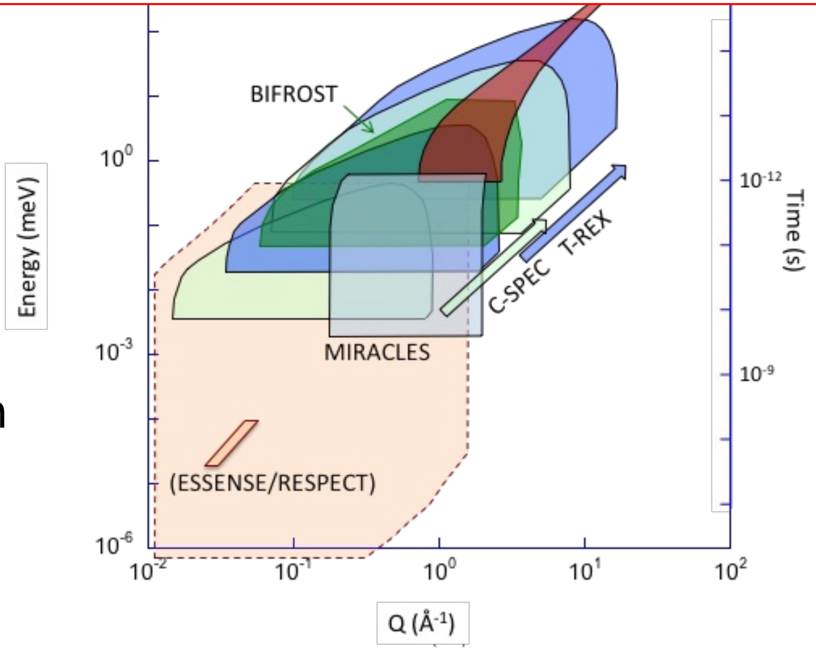
Science: Capability Gap Analysis

https://europeanspallationsource.se/instruments/capability-gap-analysis

1. High-Priority Capability Gaps
   - *Particle Physics*
   - *High-Resolution Spin-Echo*
2. Other Significant Capability Gaps
   - High Pressure Diffraction
   - Grazing-Incidence SANS
   - Very Fast Spectroscopy
   - Wide-Bandwidth Spectroscopy
   - High Magnetic Fields
3. Lower-Priority Capability Gaps
   - Bio-SANS
   - Hydrogenous-Sample Diffraction
   - Wide-Angle Spin-Echo



trade-off between building instruments 16-22 and upgrades on instruments 1-15



- Report distributed
- Input received:
  - ESS instruments teams
  - ILL-ESS user meeting 2018
  - ESS advisory panels: STAPs & SAC
- Presented to ESS Council
- Open to further ideas
- When open call for proposals?

Staff in Hot Commissioning

Science + NSS

- 3 scientists/scientific associates for each instrument in hot commissioning – mixture depending on need, working across instruments.
- Core team of technicians
- 1 data scientist for each instrument in hot commissioning
- Support from relevant parts of ESS for:
  - Sample environment
  - Detectors
  - Choppers
  - Motion Control and Automation
  - Instrument Controls
  - Data Management and Software
  - Polarisation
  - Laboratories and sample handling
- Total effort per instrument 5-8 FTE during Hot Commissioning – similar to our operations staffing level.
  - SNS experience was 12 FTE per instrument
- Number of instruments that can be commissioned simultaneously will depend on overall staff profile
- Includes in-kind staff from instrument partner institutes

Comparison with Other Facilities

Operations Staffing SOUP => 2MW steady state

	ESS[a]	ILL[b]	ESRF[c]	ISIS[d]	SNS[e]
Instruments (incl. CRGs/3)	15	31	35.6	30	18.3
Beam days for user programme	2400	3899	4404	*2678*	*2525*
per instrument	160	126	124	*89*	*138*
Number of operational days	200	158	225	*130*	*184*
Number of experiments	600	785	1358	*766*	*681*
Average Experiment Length [days]	4.0	5.0	3.2	3.5	*3.7*
Local Contacts / Instrument	2.5	2.2	3.4	2.2	2.6
Instrument Support Staff / Instr.	1.0	1.0	1.6		0.9
Sample Environment Staff / Instr.	0.5	0.5		0.6	0.9
Other Tech. Support / Instrument	4.0	3.6	4.1	3.0	6.5
Total Staff / Instrument	**8**	**7.2**	**9.0**	**5.9**	**10.8**
Total Staff / Experiment	**0.2**	**0.28**	**0.24**	**0.23**	**0.29**

Table shows **FTE** working **directly** on experiment operations. The **total staff headcount** is required to be higher to provide 24/7 support, and a core staff is needed for maintenance, installation, development, calibration and testing, and management.

Instrument Scientists Group

Introducing the Team

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