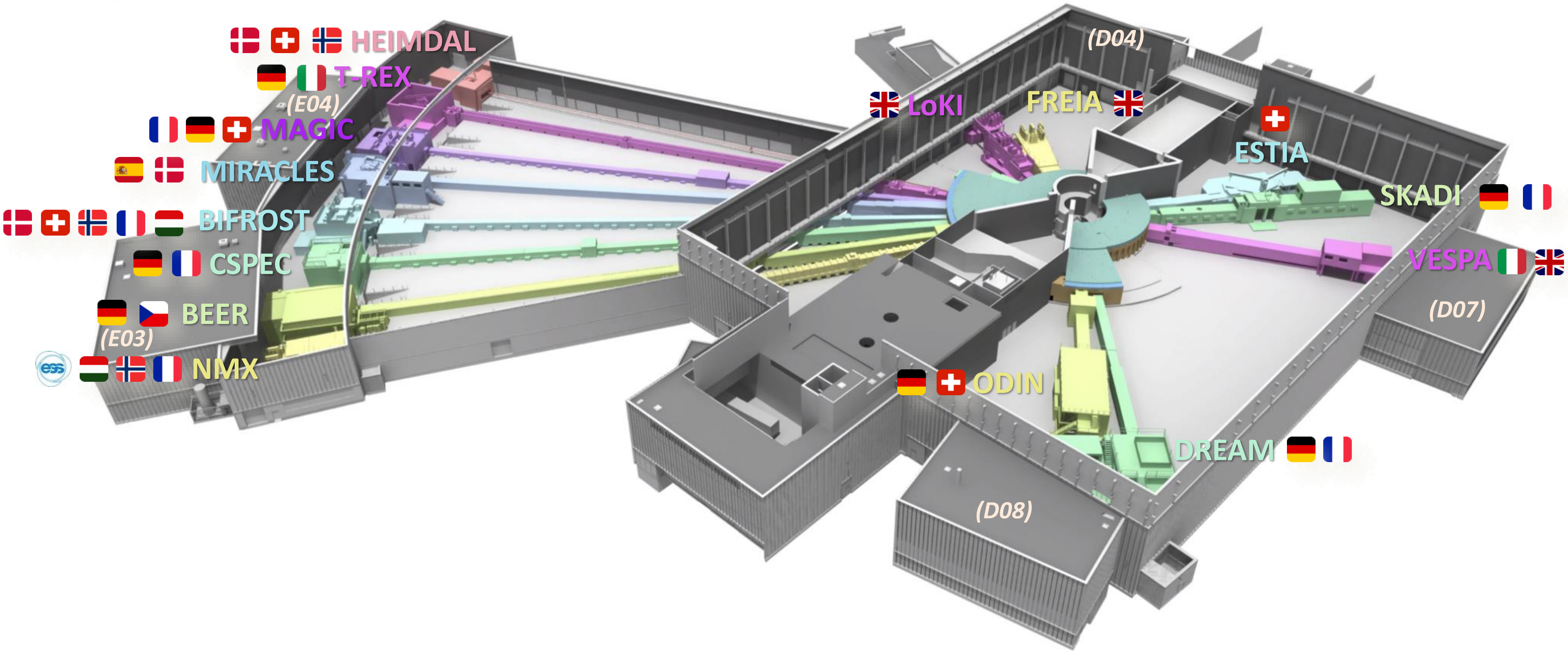
Coordinated plan to incorporate polarised neutron capabilities
Wai Tung (Hal) Lee, ESS

EUROPEAN SPALLATION SOURCE



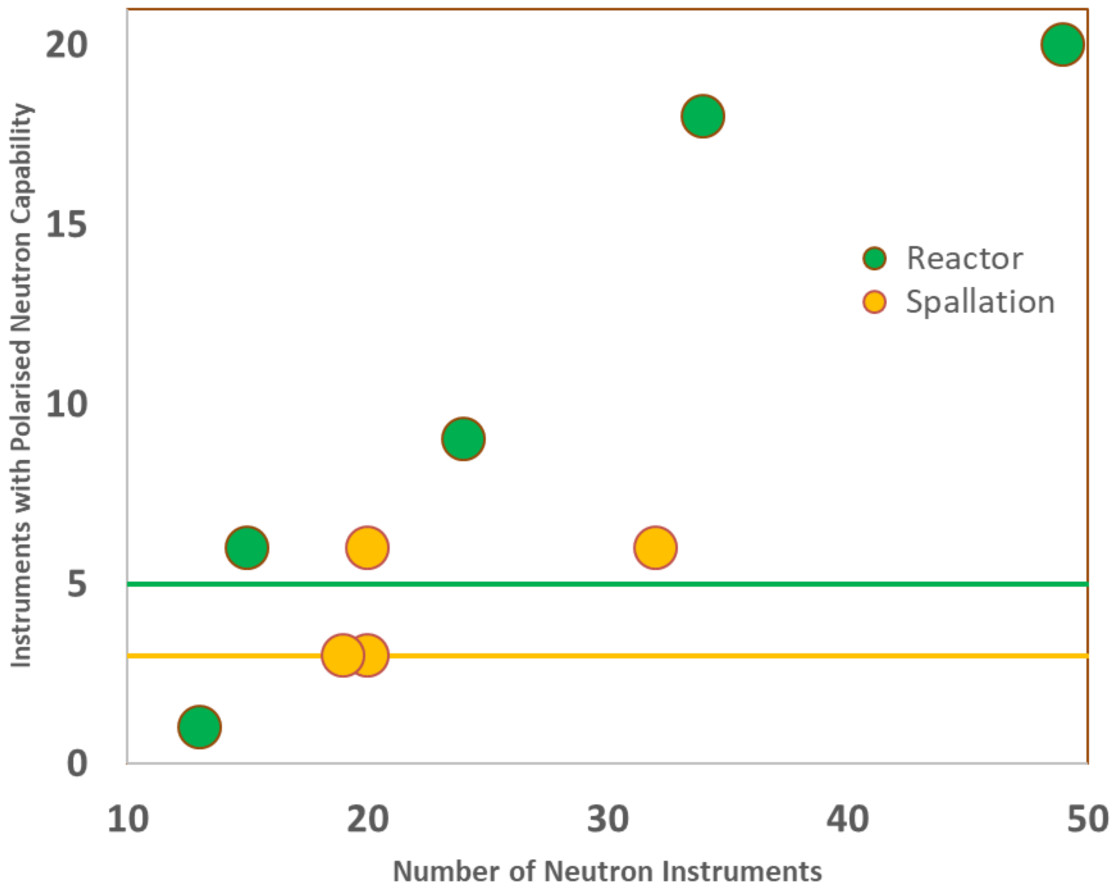
Polarisation for Scientific Studies

EUROPEAN SPALLATION SOURCE

- Polarised neutron capability has been an integral part of neutron instruments serving the user community.
  - Over 100 neutron instruments are in Europe
  - Over 40 have polarised neutrons available

- Polarised neutrons have been changing from scarced to pervasive resources thanks to advances in solid-state and polarised ^{3}He devices.

- Instruments worldwide are being upgraded to answer the user community’s call for polarised neutrons to be available on many types of instruments.

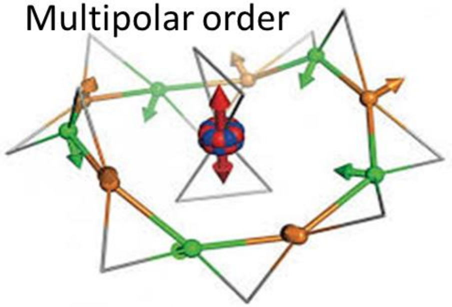


Polarisation for Scientific Studies

Spin states of matter: future based technologies

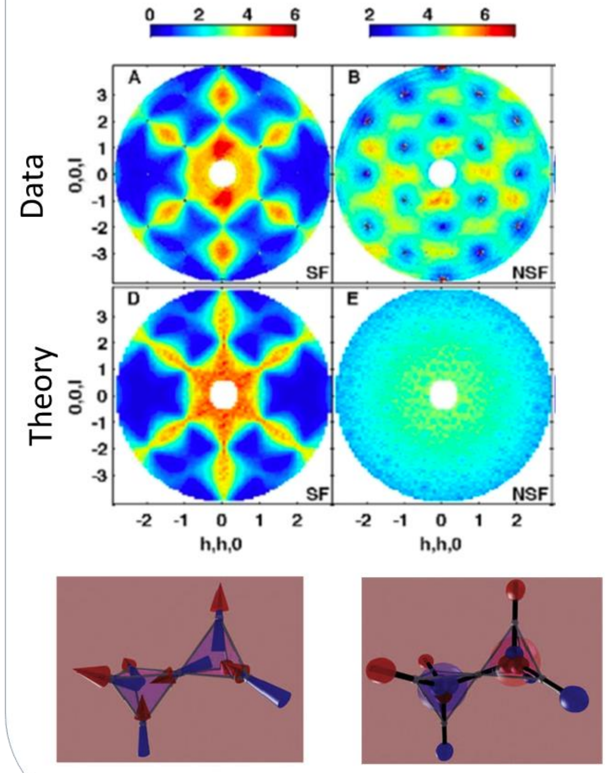
- Quantum magnetism
- Low dimensional magnetism
- Frustrated magnetism
- Topological states
- Spin-orbit coupling
- Emergent behaviour

Emergent phenomena:
Multipolar order

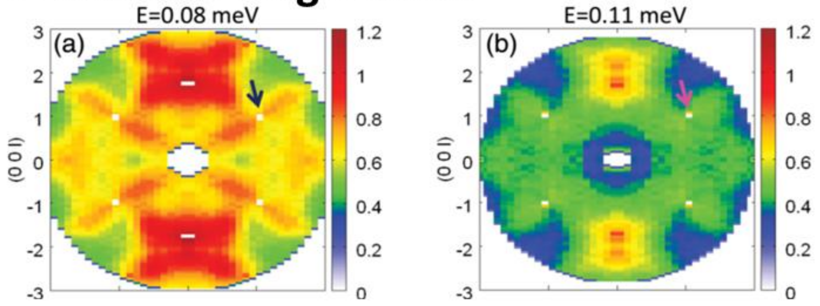


Science 350, 6257, 179

Polarisation Analysis
Determination of magnetic monopole analogues
Science 326, 415

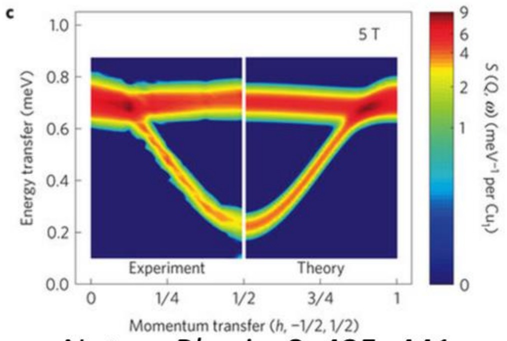


Frustrated magnetism:



Phys. Rev. B 86, 174403

Quantum magnetism:
Spinon excitations



Nature Physics **9**, 435–441

Information courtesy of Pascale Deen, ESS

Polarisation for Scientific Studies

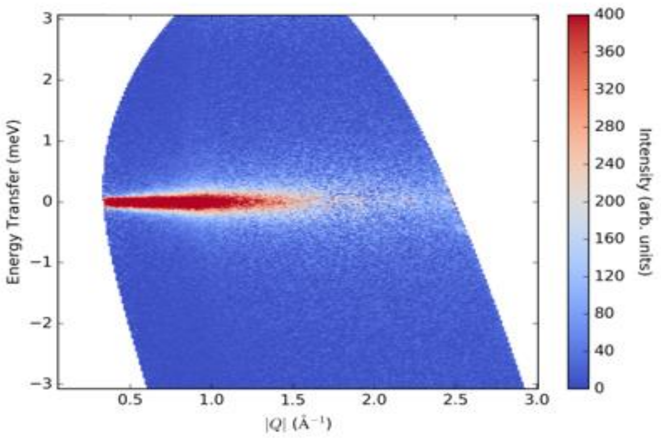
Hydrogenous materials
Polarisation analysis:
1-d guide field only
2 cross-section only

incoherent-coherent separation

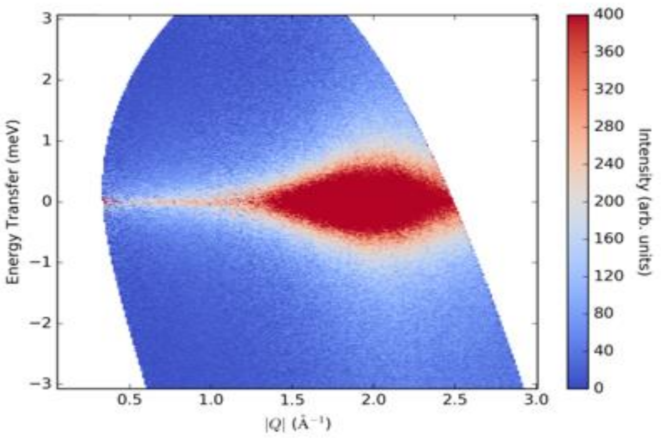
Science and Technology Facilities Council

- Quasi-elastic neutron scattering - polarization analysis can distinguish dynamic processes which occur at the same Q and E

e.g. D2O on LET (ISIS)



Incoherent: self motions



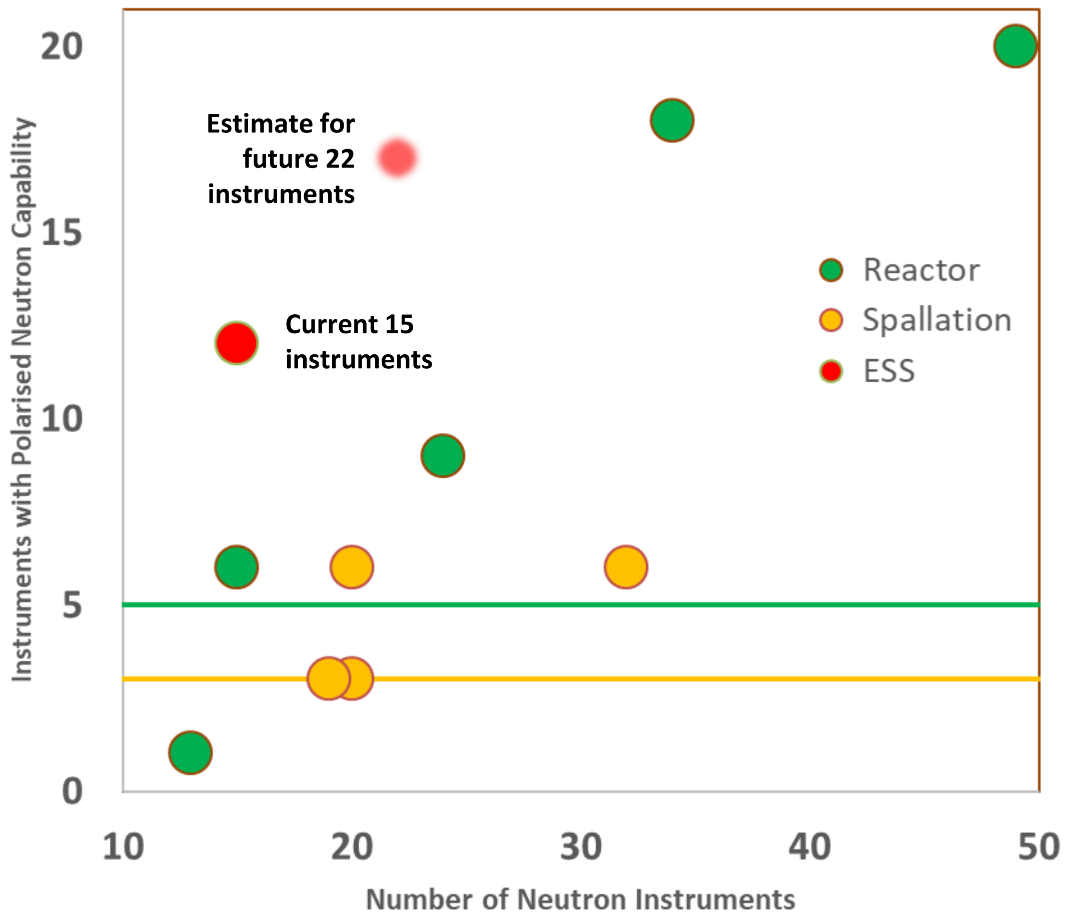
Coherent: collective + self motions

A. Arbe et. al., submitted

Information courtesy of Gøran Nilsen, STFC

ESS Plan for Polarisation

- Where do we want to be?
- Many ESS instruments have polarised neutrons in their initial scope. The ESS now intends to provide a centralised service to realise the capability.
  - (1) 12 instruments may have polarised neutrons available for users.
  - (2) We are developing a polarisation work pacakge for implementation in 2020-2025
  - (3) Work will include hardware (design, build, install, commission, operation), control software, meaurement methodology, data reduction software, and ease-of-use improvements.
  - (4) The priority is based on the schedule of the instruments
- **Scientific Advisory Committee, October 2019: "*We recommend advancing this as fast as possible in order for it to be available by 2025.*"**



Who am I?

First venture into the field of polarised neutrons

1. BIREFRINGING POLARISER: Polarised neutron interferometry - Scalar Aharonov-Bohm Effect.
2. HEUSLER CRYSTAL: Inelastic polarised neutron scattering – Chromium Spin Density Wave.

Work at ORNL

1. SUPERMIRROR: Polarised neutorn reflectometry (PNR), characterise the then-new c-benders (outposted at Argonne Lab).
2. SPIN-EXCHANGE OPTICAL PUMPING (SEOP): Developed polarised ^{3}He technique for polarised neutron scattering. Proposed Adiabatic Fast Passage (AFP) flipping of ^{3}He spin to select neutron polarisation, first use of *in-situ* polariser, deployment in SNS PNR instrument.
3. LARMOUR DEVICE: Collaborative works on Spin-Echo Scattering Angle Measurement (SESAME).
4. SELF-SHIELDED ASYMMETRIC MAGNET: Work with high-field magnet designer to show self-shielding and asymmetry work in tendem to stablise the magnet. First of its kind, a 5T "SLIM SAM" magnet at the SNS is still one of the most stable and most-requested magnets.

Work at ANSTO:

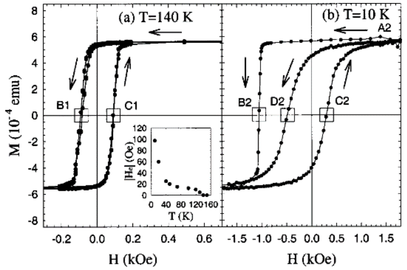
1. META-STABLE OPTICAL PUMPING (MEOP): Coordinated project to enable polarised neutorns on 6 instruments centring around the use of polarised 3He technology and MEOP ^{3}He polarising station.
2. POLARISED NEUTRON SCATTERING METHOD: Develop measurement methodology and data reduction for using polarised ^{3}He based neutron spin-filters.
3. SEOP FILLING STATION: Built polarised ^{3}He & ^{129}Xe filling station for medical imaging applications.

Who am I?

Work at ORNL

1. SUPERMIRROR: Polarised neutron reflectometry (PNR) at IPNS, while outposted to ANL with SNS division)

- Developed PNR techniques
- Characterise the performance of polarising supermirror and the then-new c-benders



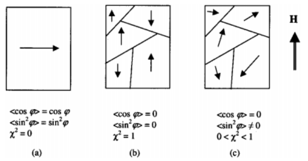
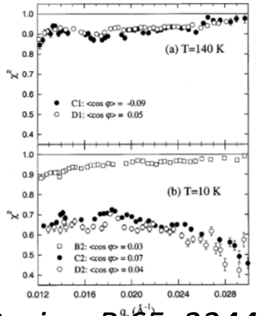


FIG. 7. Schematic diagrams illustrating some possible magnetic configurations in the thin film and the corresponding values of ⟨sin² φ⟩ and χ² (all have ⟨cos φ⟩=0): (a) single domain, (b) collinear domains with magnetization along the applied field H, (c) domains with a dispersion of magnetic orientations.



Quantitative measurement of magnetic domain dispersion. *Physical Review B 65, 224417 (2002).*

2. SPIN-EXCHANGE OPTICAL PUMPING (SEOP): Developed polarised ^{3}He technique for polarised neutron scattering

- Proposed using Adiabatic Fast Passage flipping of ^{3}He spin to select neutron beam polarisation.
- First to tested *in-situ* polarised ^{3}He setup as a modulo setup on instrument
- Deployed SEOP analyser on SNS magnetism reflectometer. Reached unprecedented 5-hour pump-up time.

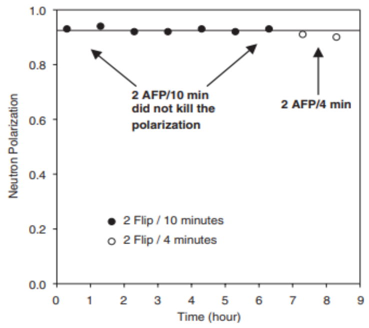


Fig. 2. Neutron measurement of the impact on ^{3}He polarization after repeated inversion via AFP.

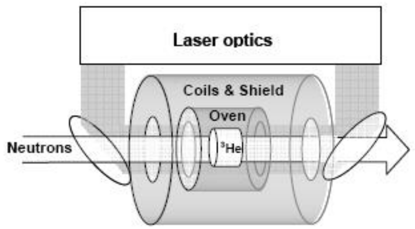


Figure 1. Schematic diagram of the analyzer. The details are explained in the text.

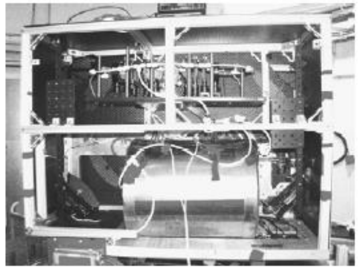


Figure 2. Analyzer setup at the reflectometer. Upper: Laser optics. Lower: Analyzer.

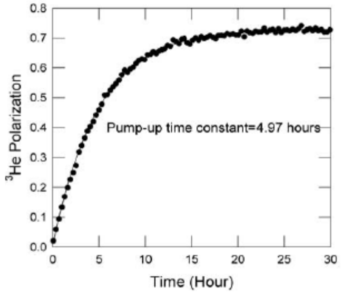


Figure 4. ^{3}He polarization as a function of ime during the polarizing process.

Physica B, 385-86, 1131 (2006).

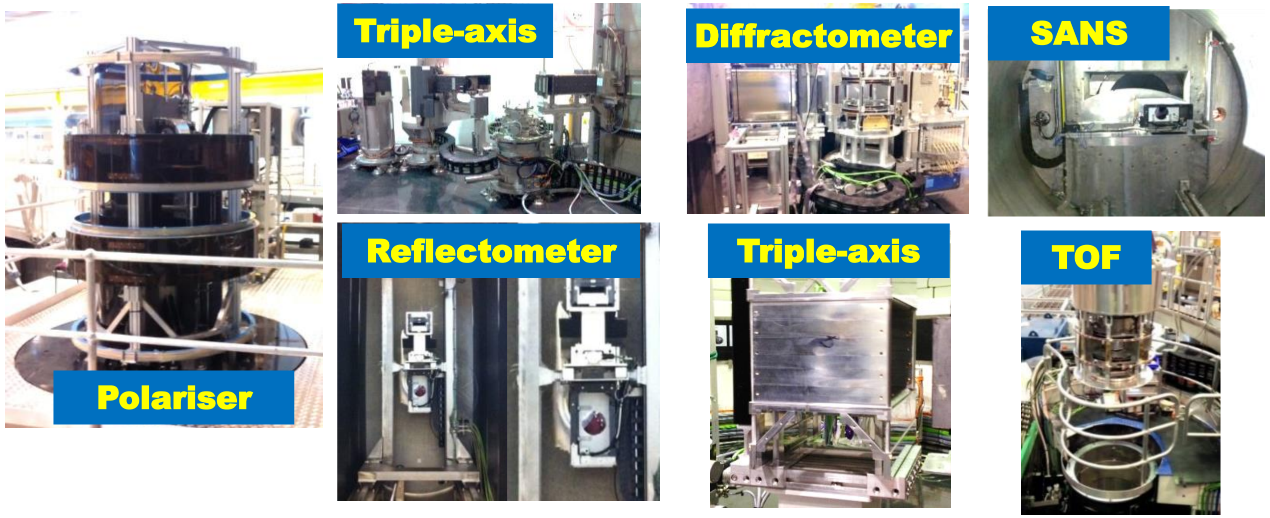
Journal of Physics: Conference Series 251, 012086 (2010).

Who am I?

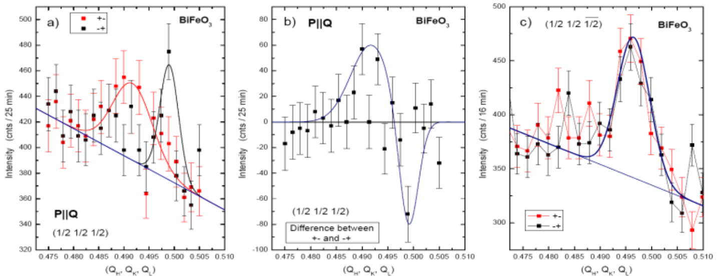
Work at ANSTO

1. META-STABLE OPTICAL PUMPING (MEOP): Coordinated project to enable polarised neutrons on 6 instruments.

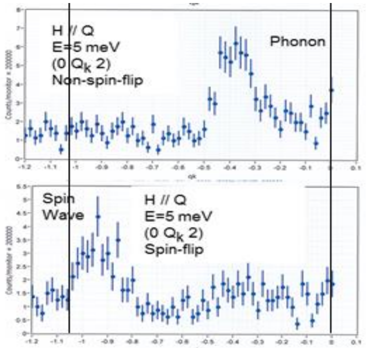
- ANSTO's reactor had been operating for nearly 10 years. The condition was right to allow an upgrade:
  - Instrument teams thoroughly understood their instruments.
  - Well-established user programme.
  - Downtime for developmental work for individual instrument was acceptable.
- Joint efforts with the ILL to deploy polarised neutron capability.



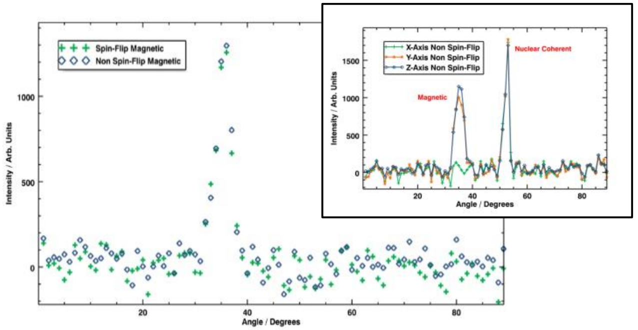
2. METHODOLOGY & DATA-REDUCTION: Measurement methods & proper data-reduction algorithm for using polarised ^{3}He



Nat. Commun. 7, Art. No. 12664 (2016).



Separate phonon & magnon on TAIPAN



"XYZ" method to identify magnetic signal on PELICAN

What have been done since joining the ESS in October 2019?

EUROPEAN SPALLATION SOURCE

ESS instruments

- First-discussion with 14 instrument teams to identify the need for polarised neutrons.
- Follow-on discussions on the detail layout of the polarised neutron setup with 12 instrument teams.
- Organising an **ESS Polarisation Workshop on 26th-27th of March** at the ESS site.
- Reported to the Scientific Advisory Committee in October.

Fact-finding

- Visited 7 neutron scattering facilities and 4 manufacturers of polarised neutron equipment.

Capability build-up

- Computation capability to do magnetic field design of polarised neutron setup on instruments:
  - COMSOL Multiphysics
  - Computation computer (soon to arrive)
- Calculation has began on individual instrument components.

Evaluation matrice based on current available technology

- We did a first-round evaluation of the polarised neutron setup based on instrument models.
- Different polarised neutron techniques have different characteristics.
- Together with the instrument teams, we have identified the options for the respective techniques to further explore.

- What follow are brief overviews of the options we are exploring for each instrument (in alphbetical order of the instrument groups and instrument names)

	NEUTRONICS					OPERATIONAL					COST	
	λ < 1.5 Å	λ > 3 Å	Large area cross-section	Large angular coverage of scattered beam	Large beam divergence	Susceptible to magnetic interference	Simple experimental setup	Lead time to change settings during experiment	Simple operation	Compact on-beam equipment	Sharable equipment	Up-front + long-term operating cost, per instrument
Supermirror - single reflective	Long baseline or small bema area	High intensity and polarisation	Difficult	No	Limited	Low	Yes, with motorised	None	Yes	Moderate	No	Moderate
Supermirror - single transmission												
Supermirror - v-cavity			Ok									
Supermirror - c-bender	High antenuation									Yes		
Supermirror - s-bender											Maybe	
Supermirror - wide-angle array	Impractically long baseline			Yes						No	No	High
Polarised 3He - MEOP	Ok	Tradeoff between polarisation and			Ok	High		1 to 3 hours	Replace polarised gas periodically	Yes	Yes	Moderate
Polarised 3He - SEOP, off-situ								1 day	Replace polarised cell periodically			
Polarised 3He - SEOP, in-situ				Impractical. Heating problem			Difficult due to infrastructure	1 day	Yes	No		

Polariser	λ < 1.5 Å				λ > 3 Å			
	long baseline		short baseline		long baseline		short baseline	
	difficult to access location	accessible location	difficult to access location	accessible location	difficult to access location	accessible location	difficult to access location	accessible location
Supermirror - single reflective								
Supermirror - single transmission								
Supermirror - v-cavity								
Supermirror - c-bender								
Supermirror - s-bender								
Polarised 3He - MEOP								
Polarised 3He - SEOP, off-situ								
Polarised 3He - SEOP, in-situ								

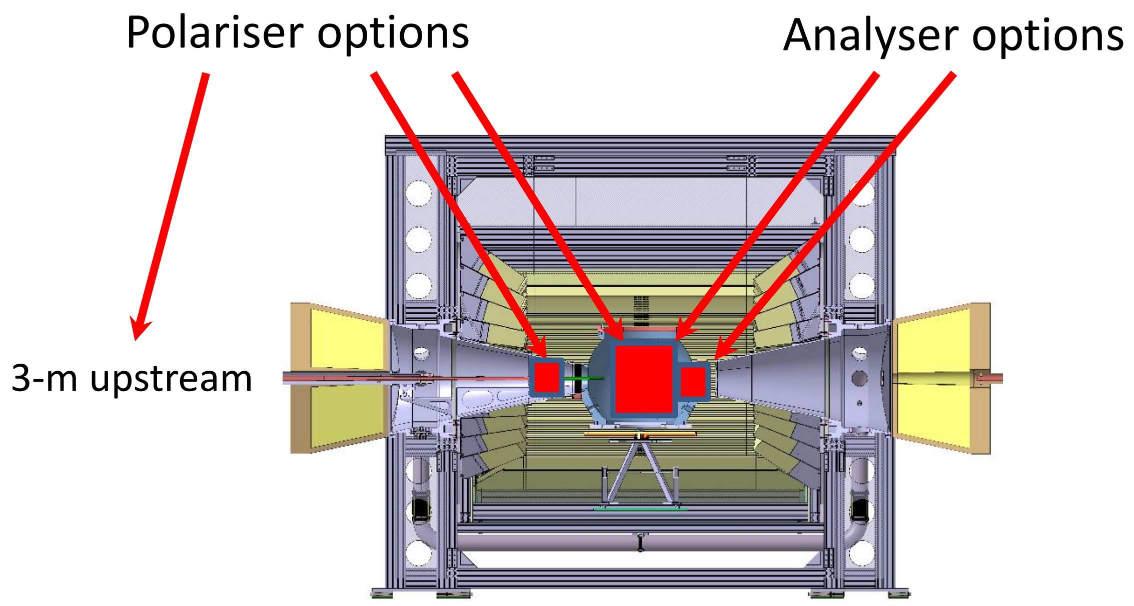
	Reflectometry				SANS, GSANS, Off-specular				Wide-angle			
Analyser	λ < 1.5 Å		λ > 3 Å		λ < 1.5 Å		λ > 3 Å		λ < 1.5 Å		λ > 3 Å	
	With high-field magnet	With guide field only	With high-field magnet	With guide field only	With high-field magnet	With guide field only	With high-field magnet	With guide field only	With high-field magnet	With guide field only	With high-field magnet	With guide field only
Supermirror - single reflective												
Supermirror - single transmission												
Supermirror - v-cavity												
Supermirror - c-bender												
Supermirror - s-bender												
Supermirror - wide-angle array												
Polarised 3He - MEOP												
Polarised 3He - SEOP, off-situ												
Polarised 3He - SEOP, in-situ												

Conceptual polarised neutron setup

Diffraction – DREAM

Mikhail Feygenson, Instrument Scientist
Peter Harbott, Lead Engineer

- Magnetism & hydrogenous materials
- Polarise ^3He with ^3He spin-flipping most likely for both polariser and analyser.
- Different combinations of polarised ^3He techniques and placements of the polariser & analyser are being explored.
- *In-situ* SEOP possible for polariser and low-angle analyser.

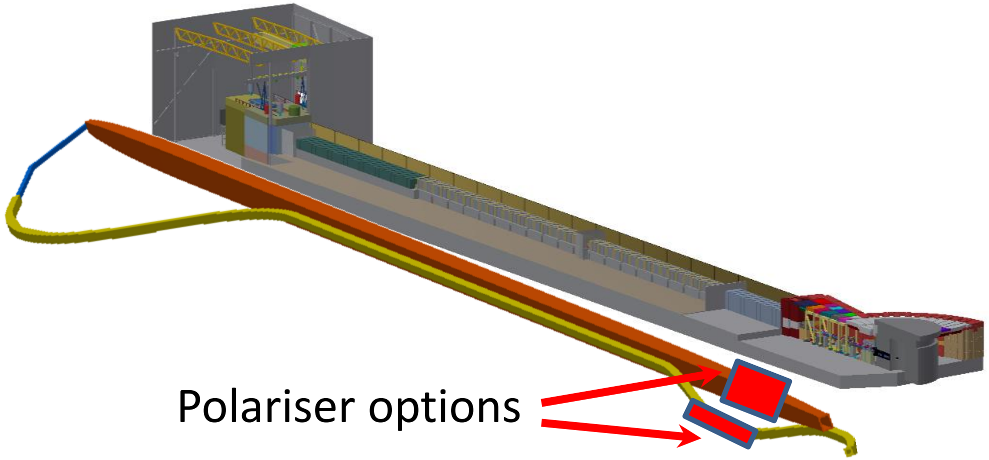


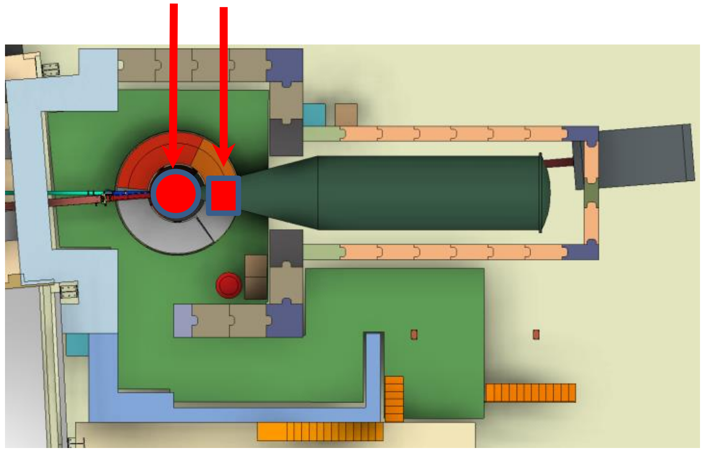
DREAM Detector Tank

Conceptual polarised neutron setup

Diffraction – HEIMDAL
Dan Mannix, Instrument Scientist
Kåre Iversen, Lead Engineer

- Magnetism & hydrogenous materials
- Incident: Solid state polariser for cold incident beam. Polarise ^3He with ^3He spin-flipping for thermal beam
- Scattered: Polarised ^3He analyser.
- Different combinations of polarised ^3He techniques and placements of the polariser & analyser are being explored.
- *In-situ* SEOP possible for polariser and low-angle analyser.





Conceptual polarised neutron setup

Diffraction - MAGiC

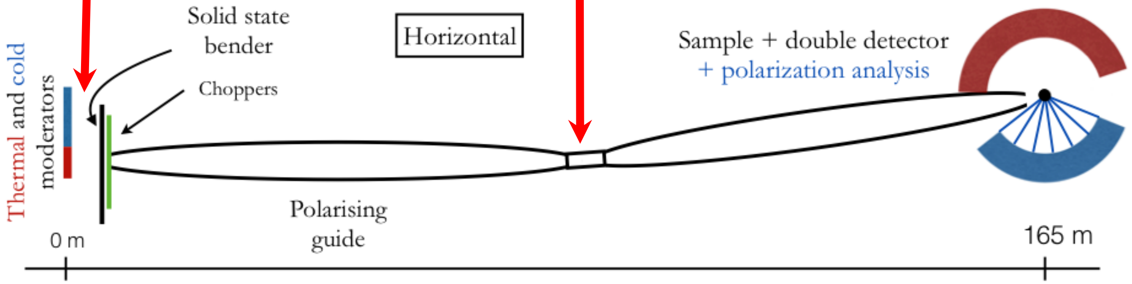
Xavier Fabrèges, Instrument Scientist

Sergey Klimko, Lead Engineer

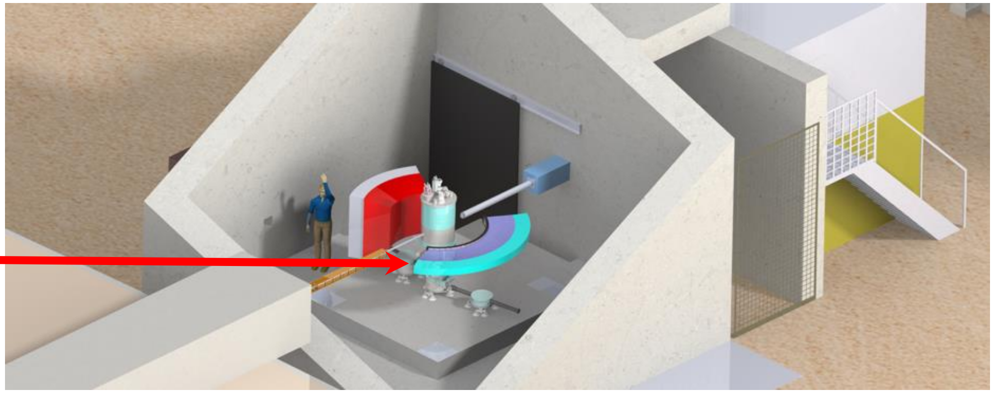
- Magnetism
- Polarising supermirror for both polariser and analyser. Spin-flipper for incident beam.
- Dedicated polarised neutron instrument
- Polarised neutron equipment part of in-kind contribution
- Polarised ^3He wide-angle analyser can be a valuable tool for the commissioning of supermirror analyser.

C-bender (cold)

Polarising guide (thermal)



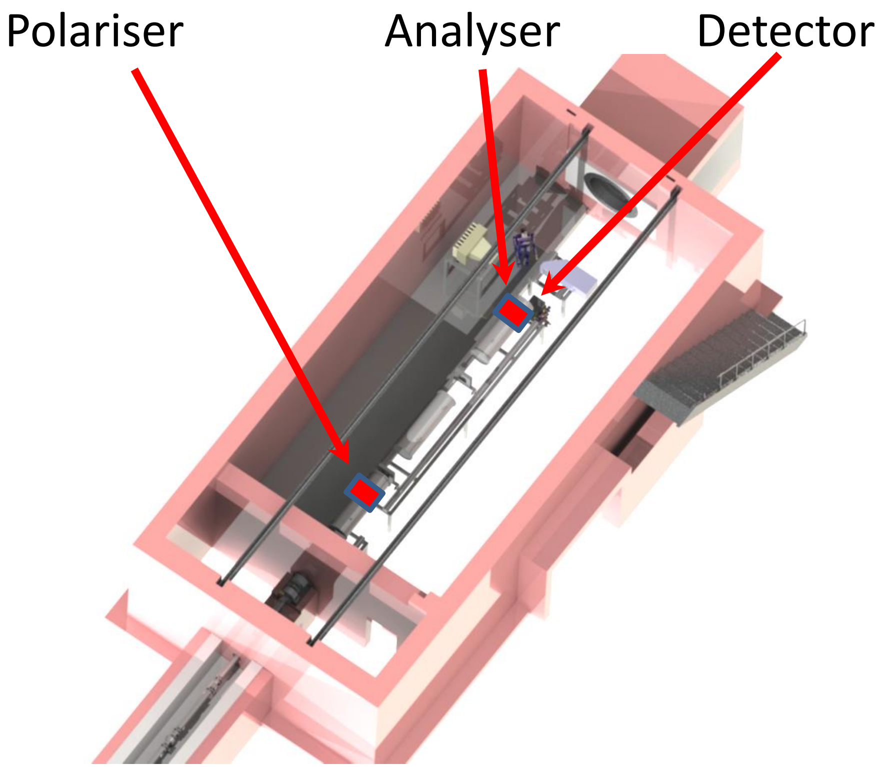
Analyser



Conceptual polarised neutron setup

Engineering and Industrial - ODIN
Aureliano Tartaglione, Instrument Scientist
Manuel Morgano, Instrument Scientist
Elbio Calzada, Lead Engineer

- Polarising supermirror for polariser
- Polarising supermirror or polarised ^{3}He for analyser, depending on application
- For imaging, the sample-to-detector distance is limited for achieving good resolution. This places a constraint on the analyser.



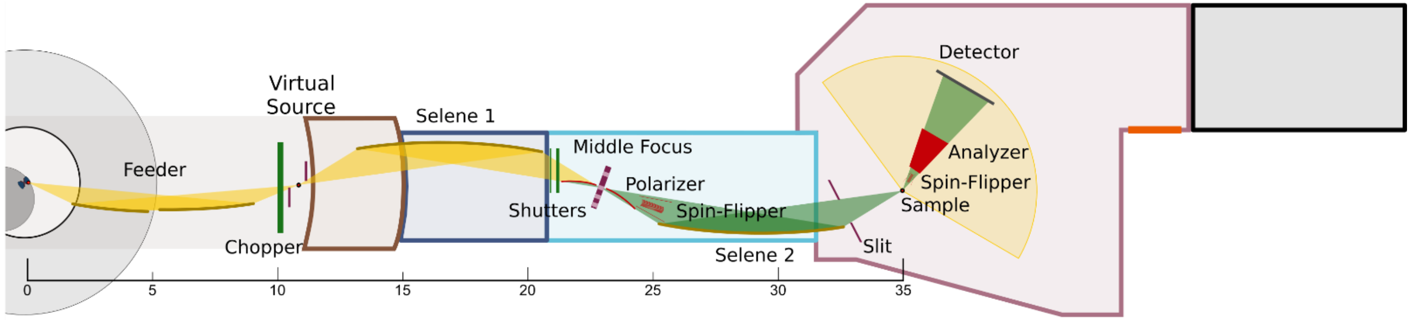
Conceptual polarised neutron setup

Large Scale Structure – ESTIA

Artur Glavic, Instrument Scientist

Sven Schütz, Lead Engineer

- Magnetism
- Polarising supermirror for both polariser and analyser. Spin-flippers for incident beam and scattered neutrons.
- Dedicated polarised neutron instrument
- Polarised neutron equipment part of in-kind contribution
- Polarised ^3He analyser will serve as optional test device.



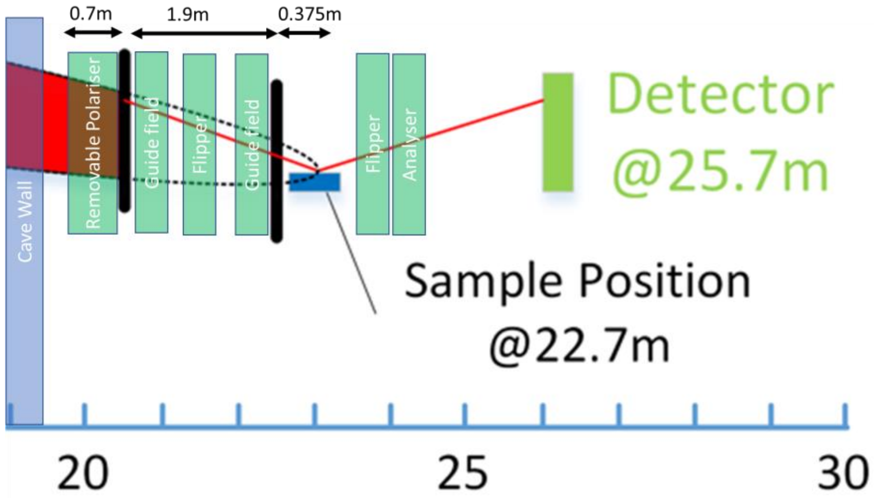
Conceptual polarised neutron setup

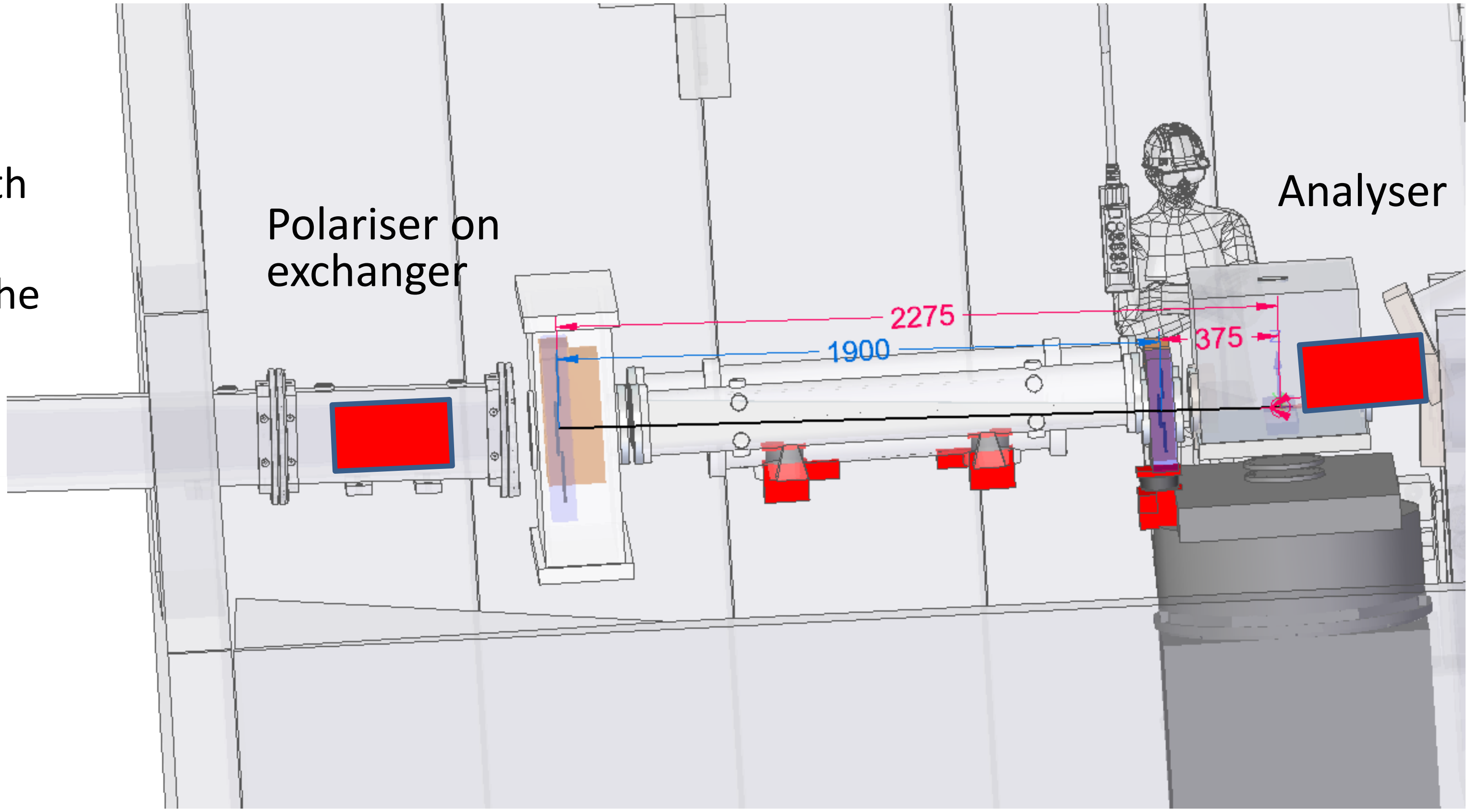
Large Scale Structure – FREIA

Tom Arnold, Instrument Scientist

Jon Elmer, Lead Engineer

- Hydrogenous materials
- Polarise ^{3}He with ^{3}He spin-flipping for both polariser and analyser
- Large vertical height coverage would be the main challenge
- *In-situ* SEOP may be possible.

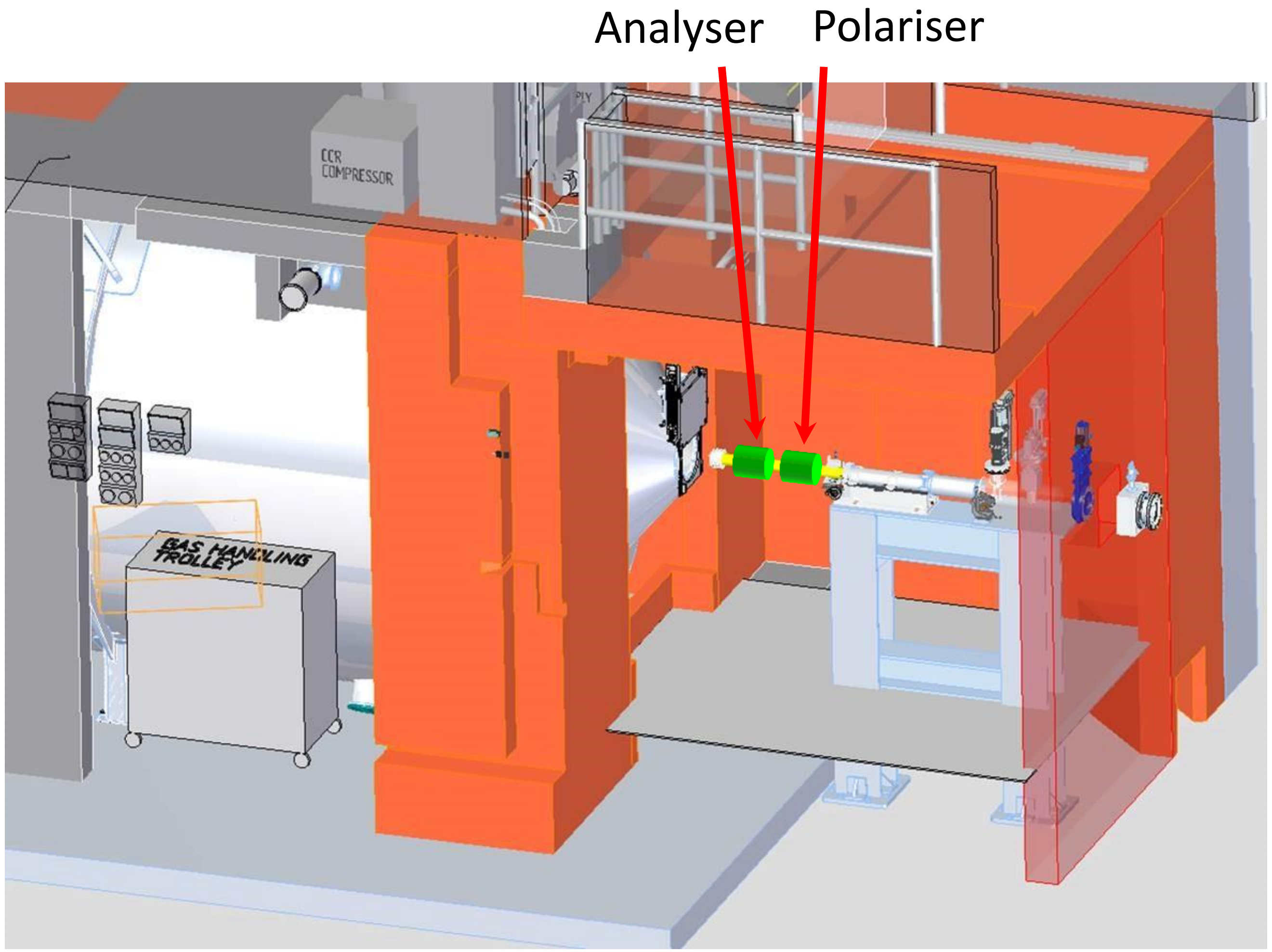




Conceptual polarised neutron setup

Large Scale Structure – LoKI
Judith Houston, Instrument Scientist
William Halcrow, Lead Engineer

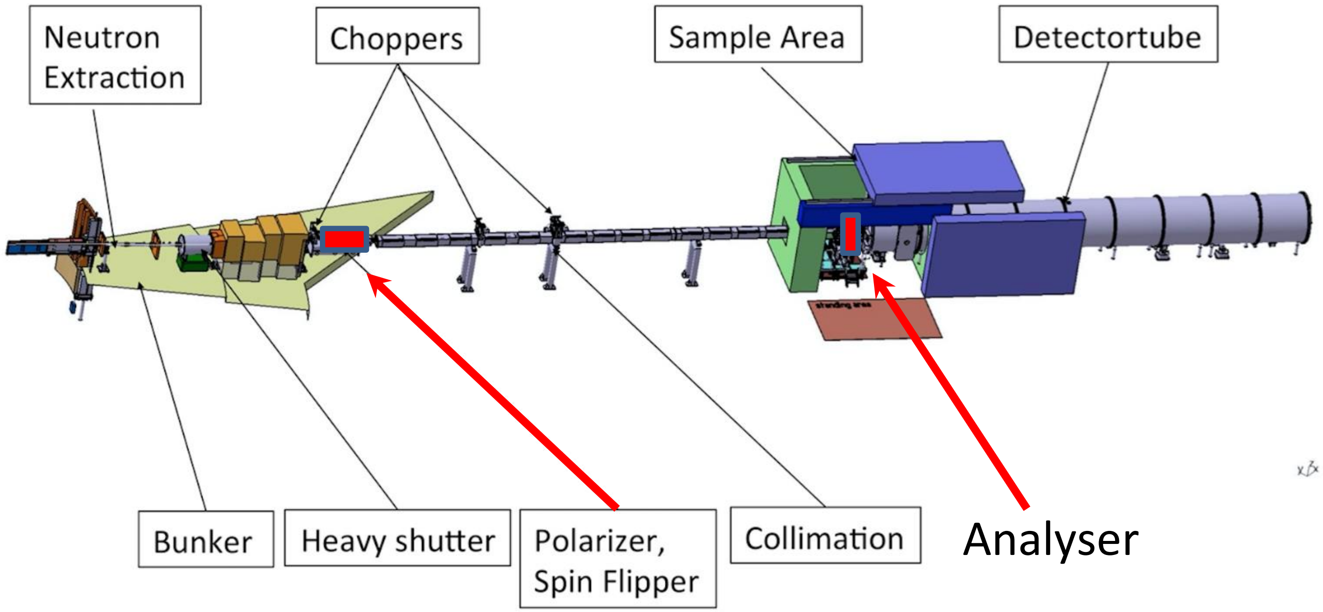
- Hydrogenous materials
- Polarise ^3He with ^3He spin-flipping for both polariser and analyser
- Compact setup at sample area
- *In-situ* SEOP may be possible.



Conceptual polarised neutron setup

Large Scale Structure – SKADI
Sebastian Jaksch, Instrument Scientist
Romuald Hanslik, Lead Engineer

- Magnetism
- Incident: Polarising supermirror polariser, spin-flipper
- Scattered: Polarised ^{3}He with ^{3}He spin-flipping for analyser
- 2d translation of analyser needed
- Shielded high-field magnet needed to work with polarised ^{3}He
- *In-situ* SEOP may be possible.

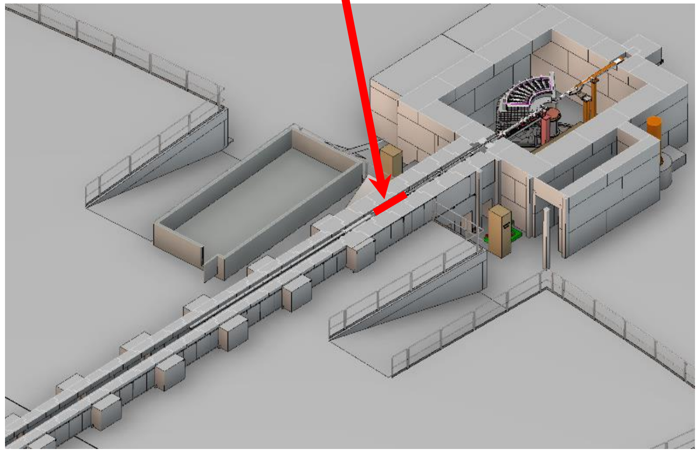


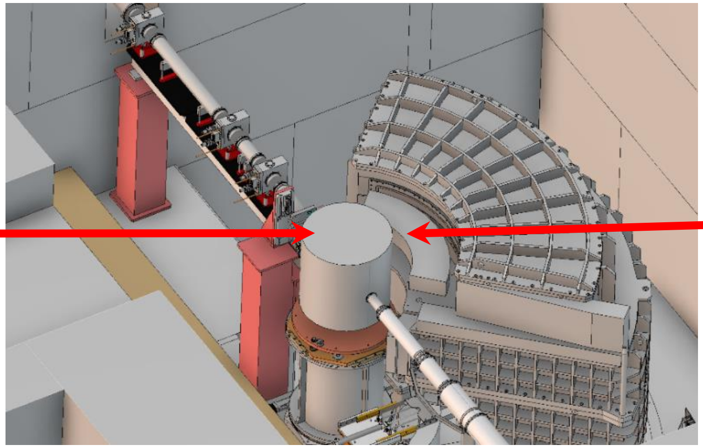
Conceptual polarised neutron setup

Spectroscopy, indirect geometry – BIFROST
Rasmus Toft-Petersen, Instrument Scientist
Liam Whitelegg, Lead Engineer

- Magnetism & hydrogenous materials
- Incident: Polarising s-bender, spin-flipper
- Scattered: Polarised ^{3}He wide-angle analyser, limited coverage supermirror analyser, possible upgrade to wide-angle supermirror analyser.

Polariser, spin-flipper





Polarised ^{3}He wide-angle analyser (showing 3-d field coil region)

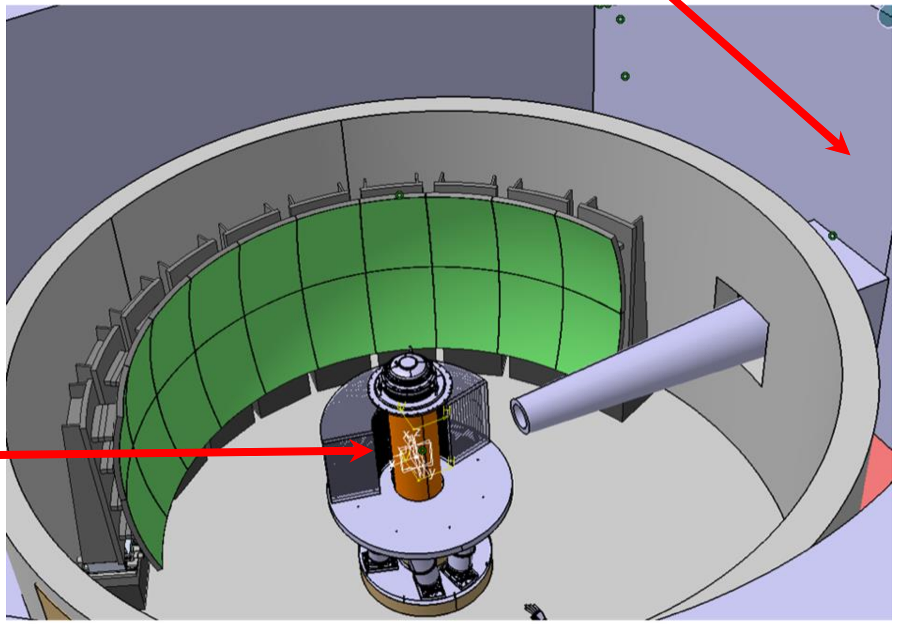
Supermirror analyser (showing full wide-angle analyser)

Conceptual polarised neutron setup

Spectroscopy, indirect geometry – MIRACLES
Félix J. Villacorta, Instrument Scientist

- Hydrogenous materials
- Incident: Polarising supermirror, spin-flipper
- Scattered: Polarised ^{3}He wide-angle analyser

Guide exchanger housing polariser, spin-flipper (not shown)



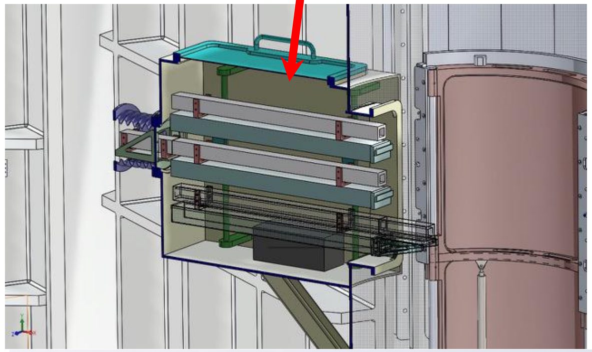
^{3}He wide-angle analyser between sample tank and collimator

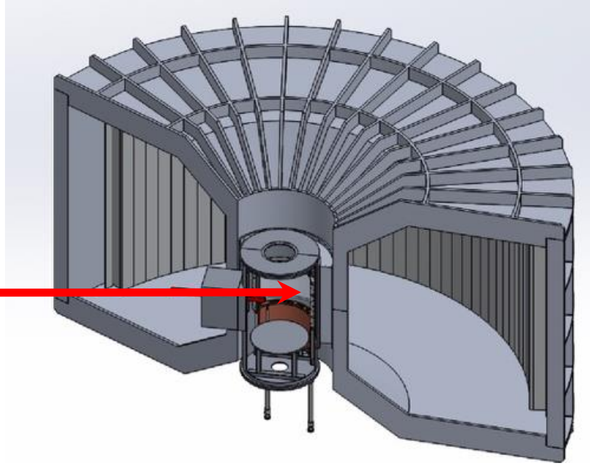
Conceptual polarised neutron setup

Spectroscopy, direct geometry – CSPEC
Pascale Deen, Instrument Scientist
Fernando Yamil Moreira, Lead Engineer

- Magnetism & hydrogenous materials
- Incident: Polarising supermirror, spin-flipper
- Scattered: Polarised ^{3}He wide-angle analyser

Guide exchanger housing polariser, spin-flipper



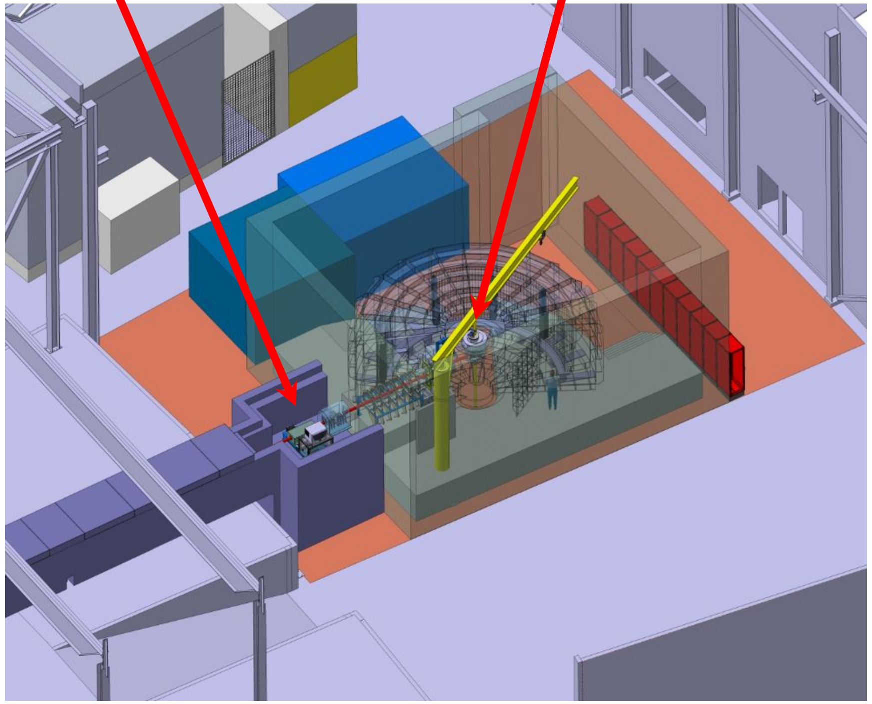


Sample area to house ^{3}He wide-angle analyser

Conceptual polarised neutron setup

Spectroscopy, direct geometry – T-REX
Nicolò Violini, Instrument Scientist
Hans Kämmerling, Lead Engineer

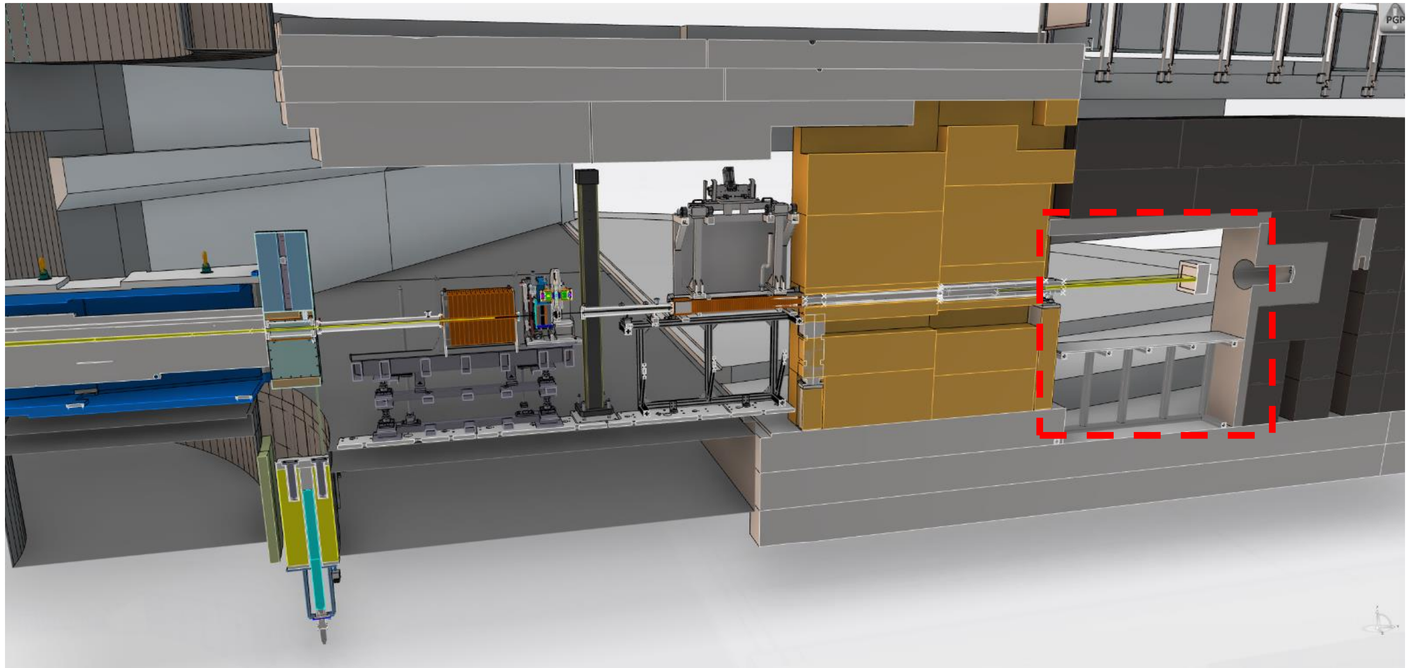
- Magnetism
- Incident: Polarising supermirror, spin-flipper and/or *in-situ* ^{3}He polariser
- Scattered: Polarised ^{3}He analyser



Conceptual polarised neutron setup

Test Beam Line
Robin Woracek, Instrument Scientist
Nicolas Breton, Lead Engineer

- Beam line for testing polarised neutron devices –
  - Polarising supermirror
  - Polarised ^{3}He neutron spin-filter
  - Spin-flipper
  - Resonance coil



Summary of the polarised neutron setup options being evaluated

POLARISER	DIFFRACTION			ENG.	LARGE-SCALE STRUCTURE				SPECTROSCOPY			
	DREAM	HEIMDAL	MAGiC	ODIN	ESTIA	FREIA	LoKI	SKADI	BIFROST	CSPEC	MIRACLES	TREX
Supermirror - reflection		■	■		■			■				
Supermirror - stack transmission				■							■	
Supermirror - v-cavity				■				■			■	■
Supermirror - c-bender			■									
Supermirror - s-bender				■					■	■	■	
Polarised 3He - MEOP, cylindrical cell	■	■		■		■	■		■	■	■	■
Polarised 3He - SEOP, in-situ, cylindrical cell	■	■		■		■	■		■	■	■	■

ANALYSER	DIFFRACTION			ENG.	LARGE-SCALE STRUCTURE				SPECTROSCOPY			
	DREAM	HEIMDAL	MAGiC	ODIN	ESTIA	FREIA	LoKI	SKADI	BIFROST	CSPEC	MIRACLES	TREX
Supermirror - reflection					■							
Supermirror - stack transmission				■								
Supermirror - v-cavity												■
Supermirror - c-bender												
Supermirror - s-bender												■
Supermirror - wide-angle array			■									
Polarised 3He - MEOP - wide-angle cell	■	■	■						■	■	■	■
Polarised 3He - MEOP - cylindrical cell	■	■		■	■	■	■	■				
Polarised 3He - SEOP, in-situ, cylindrical cell	■	■		■	■	■	■	■				

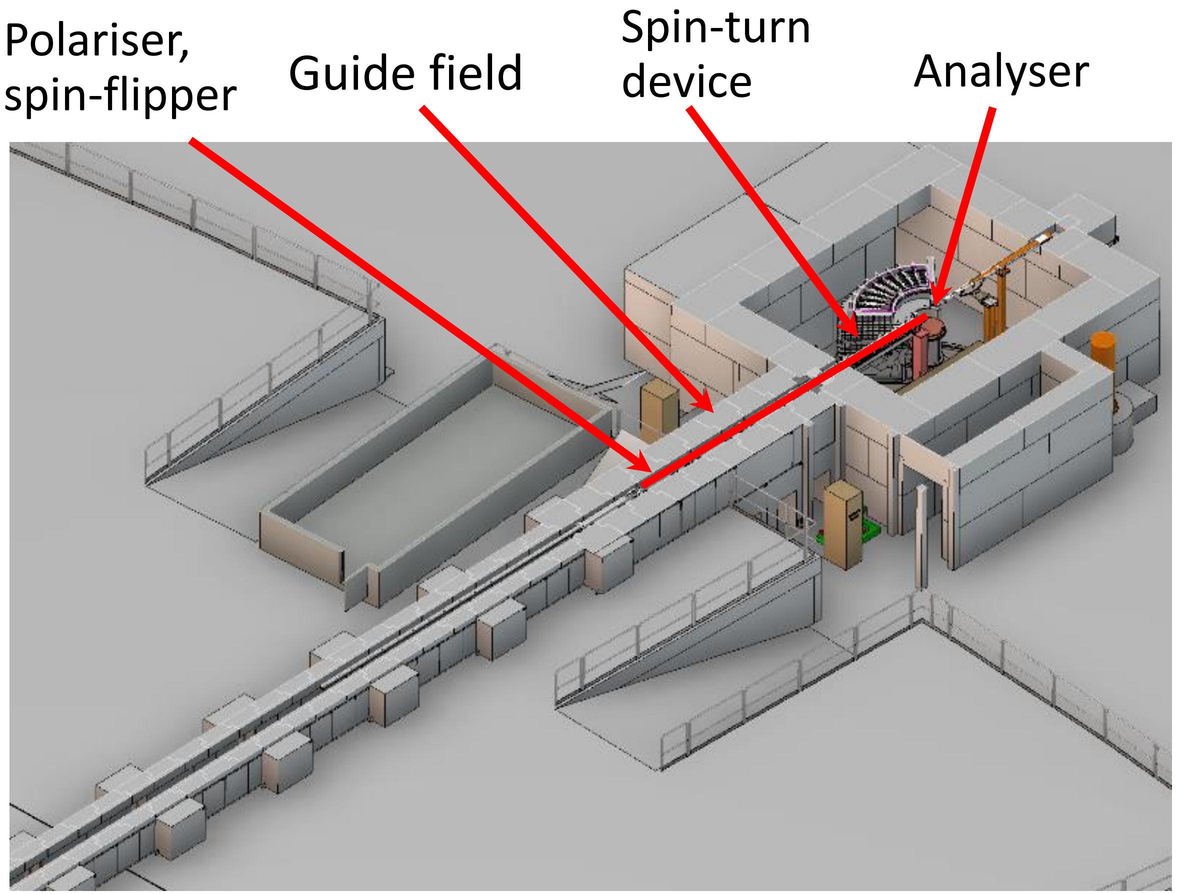
Each combination of plausible setup will be evaluated on its merits.

- Solid state devices being evaluated on 6 instruments.
- Cylindrical polarised ^{3}He cell, either in-situ SEOP or MEOP being evaluted on 9 instruments.
- There are overlaps of solid state devices and polarised ^{3}He devices in some instances. The mertis of each is to be evaluated.
- Wide-angle cell, MEOP being evaluated on 7 instruments

Design considerations – Magnetic field design

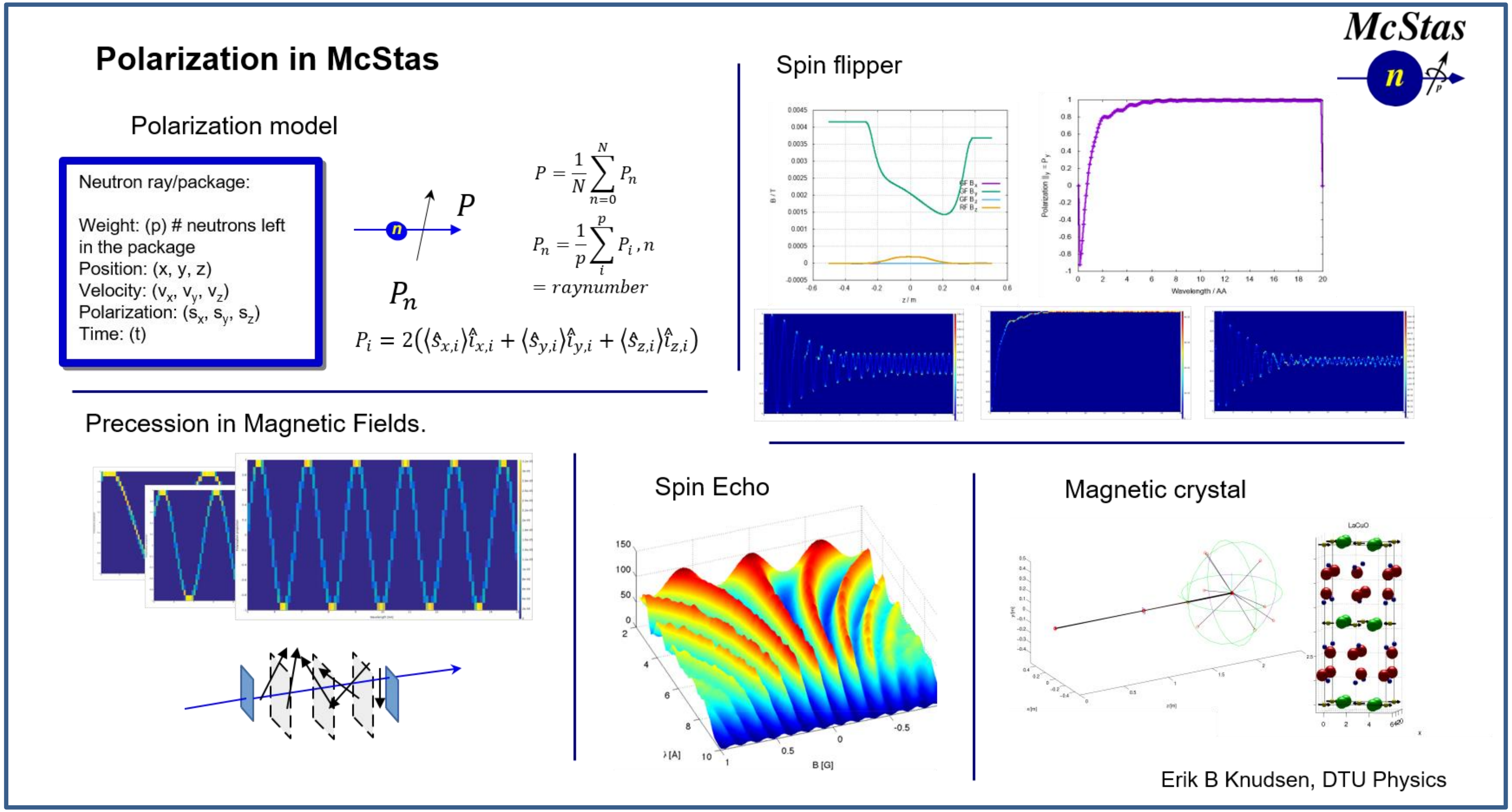
- Polarised neutron setup
  - Magnetic field from the polariser to the sample and to the analyser.
  - Uniform magnetic field for ^{3}He polarisation

- Proper magnetic field design based on instrument model is critical



Design considerations – Monte Carlo simulation

- Polarised neutron components also change the beam characteristics. Monte Carlo simulation will therefore be part of the design process.

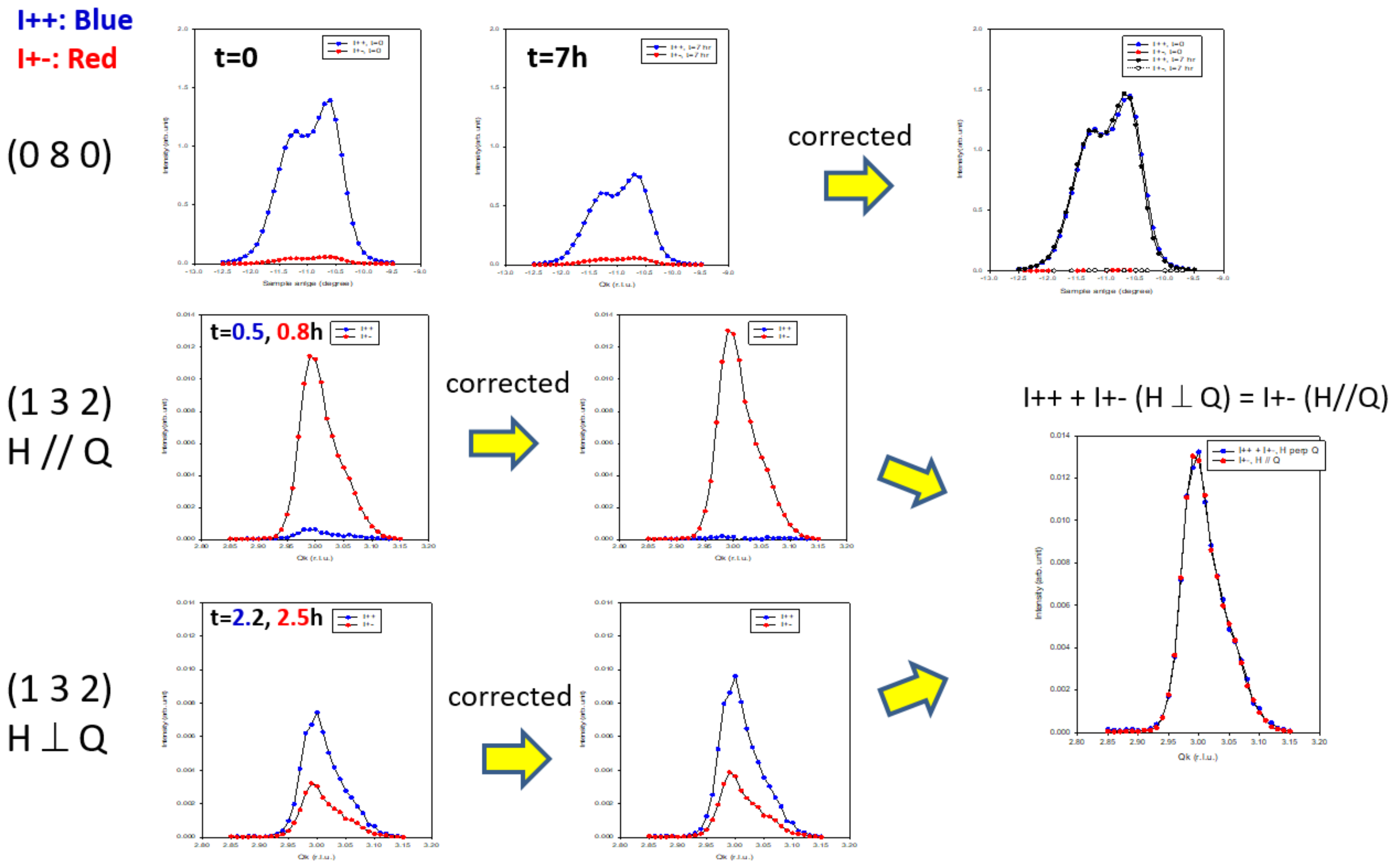


Wai Tung (Hal) Lee, ESS. IKON 18. 2020-02-24.27. Lund

Measurement methodology and data reduction

- Data reduction: polarised neutron more complex than unpolarised neutron.
  - Both non-spin-flip and spin-flip measurements often need to be done.
  - Reference measurements also need to be for non *in-situ* polarised ^{3}He device

- Discussion next week with DMSC colleagues to develop the methodology and data reduction resources.



Interface with Sample Environment

EUROPEAN
SPALLATION
SOURCE

- There are two issues needing more extensive coordination with Sample Environment group:

  1. Magnetic interference: Polarised neutrons and polarised ^{3}He devices are susceptible to magnetic interence in the vicinity.

  2. To guarantee spin-transport, asymmetric high-field magnet is needed for polarised neutron work.

ESS Polarisation Workshop

As a lead-up to develop the polarisation work package, we are organising a workshop:

ESS Polarisation Workshop, 26th-27th of March, ESS site
https://indico.esss.lu.se/event/1390/

The workshop will be a focal point to

- highlight the sciences that can be done on ESS instruments using polarised neutrons from the perspectives of the user community,
- share the experiences in polarised neutorn instrumentation R&D and in operations for experiments using polarised neutrons,
- provide an overview of the neutron polarisation setup options,
- advise the ESS on the developmental road map to incorporate polarised neutron capabilties, and
- write a workshop report to serve as the basis of the ESS Polarisation Work Plan

Summary

- The ESS intends to provide a coordinated service to assist instruments to incorporate polarised neutron capability.
  1. (1) 12 instruments may have polarised neutrons available for users.
  2. (2) We are developing a polarisation work pacakge for 2020-2025.
  3. (3) Work will include hardware (design, build, install, commission, operation), control software, meaurement methodology, data reduction software, and ease-of-use improvements.
  4. (4) The priority is based on the schedule of the instruments.

- **Scientific Advisory Committee, October 2019: "*We recommend advancing this as fast as possible in order for it to be available by 2025.*"**

- ESS Workshop on Polarisation will be held on 26th-27th of March at the ESS site. https://indico.esss.lu.se/event/1390/

Acknowledgement

EUROPEAN SPALLATION SOURCE

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Auxiliary Slides

Who am I?

First venture into the field of polarised neutrons

1. BIREFRINGING POLARISER: Polarised neutron interferometry - Scalar Aharonov-Bohm Effect

- An array of prime-shaped field splitted an unpolarised beam to 2 polarised beam.
- Single-crystal silicon reflections then selected the polarised beam.

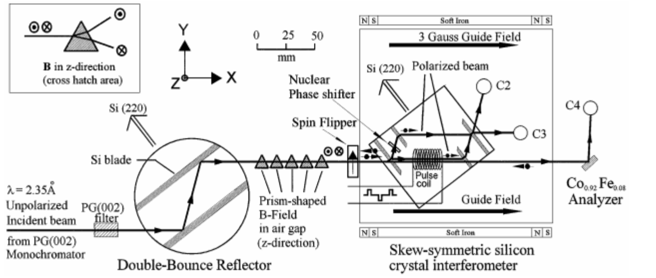


FIG. 1. Schematic drawing of the experimental setup. The polarizer consists of the perfect silicon crystal double-bounce reflector and the series of five prism-shaped air-gap magnetic fields. The silicon skew-symmetric interferometer and the pulse coil are the key components to observe the SAB effect. A static type spin flipper is placed between the polarizer and the interferometer to rotate the neutron spins from the z direction to the longitudinal x direction. The permanent magnet guide field maintains this direction of polarization throughout the region of the interferometer. Behind the interferometer is a magnetically saturated $Co_{0.92}Fe_{0.08}(111)$ crystal to analyze the classical spin orientation.

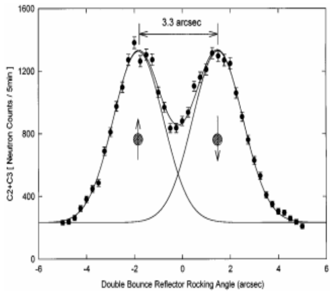


FIG. 2. Rocking curve of the double-bounce reflector against the interferometer, showing the birefringence splitting of 3.3 arcsec. The two neutron peaks have opposite polarization. The total intensity C2 + C3 is shown.

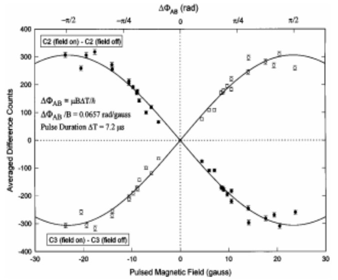


FIG. 5. SAB interference intensity, shown as difference counts of positive and negative field pulses relative to the zero-field counts, plotted as a function of the pulsed B-field strength. Each point is an average of four points at the center of the peak plateaus in the TOF patterns (Fig. 4). The solid lines are fits of a sinusoid to the data, with the pulse duration ΔT as the adjustable parameter.

Physical Review Letters, Vol. 80, 3165 (1998).

2. HEUSLER CRYSTAL: Inelastic polarised neutron scattering – Chromium Spin Density Wave

Heusler 111 polariser & analyser in triple-axis spectrometer

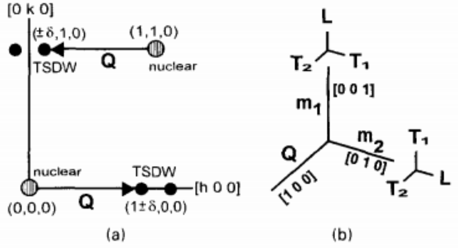


Fig. 1. (a) TSDW satellites in reciprocal space. (b) The polarizations $\Delta\boldsymbol{m}$ of the modes of magnetic excitation (T_1, T_2, L) associated with the TSDW polarizations $\boldsymbol{m}_1$ and $\boldsymbol{m}_2$.

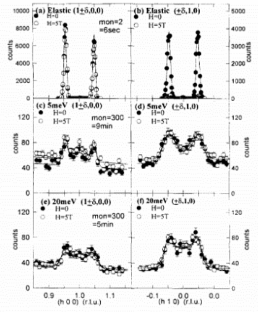


Fig. 2. Constant energy scans across the TSDW satellites. The filled circles are $H = 0$ data. The opened circles are $H = 5$ T data. The solid lines are curve fits with Gaussians.

Physica B, Vol. 241, 622 (1997)

Who am I?

Work at ORNL

3. SELF-SHIELDED ASYMMETRIC MAGNET

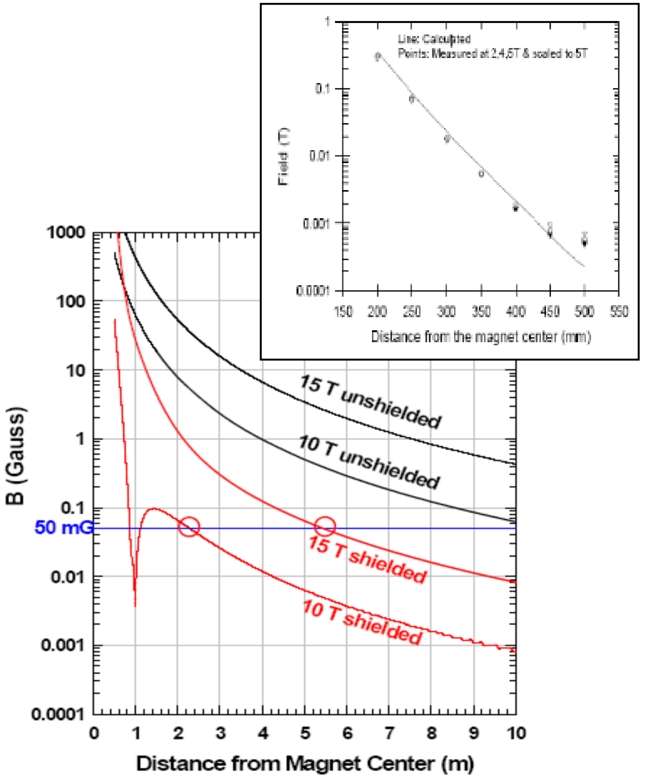
- Design study up to 15T.
- Asymmetric and self-shielding work in tandem to stablise the magnet

- First of its kind: 5 T “Slim-Sam”. Still one of the most-stable & most-requested work horse at the SNS

- No relationship to 16T/14T magnet which is a symmetric magnet running asymmetrically (unstable).

Problem: Magnetic interference

Solution: Self-shielded asymmetric magnet



4. Monte Carlo simulation for neutron scattering instrumentation design

5. R&D works of SESAME (Spin-Echo Scattering Angle Measurement)