Heimdal Instrument Diffraction STAP Meeting

Dan Mannix

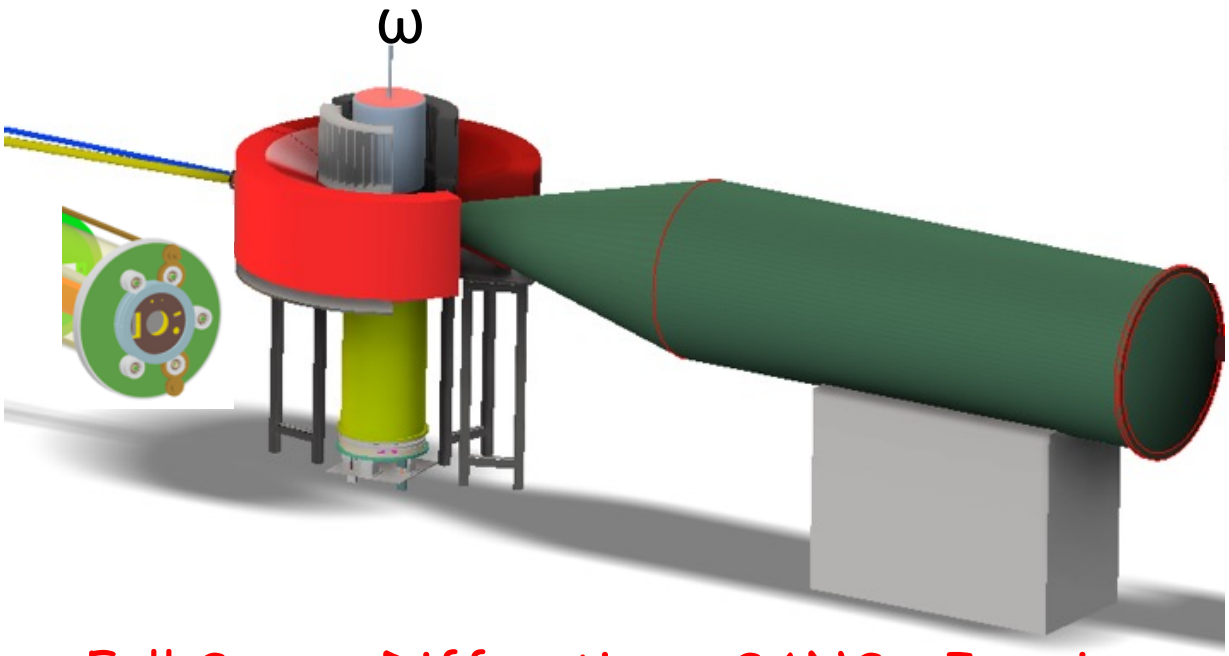
Lead Scientist Heimdal Instrument ESS, Lund Sweden

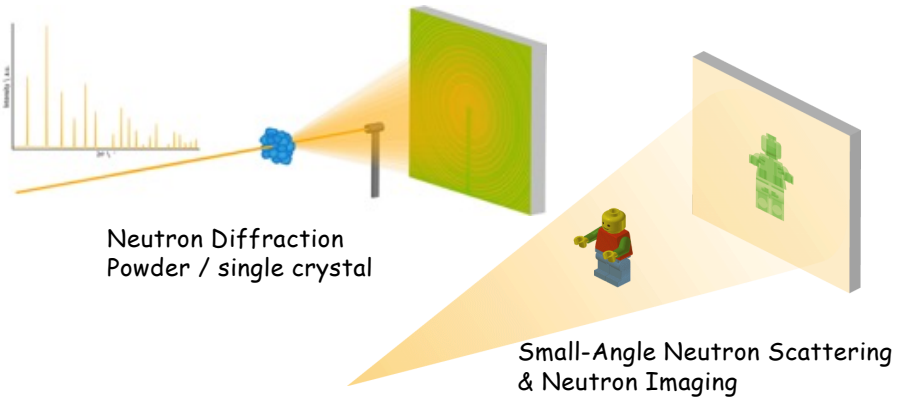
ESS - October 2024

HEIMDAL – Hybrid Diffraction

Multi Length Scale Neutron Scattering Instrument: 10^{-2} – 10^{8} nm

EUROPEAN SPALLATION SOURCE





Full Scope: Diffraction + SANS + Imaging

(1) Thermal Diffraction (SOUP 2028)
(2) SANS - Cold Guide (75% complete)
(3) Imaging (future upgrade)

Rescoping Instruments
Under discussion @ ESS

Heimdal was heavily descoped !

Heimdal Team

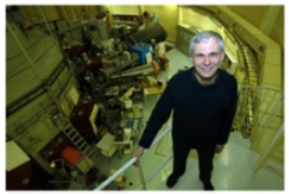
Isabel Llamas
Scientist (IFE)

Dan Mannix
Lead Scientist
(ESS/AU)

Siamak Kianzad
Lead Engineer
(ESS/NSS)

Kåre Iversen
Engineer
(AU scope)

Bengt Jönsson
Engineer
(ESS/AU)



Bjørn Hauback
In-kind Partner IFE

P.I Mogens Christensen
In-Kind Partner AU

Autur Glavic
In-kind Partner PSI

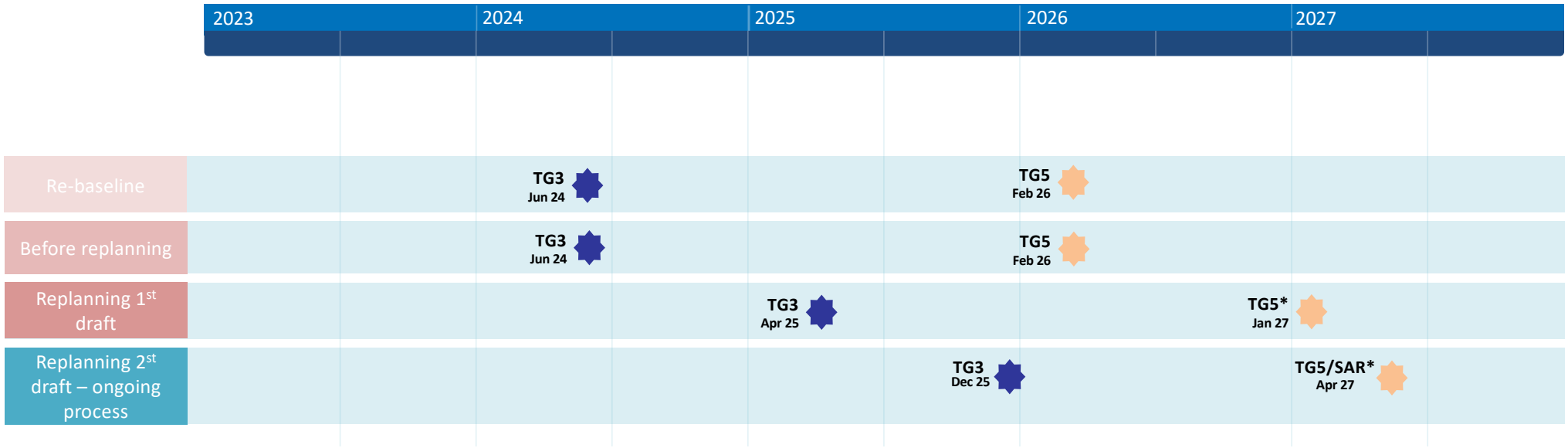
New Resources:

Siamak: New Lead Engineer (ESS)
Bengt: Engineer (ESS)
Kåre: Engineer (AU)

More Engineering support
To gear up to TG3 & TG5
Outsource & ESS/AU

Documentation Support 2025
Harald Lang (PSI – Estia)
Isabel Llamas (IFE)

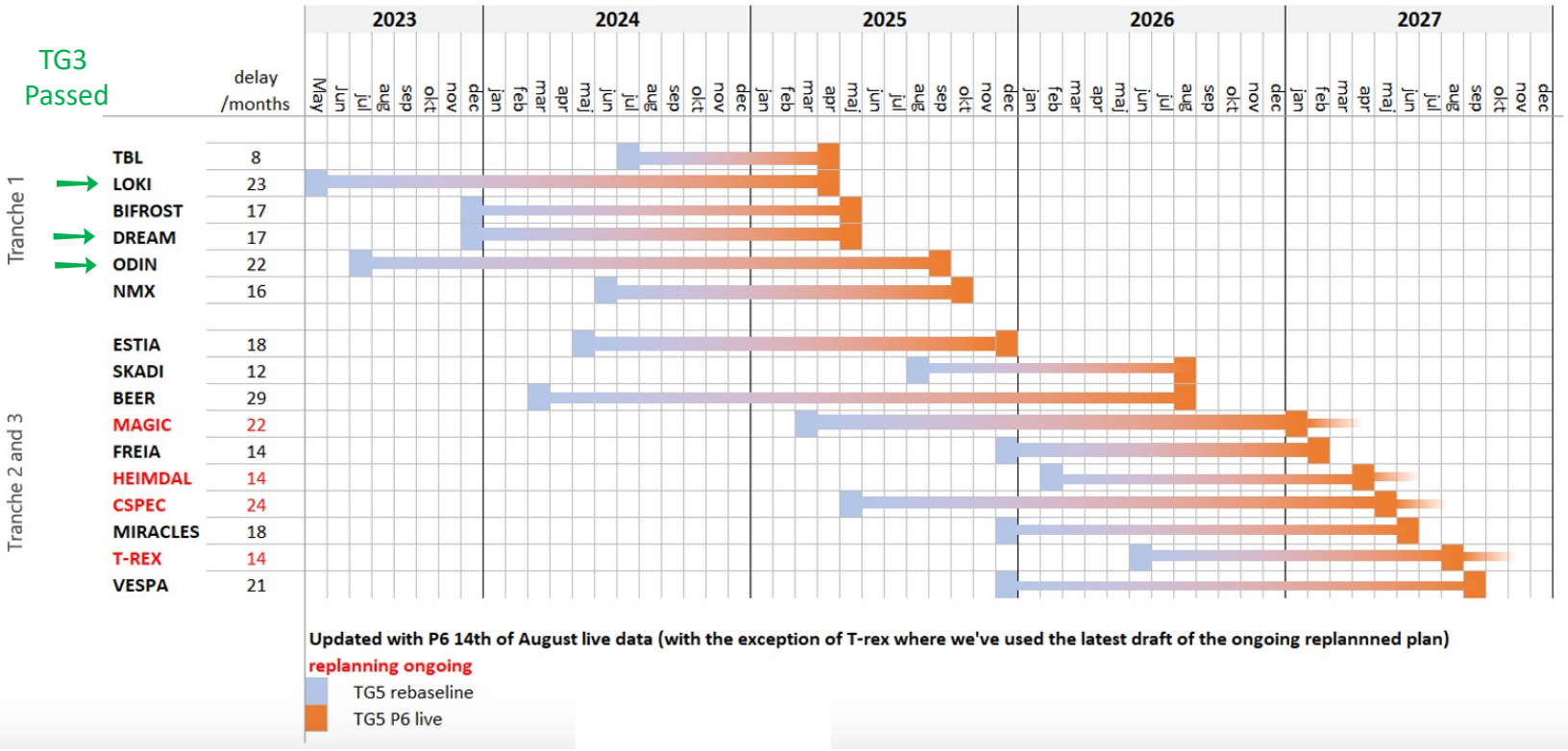
HEIMDAL Schedule overview



Instrument Replanning

Re-planning of later instruments

Delay of TG5 milestone for all instruments

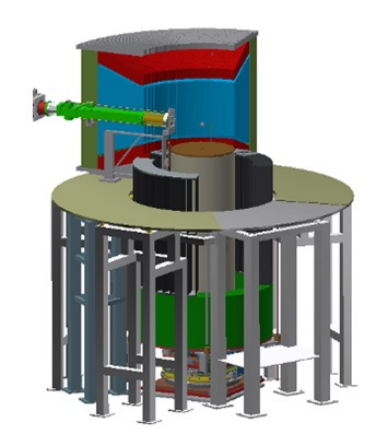


2018 TG3

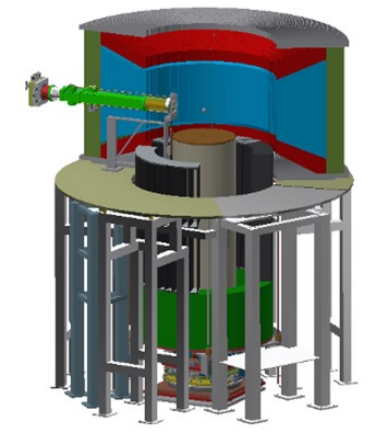
ESS Instrument Rescoping

EUROPEAN SPALLATION SOURCE

Scope 1.0sr. (80°)

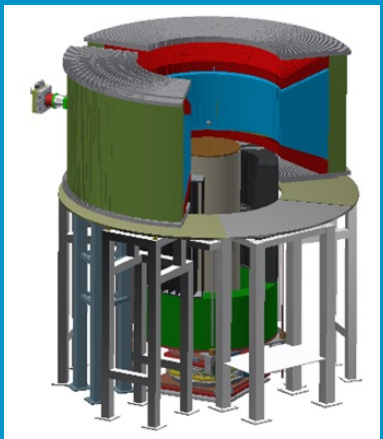


UG1 2.0sr. (1.8M€)

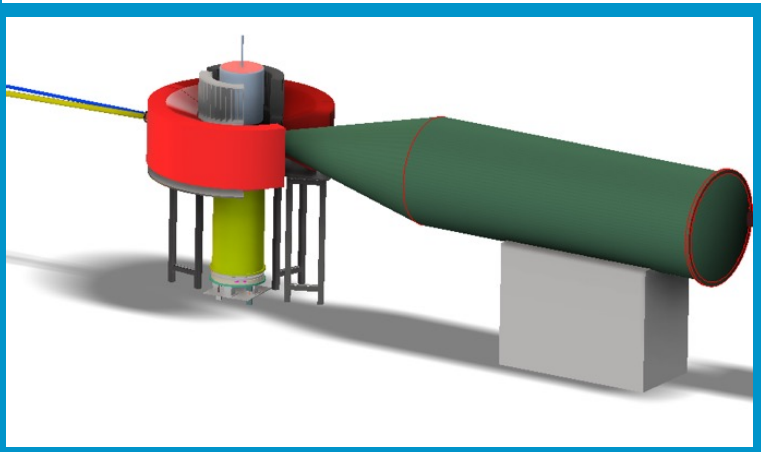


ESS Resources:
CUP/CEP
Detector Group
DMSC…

UG2 3.0sr. (3.6M€)



Full Scope: Diffraction + SANS + Imaging (6.2M€)

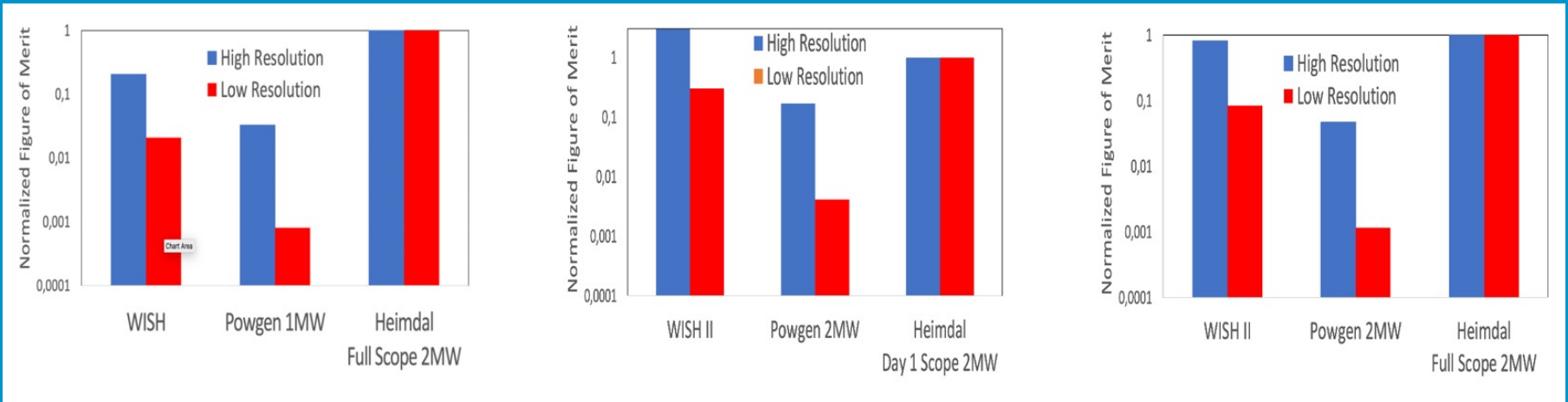


Upgrade Item	Cost k€
rescope 1: Diffraction Detectors current scope 1sr 80-170°	
Double Dector coverage 1.0sr - 2.0sr Costed CDT (2023) 10-80°	1800
Triple Detector coverage 2.0sr ->3.0sr costed CDT (2023) 190-290°	1800
Subtotal rescope 1:	**3600**
rescope 2: SANS Scope	
Wide Shielding (Mirrotron offer)	265
Final 40m Cold guide (Swissneutronics)	464
SANS TANK (estimate)	75
2 x Cold Choppers ESS Common	400
SANS Detector 1 (BANDGEM) 0-4°	500
SANS detector 2 (BANDGEM) 4-10°	500
Subtotal rescope 2: SANS	**2204**
Rescope 3: Imaging	
Imaging detector (timepix 28x28)	150
Detector Mounting motorisation	50
Subtotal Rescope 3: Imaging	**200**
Total 2sr Detector + SANS	**4004**
Total full scope	**6229**

ESS Instrument Rescoping

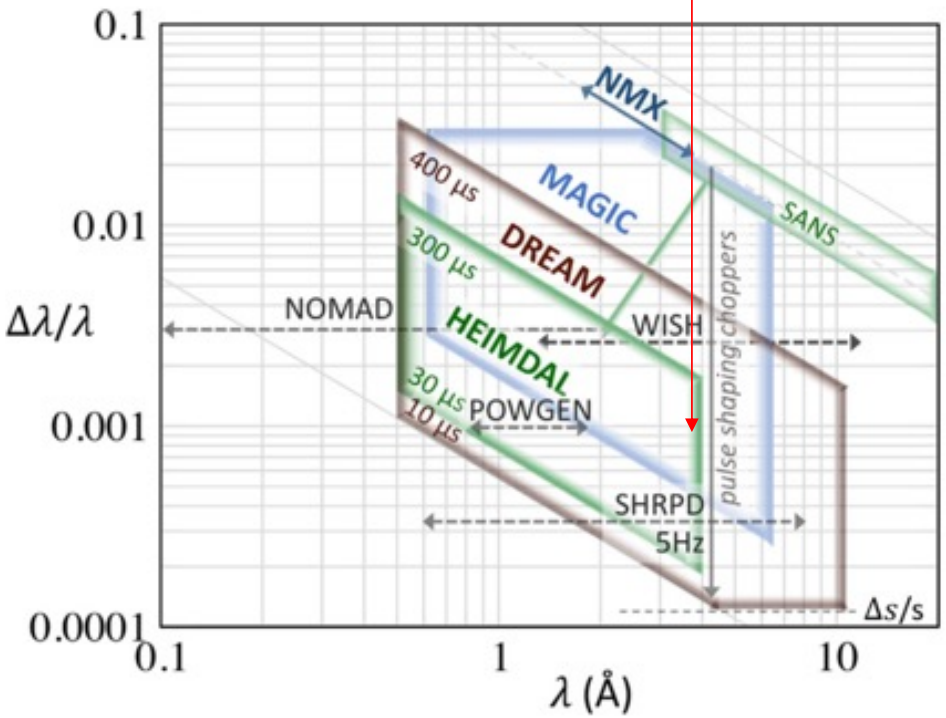
EUROPEAN SPALLATION SOURCE

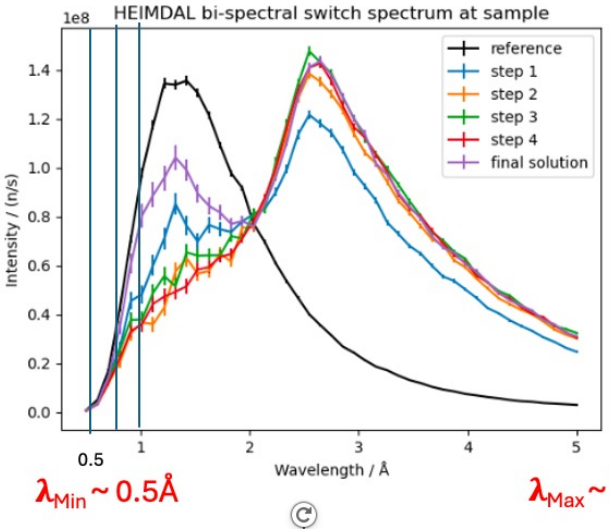
$$FOM = Flux * Detector\ Efficiency * \frac{DetectorCoverage}{SampleSize}$$

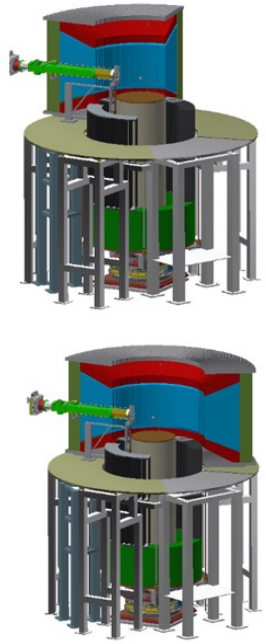


2D Detector & Rescoping

High Resolution + High Flux $Q = 4\pi \sin(\theta) / \lambda$ $d = 2\pi / Q$

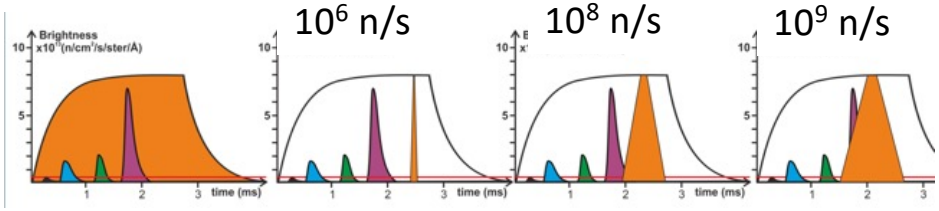






Optimum flux 0.8Å–3.5Å

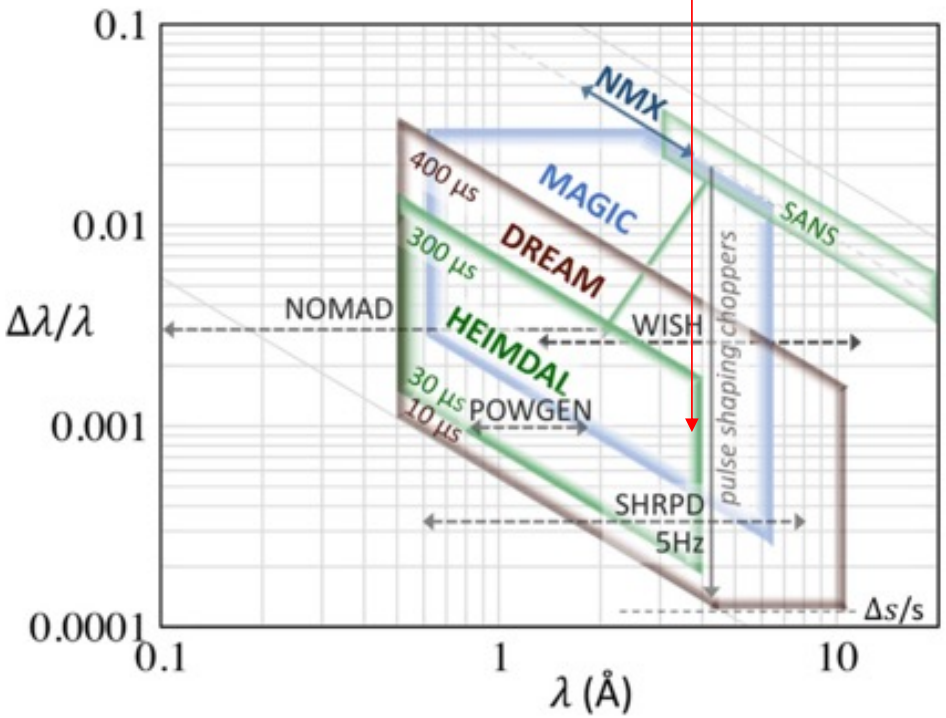
Obtainable flux 0.5Å - 6Å +

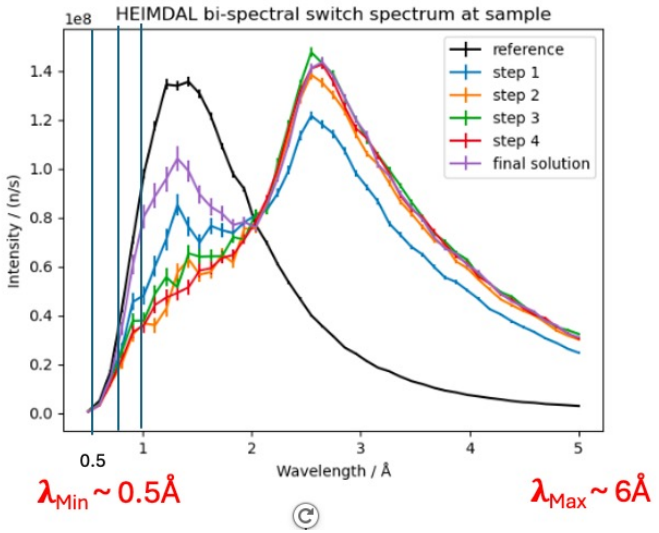


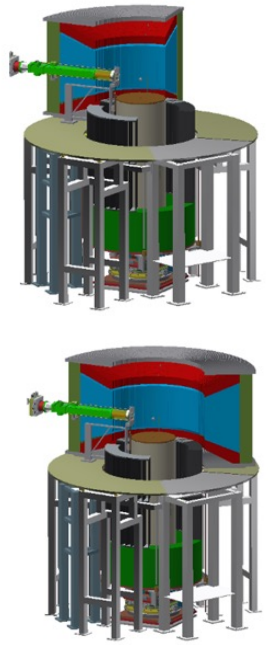
Wavelength			λ = 0.5Å		λ = 4.0Å	
Detector Position	2θ Max	2θ Min	Q Max (Å^{-1})	Q Min (Å-1)	Q Max (Å-1)	Q Min (Å-1)
Back scatt.	172	92	25,0707797	18,0784479	3,13384746	2,25980598
Low-Q	90	10	17,7710076	2,19039813	2,22137595	0,27379977
rescoped	172	10	25,0707797	2,19039813	3,13384746	0,27379977

2D Detector & Rescoping

High Resolution + High Flux Q =4π Sin(θ) / λ d =2π / Q







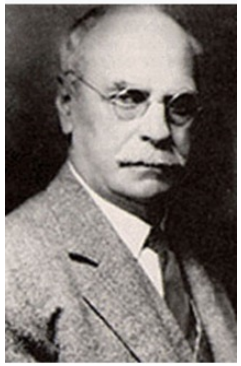
Optimum flux 0.8Å–3.5Å
Obtainable flux 0.5Å - 6Å +

Wavelength			λ = 0.5Å		λ = 0.5Å		λ = 4.0Å		λ = 4.0Å	
Detector Position	2θ Max	2θ Min	Q Max ($Å^{-1}$)	Q Min (Å-1)	d Min (Å)	d Max (Å)	Q Max (Å-1)	Q Min (Å-1)	d Min (Å)	d Max (Å)
Back scatt.	172	92	25,0707797	18,0784479	0,25061787	0,34755115	3,13384746	2,25980598	2,00494293	2,78040918
Low-Q	90	10	17,7710076	2,19039813	0,35356382	2,86851291	2,22137595	0,27379977	2,82851054	22,9481033
rescoped	172	10	25,0707797	2,19039813	0,25061787	2,86851291	3,13384746	0,27379977	2,00494293	22,9481033

Spin Caloritronics ?

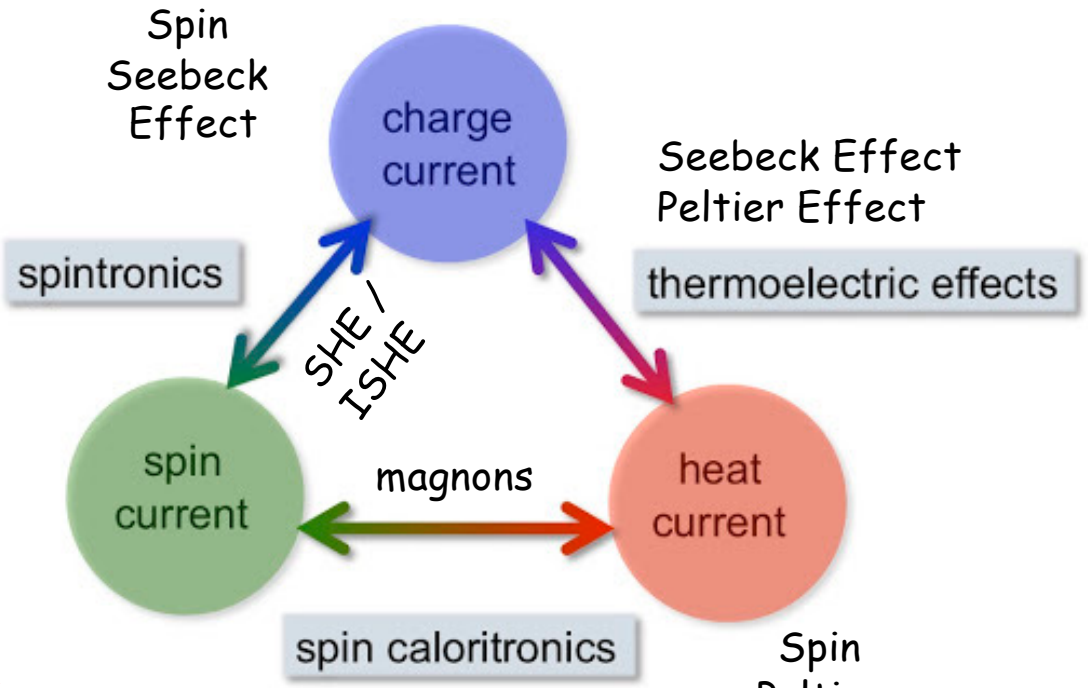
A New Spin on Old Physics

EUROPEAN SPALLATION SOURCE



Hall Effect
1879

Heimdal Early Science Impact



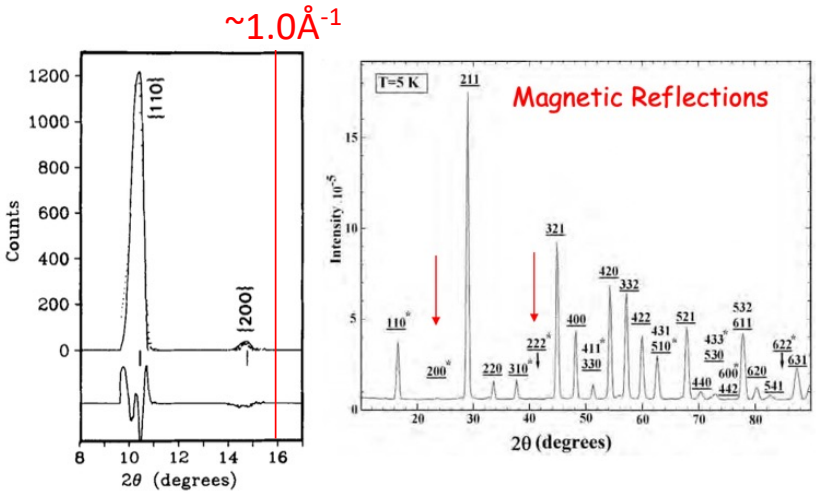
Interconversion of heat, charge and spin currents

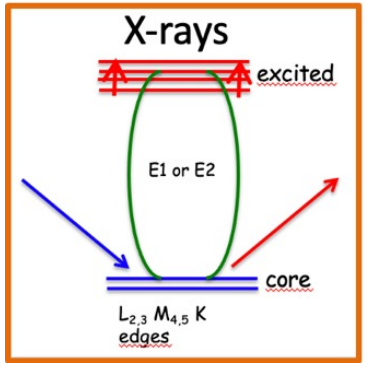
Spintronic + Thermoelectric Functionality

Seebeck Effect
1822

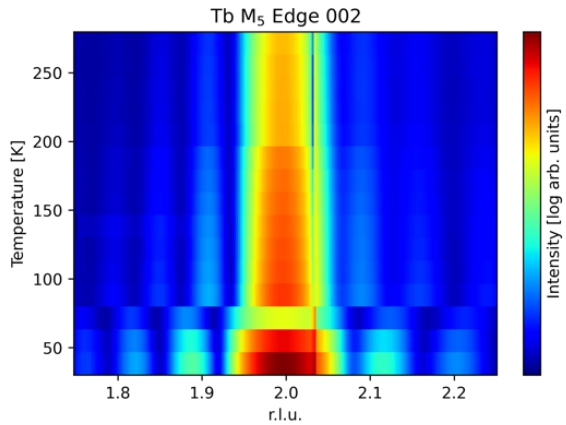
Peltier Effect
1834

Spin Caloritronics ($Re_3Fe_5O_{12}$)

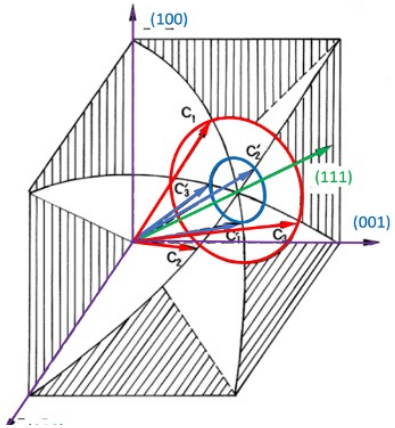


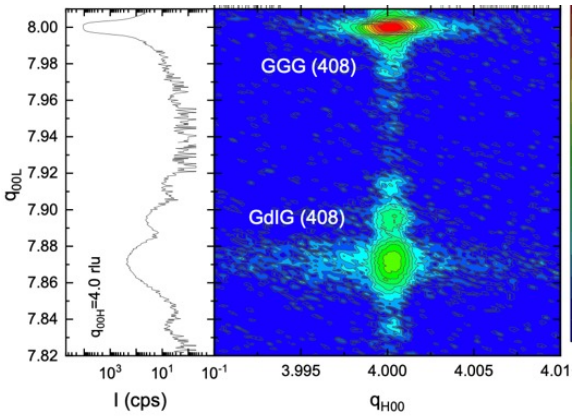


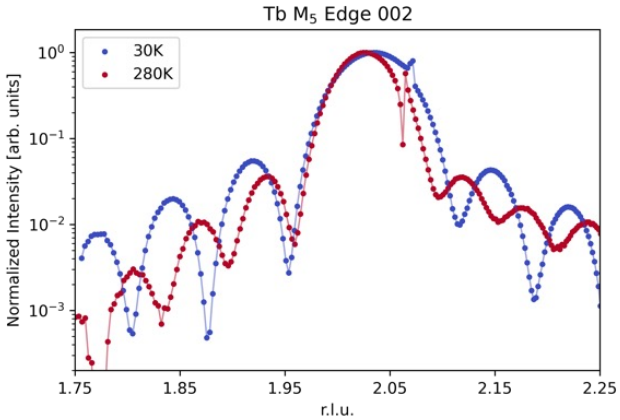
30nm Thin Film:



XRS I10 Diamond
Nano-structure Powder





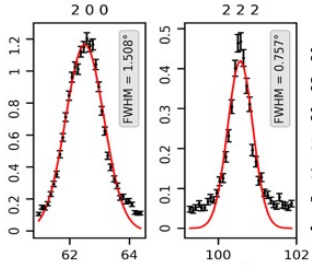


Neutron X-ray Synergies -> Spin Caloritronics

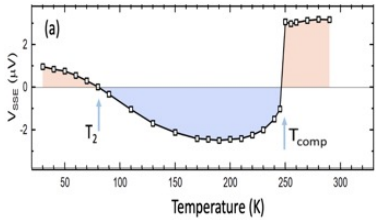
EUROPEAN SPALLATION SOURCE

XFEL: LCLS

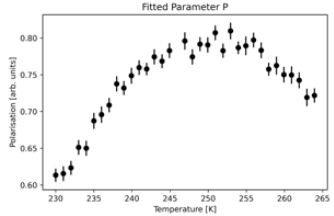
Neutron Single Crystal Diffraction



Spin Seebeck Magnons $Tb_3Fe_5O_{12}$



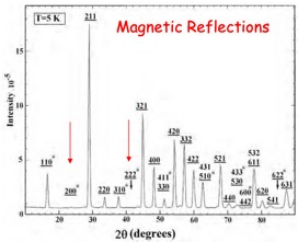
Neutron Spin Echo $Tb_3Fe_5O_{12}$ _ lifetimes?



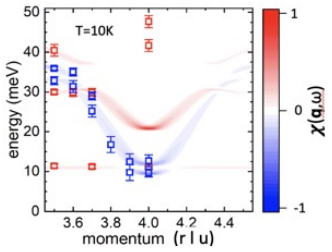
← Bulk

Picosecond →

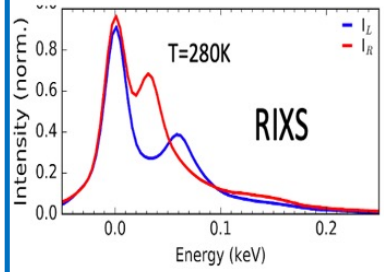
Nanometer ↓



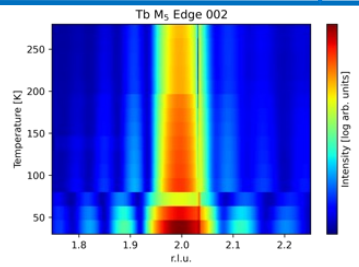
Neutron Powder Diffraction $Tb_3Fe_5O_{12}$



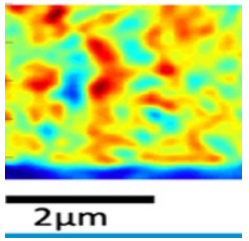
Polarised Neutron Inelastic Scattering $Tb_3Fe_5O_{12}$



RIXS $Gd_3Fe_5O_{12}$ Circular Polarised

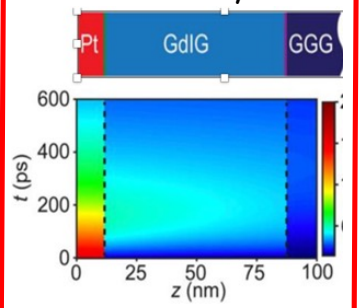


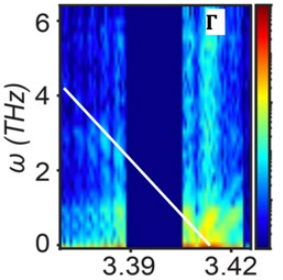
REXS: Films 28nm $Tb_3Fe_5O_{12}$



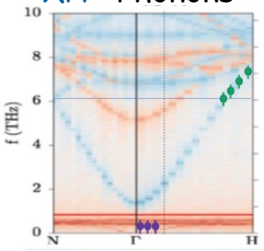
Ptychography $Gd_3Fe_5O_{12}$

XPP: Heat Dynamics





XPP: Phonons



XPP: Magnons ?

Invited Talk ESRF "Coherence ESRF EBS 4th Generation synchrotron sources October 2024

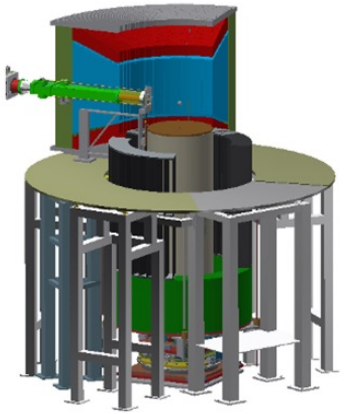
Contributed Talk ILL/ESS User meeting Flipper Polarised Neutrons – Smart Materials December 2024

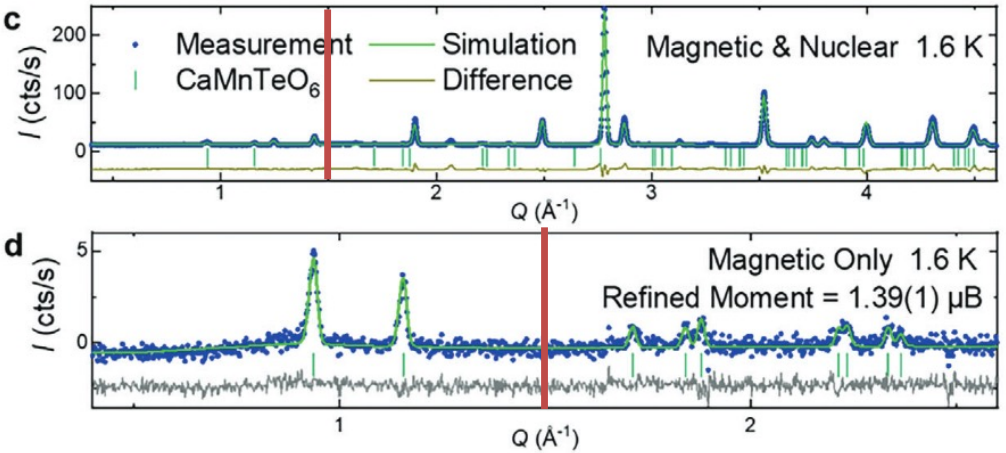
Science Cases

Science Cases & Detector coverage

High Angle only: 92-172º
High resolution, Bond-lengths & PDF
Excludes large & magnetism
Q ~ 2,21-25.0 Å^{-1}
Length scales d: 0.25-2.8Å

Low Angle Only: 10-90º (1-81º)
Large d-space materials & magnetism
Excludes High resolution & PDF ?
Q ~ 0.27-17,7 Å^{-1} (0.03-16,3 Å^{-1})
Length Scales d: 0.35-22.9Å

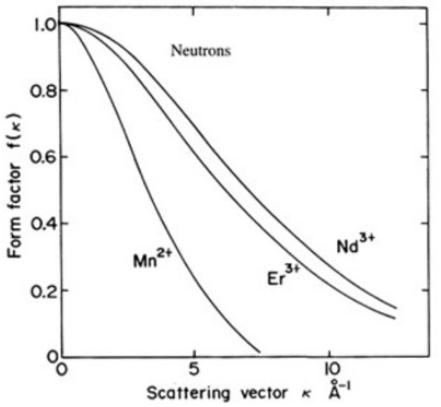




Qmin (6Å) 2θ =92º. ~1.5Å^{-}
Qmax (0.5Å) 2θ =172º ~2.5Å

Qmin (6Å) 2θ =10º ~0.2Å^{-1}
Qmax(0.5Å) 2θ =90º ~17Å^{-1}

Qmin (6Å) 2θ =30º ~0.5Å^{-1}
Qmax(0.5Å) 2θ =120º ~21Å^{-1}

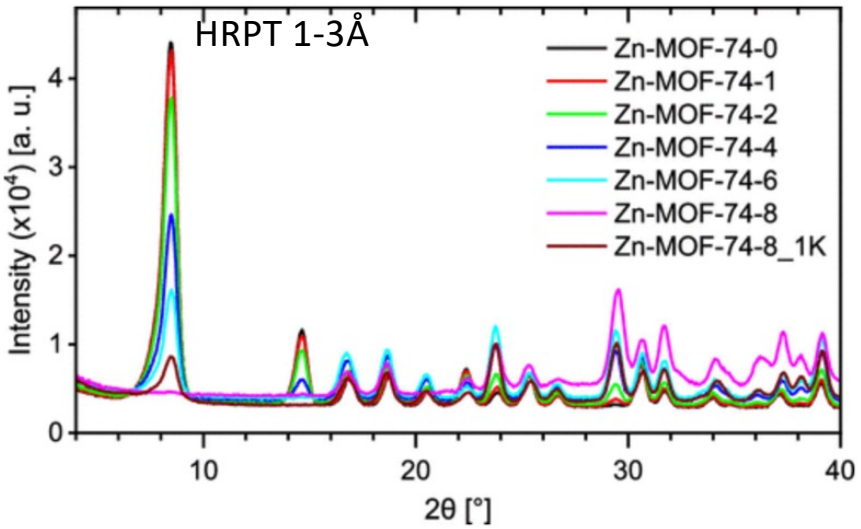


Large d-spacing e.g. MOFs

Science Cases & Detector coverage: Large unit cells cells & metal organic frameworks etc.

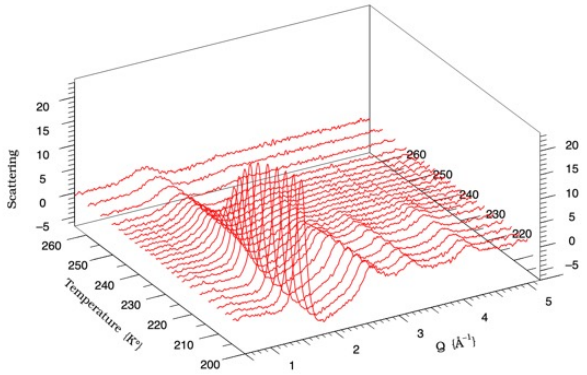
C: PHYSICAL PROPERTIES OF MATERIALS AND INTERFACES | August 16, 2023

In Situ Neutron Diffraction of Zn-MOF-74 Reveals Nanoconfinement-Induced Effects on Adsorbed Propene



Structural and Dynamic Studies of Water in Mesoporous Silicas using Neutron Scattering and Nuclear Magnetic Resonance

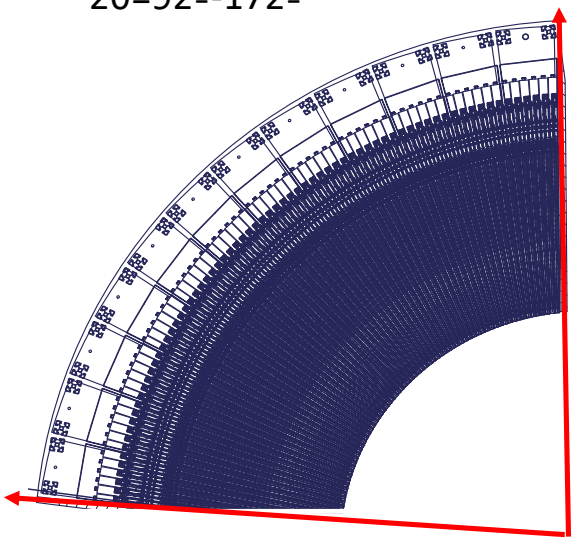
Article in Journal of Physics: Condensed Matter · November 2004



Fixed 2D Detector Position

EUROPEAN SPALLATION SOURCE

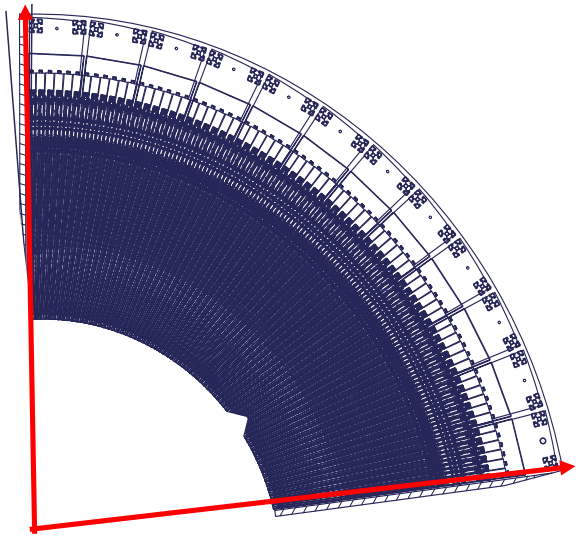
2θ=92º-172º



Qmin (6Å) 2θ =92º. ~1.5Å^{-}
Qmax (0.5Å) 2θ =172º ~25Å

PDF & High resolution. 🙂
Magnetism & large d-spacings ☹️

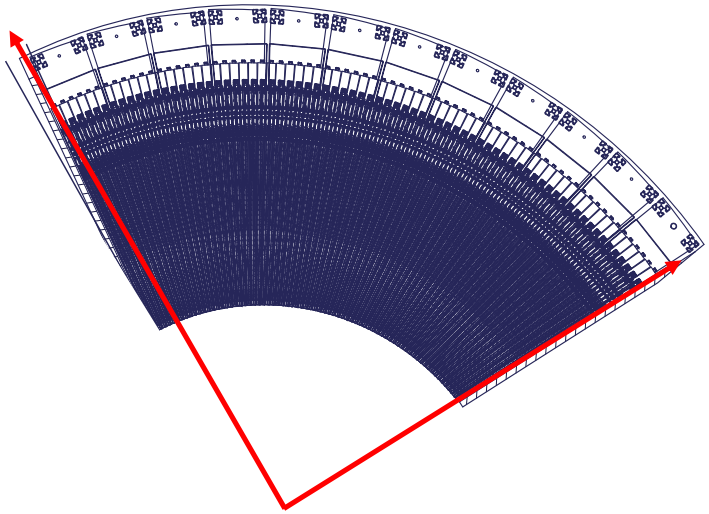
2θ=10º-90º



Qmin (6Å) 2θ =10º ~0.2Å^{-1}
Qmax(0.5Å) 2θ =90º ~17Å^{-1}

PDF & High resolution. ☹️
Magnetism & large d-spacings 🙂

2θ=30º-120º



Qmin (6Å) 2θ =30º ~0.5Å^{-1}
Qmax(0.5Å) 2θ =120º ~21Å^{-1}

PDF & High resolution. 😐
Magnetism & large d-spacings 😐

Or Should we move the detector on rail 0-172 degrees ? ~100k Euros

2D Detector & Rescoping

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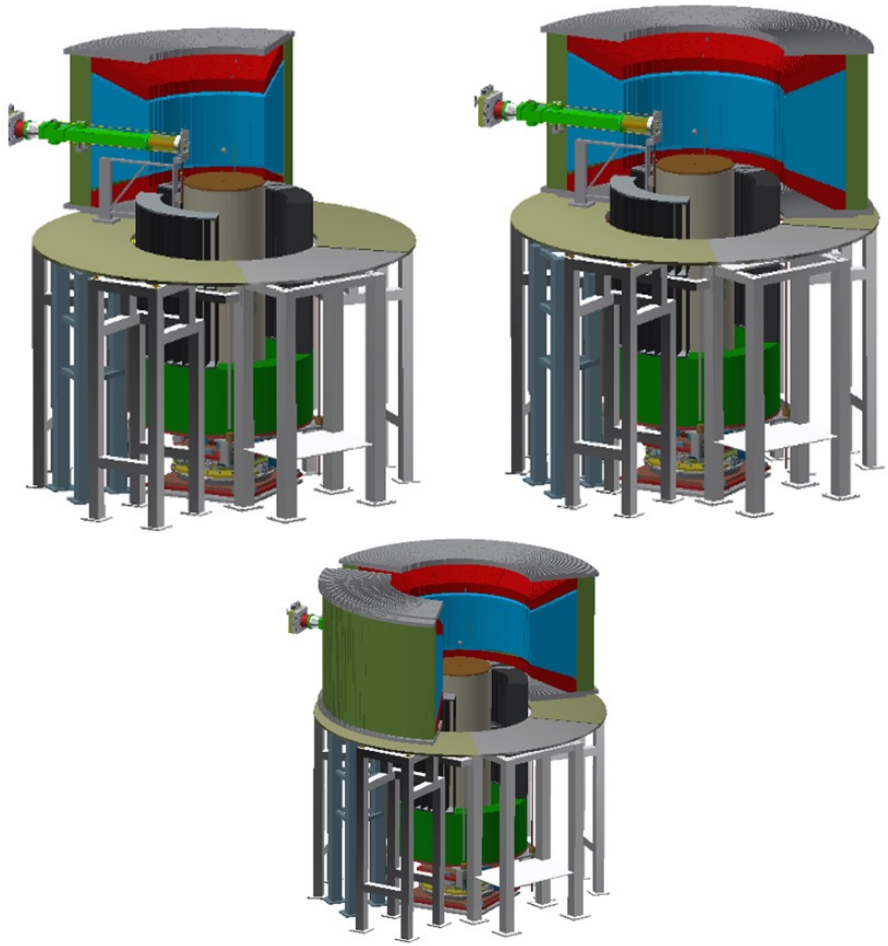
STAP Advice:

(1) Rescope 2D detector 1sr-2sr before HC&FS mid 2027.
- Need agreement with NSS to start procurement now (after dream).
Costs 2.8M Euros.

(2) Go for movable detector support?
Need to start design now to avoid delays to TG3/TG5.
Cost 100k Euros

(3) Stay with fixed 2D detector support?
Which position? 90-172? 10-92? 30-120?
PDF / Magnetism etc. science cases.
No extra cost or delay risks.

(4) Moveable 2D detector & push for SANS upgrade ~3m Euros ?



Heimdal Guide (PSI) Project
Progress with Swiss Neutronics

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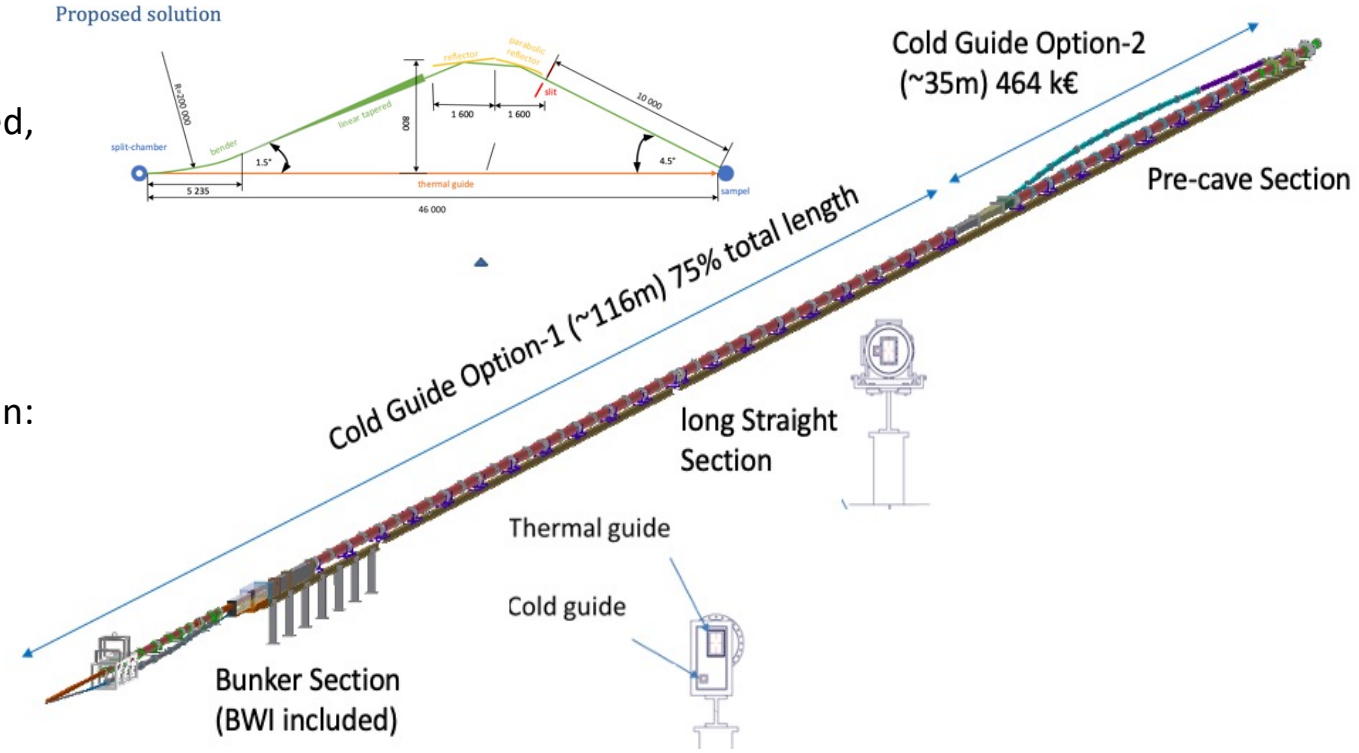
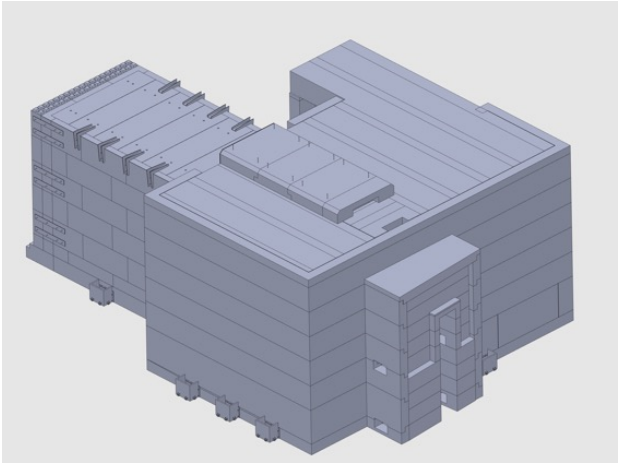
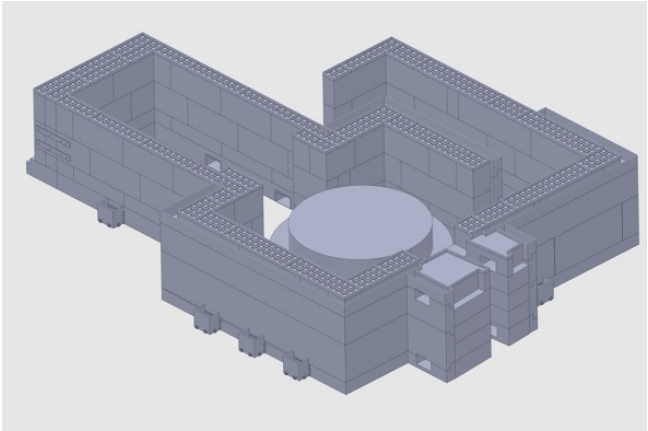
1. BWI: Installed 24/06
2. Long Straight 1: Fabricated, FAT accepted, to be delivered to ESS expected soon.
3. Long Straight 2: Fabricated, FAT documentation received.
4. In-Bunker : SubTG3 planned 14/11, documentation @ESS for review
5. Merge Chamber and final focusing section: Detail design ongoing
6. Split Chamber: Detail design ongoing

7. Cold Guide SANS collimating section redesigned using reflectors.



Experiment Cave

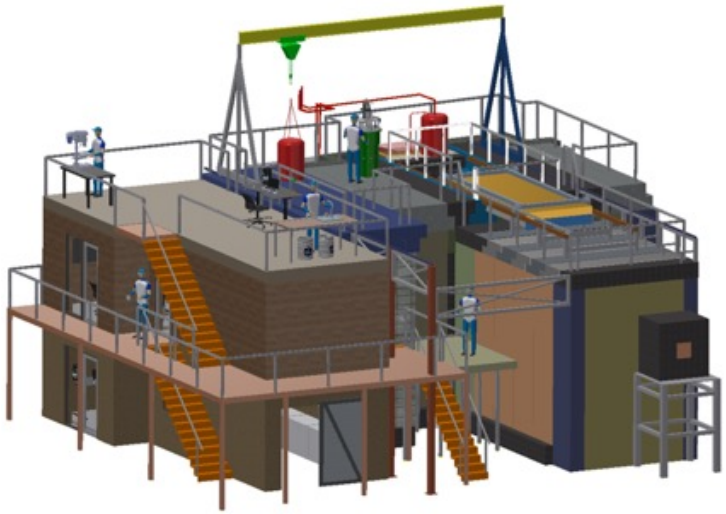




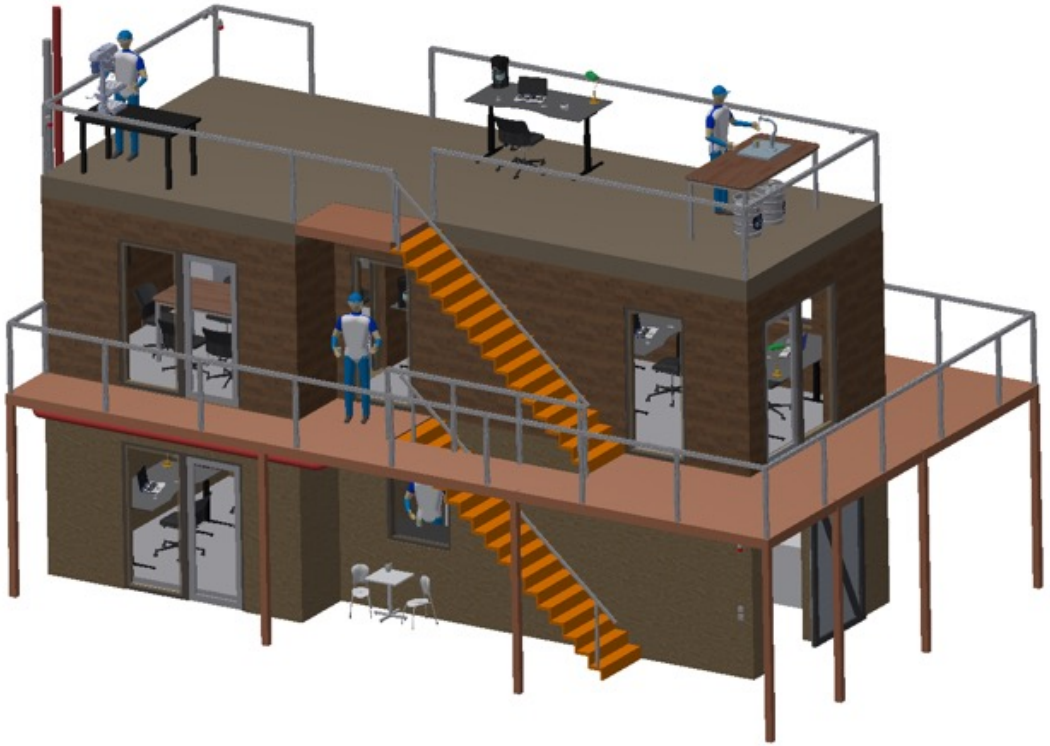
Mirrotron: New PDR.

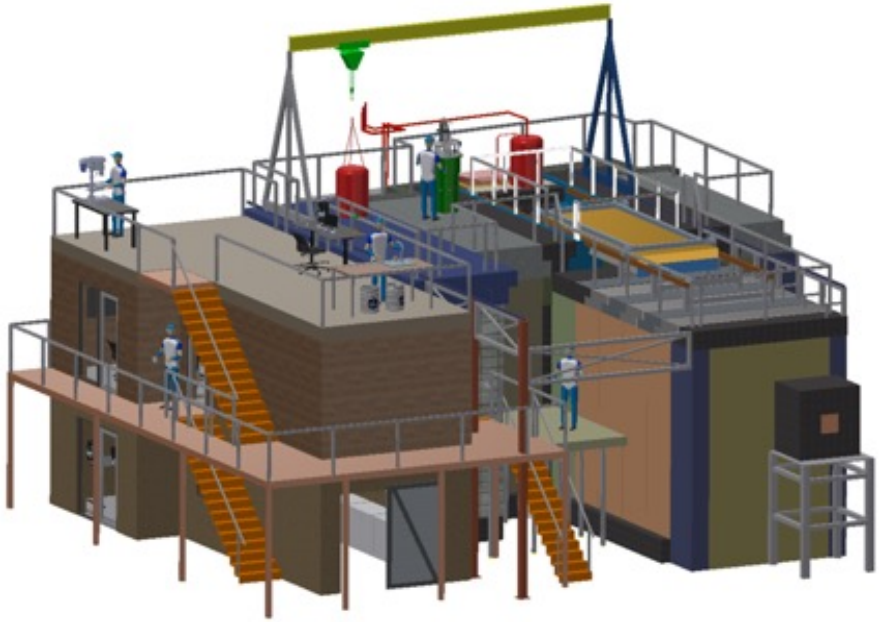
Integration review ESS
October 2024.

8M SANS cave
Extendible to 10m



Experiment Cabin





Decided to go to new tender to optimize costs

ESS FM 200k Euros.

Heimdal RISK Register

RISK to Schedule due to lack of Engineering resources	High workload on Engineering and documentation for TG3 milestone. RISK to delay in TG3, and TG5	ESS (Dan Mannix & Susanna Domeij)	ESS	Open	Avoid	Dedicated resource added for the cave.	8
RISK to TG3 milstone delay due to lack of Resources	Heavy documentation workload period to make TG3 milestone. Can be resolved by using a technical writer proposed by PSI	PSI (Artur Glavic)	ESS	Open	Avoid	Technical writer support proposed by PSI on PSI budget.	9
Instrument software	Rist to delay of SOUP due to no resources to work on instrument software at DMSC	Mikhail Feygenson	ESS	Open	Observe	Currently no resources availiable at DMSC. Issue to be brought to higher level. Recruitments required at DMSC?	25
Cave Infrastructure CUP/CEP	Risk to cost overspend on IFE budget or reduction in science scope of instrument due to cost of CUP/CEP overspend on IFE budget	IFE (Bjørn Hauback)	ESS	Open	Reduce	Predicted costs of CUP/CEP greater than budget. Find funding or trim scope?	20
RISK of overspend on AU budget	Risk due to scope not being contracted and uncertainties in cost. RISK also due to extended Salary costs on AU budget.	AU (Mogens Christensen)	ESS	Open	Avoid	Priortize AU comitment to engineering scope. Find solution to continue personell resources funding.	25

Engineering and technical resources added -> RISKS Reduced

Nothing changed at DMSC on software? IFE Budget ok for now! Au Budget & resources in discussion

Summary

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Major items now contracted: Guide shielding (ESS), Choppers (ESS), Cave (Mirrotron), Guides (swissneutronics), 2D detector (CDT) – Costed & within budget and spec.

Starting manufacture and delivery to ESS e.g. Guide Long straight sections thermal *& cold.

New rescheduling for Tranche-2&3 instruments: Final TG3 Q2-2025. TG5 mid 2027

New injection of Engineering resources & possible more to keep on new timeline track

Main Issues for Heimdal to STAP ? Please Feedback
2D Detector & rescoping. Current Diffraction 2D detector limited to only 80 degrees 1sr.
This will limit first science opportunities on Heimdal.
Can we have the rescope 2D detector (2.0sr) in time for 1st science 2027 ?
Do we work to design moveable 2D detector (1.0sr) to optimize instrument & science scope day 1 ?
If detector is fixed what angles do we cover with 80 degrees?


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