CSPEC

The Cold Chopper spectrometer of the ESS

Agenda:
13:00 - 13:15 Aims of the ICEB. (PD)
13:15 - 13:30 CSPEC Overview and components reminder. In scope / future plans. (PD)
13:15 - 14:30 Project update: (Overview of project, schedule & budget)) (CSPEC/ESS) (FM)
14:20 - 15:40 Installation (FM)
15:40 - 16:00 Risks (FM)
14:30 - 15:00 DMSC, data management. (JT)
15:00 - 15:20 Sample environment (DN)
16:00 - 16:30 Discussion, actions, decision on risks, issues to follow up.

Aim:

Provide an overview of the project (inclusive of risks) to partners.

Time decisions.

Costing decisions.

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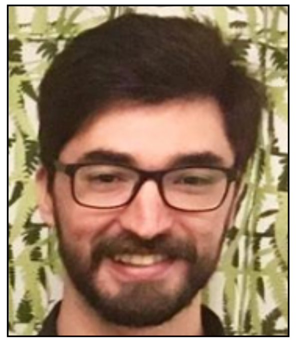
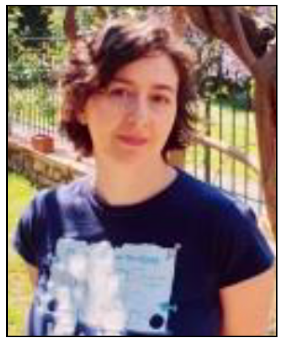
The Cold Chopper spectrometer of the ESS

Scientists: P.P. Deen, D. Noferini (TUM)

Engineer: Fernando Moreira (Lead, LLB), Luis Loaiza (TUM), Gregoire Fabrèges (LLB)

TUM: W. Lohstroh

LLB: S. Longeville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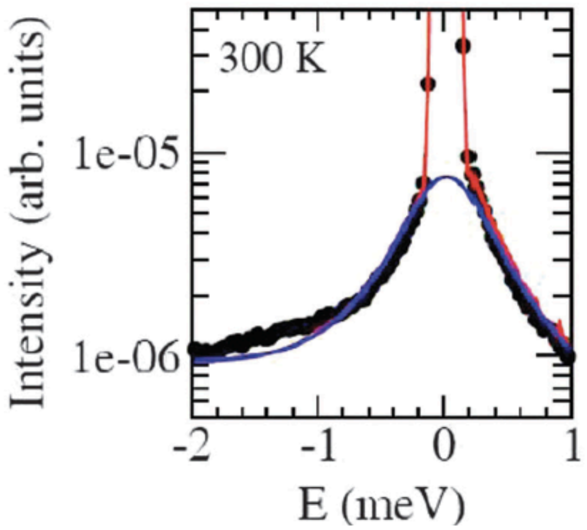
Chem. Soc. Rev., 2012, 41, 6778–6786

Quasielastic scattering:

Translational dynamics

Diffusive dynamics

Rotational dynamics



Chem. Soc. Rev., 2012, 41, 6778–6786

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

Soft matter: Polymer nanocomposites, organic photovoltaics, polymer electrolytes

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

Chemistry: ionic liquids, clays, complex fluids

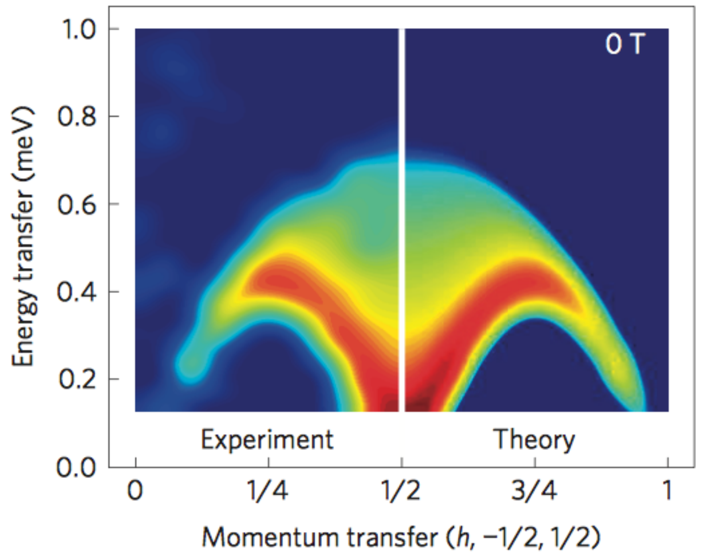
Low lying energy modes:

Spin dynamics

Critical scattering

Collective excitations

Quasiparticles



Nature Physics **9**, 435–441 (2013)

Magnons, phonons, polarons

Topological states of matter: Majorana fermions.

RVB states, Quantum spin liquids, emergent behaviour.

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CSPEC: enable the study of low lying excitations of materials with a focus on in-operando/kinetic behaviour.
Need 10-50x current day signal to noise to perform adequately

- The cold chopper spectrometer of the ESS (2 - 20 Å).
- **Cold neutrons (2-20 Ang) with ΔE/E = 1.5 % @ 4 Å (Ei, ΔE = ∞ < E_i < 0.2E_i).**
- Focus flux on range of sample areas 4 x 2 cm^2 → 1 x 1 cm^2.
- **Signal to noise = 10^5 (@5 Å, Vanadium).**
- Detector will provide angular range of -30 < 2θ < 140^o in the horizontal plane and +/- 26.5 ^{o} in the vertical plane with a planar sample to detector distance = 3.5 m.
- **Enhanced sample environment : in-situ/kinetic phenomena. < 1 min resolution.**
- Multiple characterisation techniques.
- Much improved coupling of neutron scattering with theory.
- Polarisation analysis.

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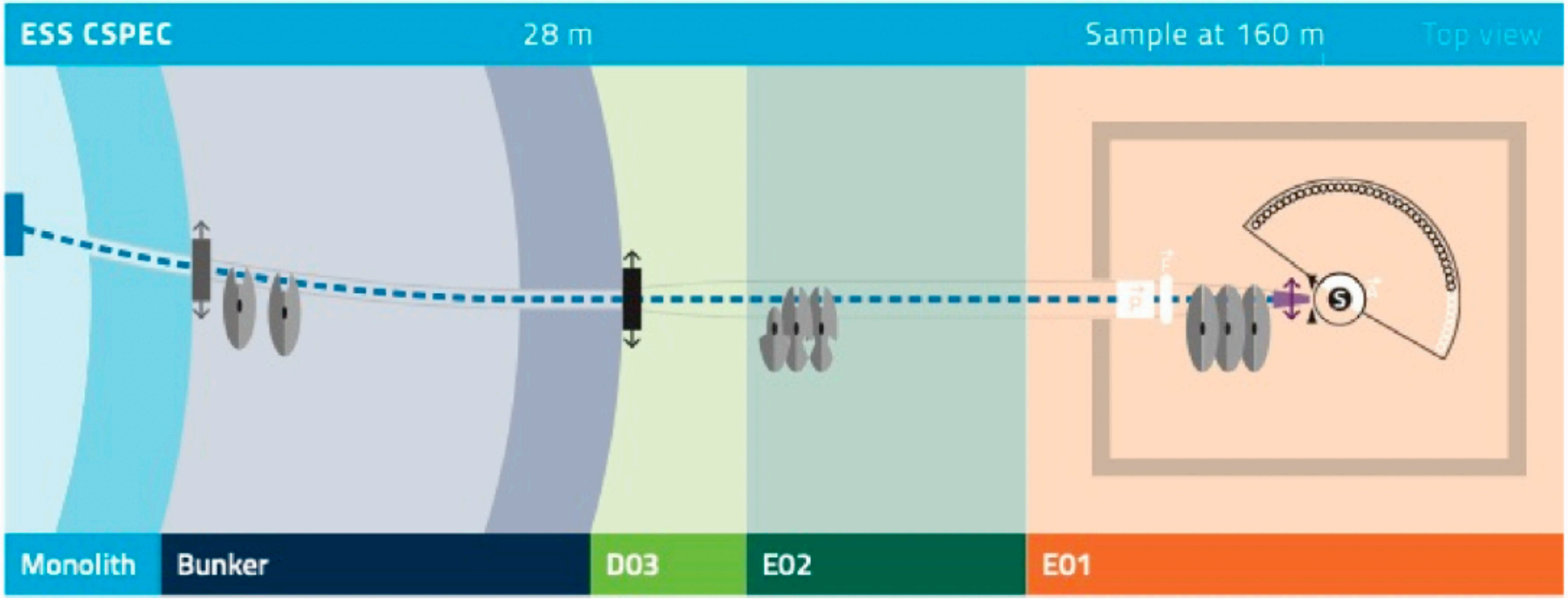
The Cold Chopper spectrometer of the ESS



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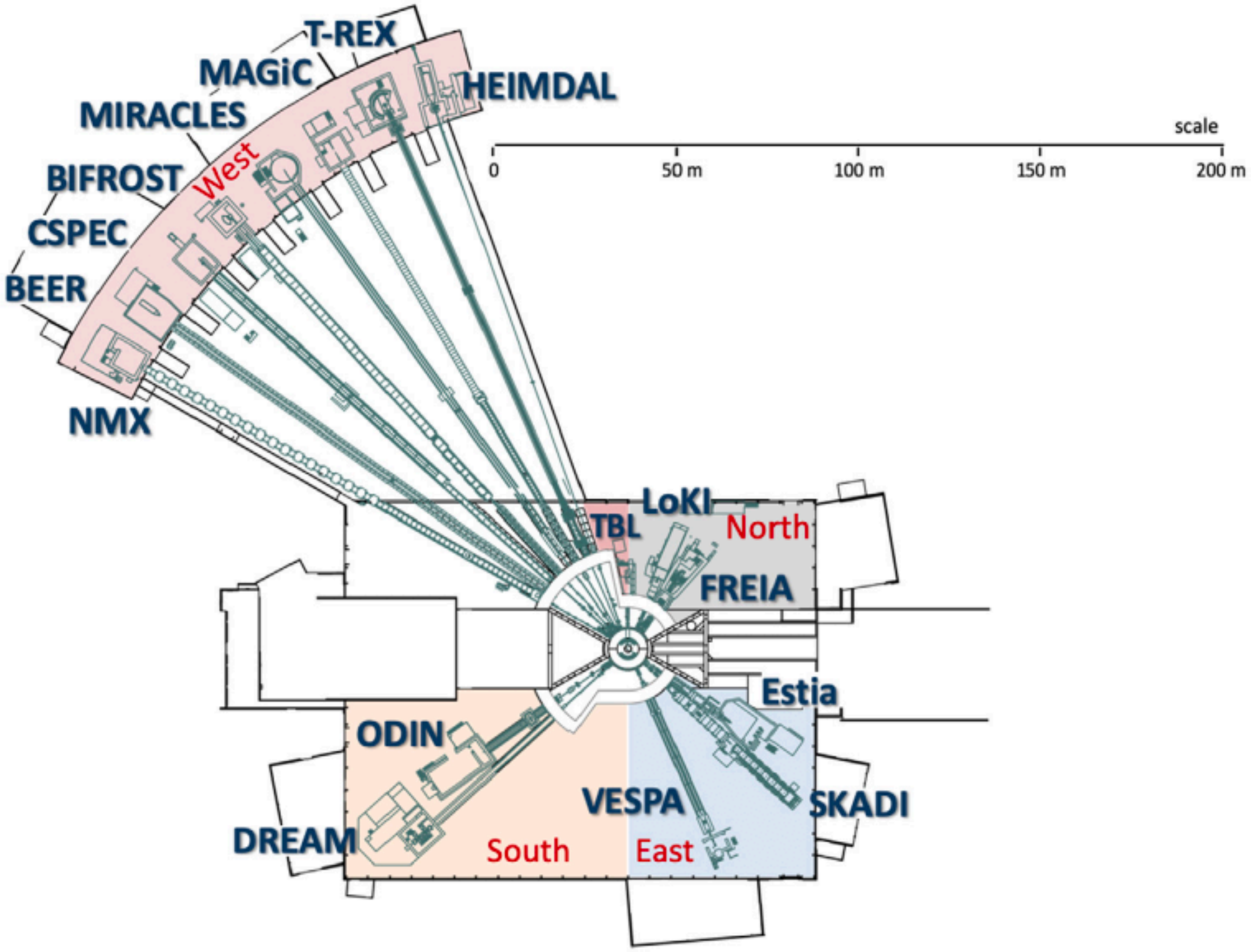
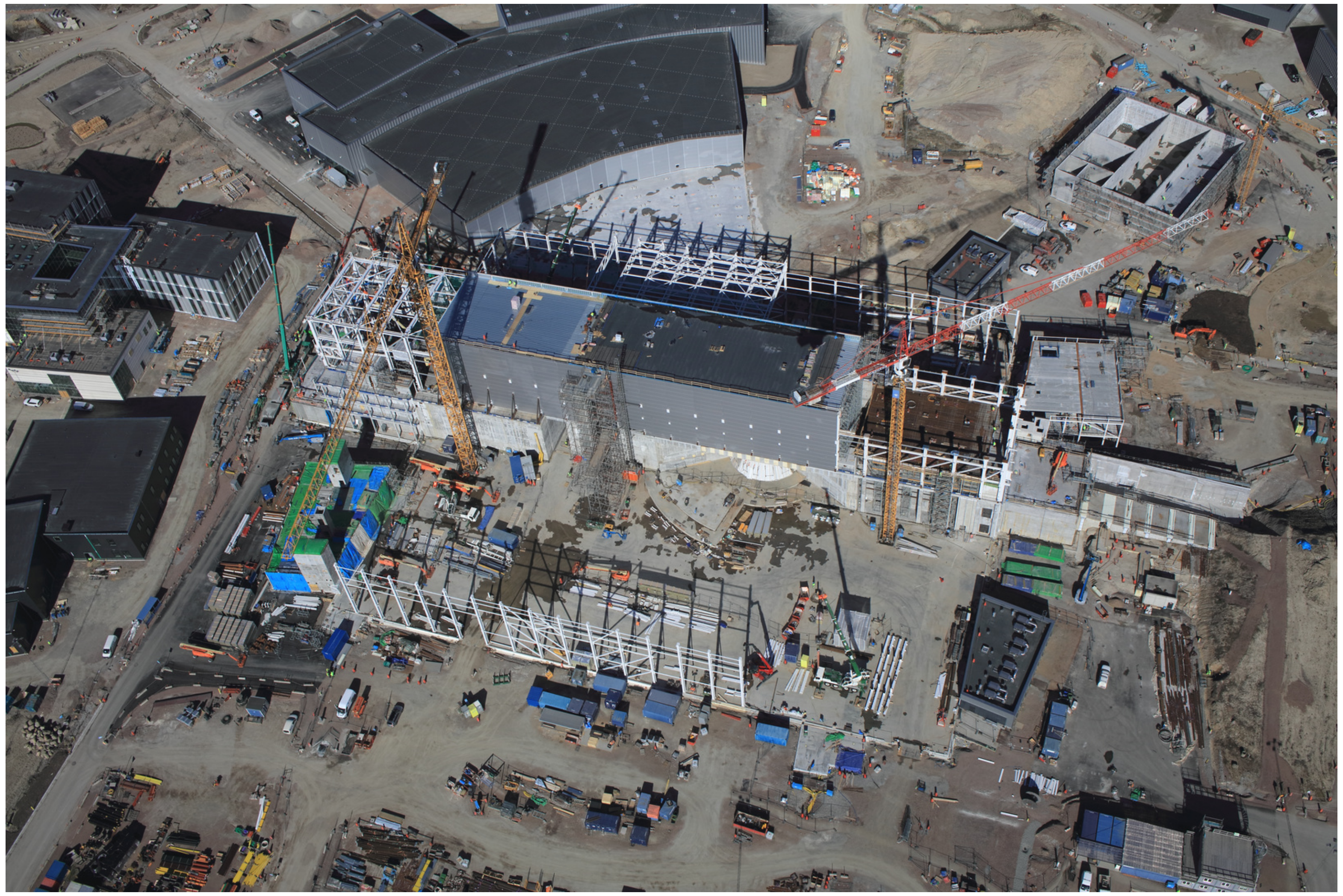
ESS April 2020





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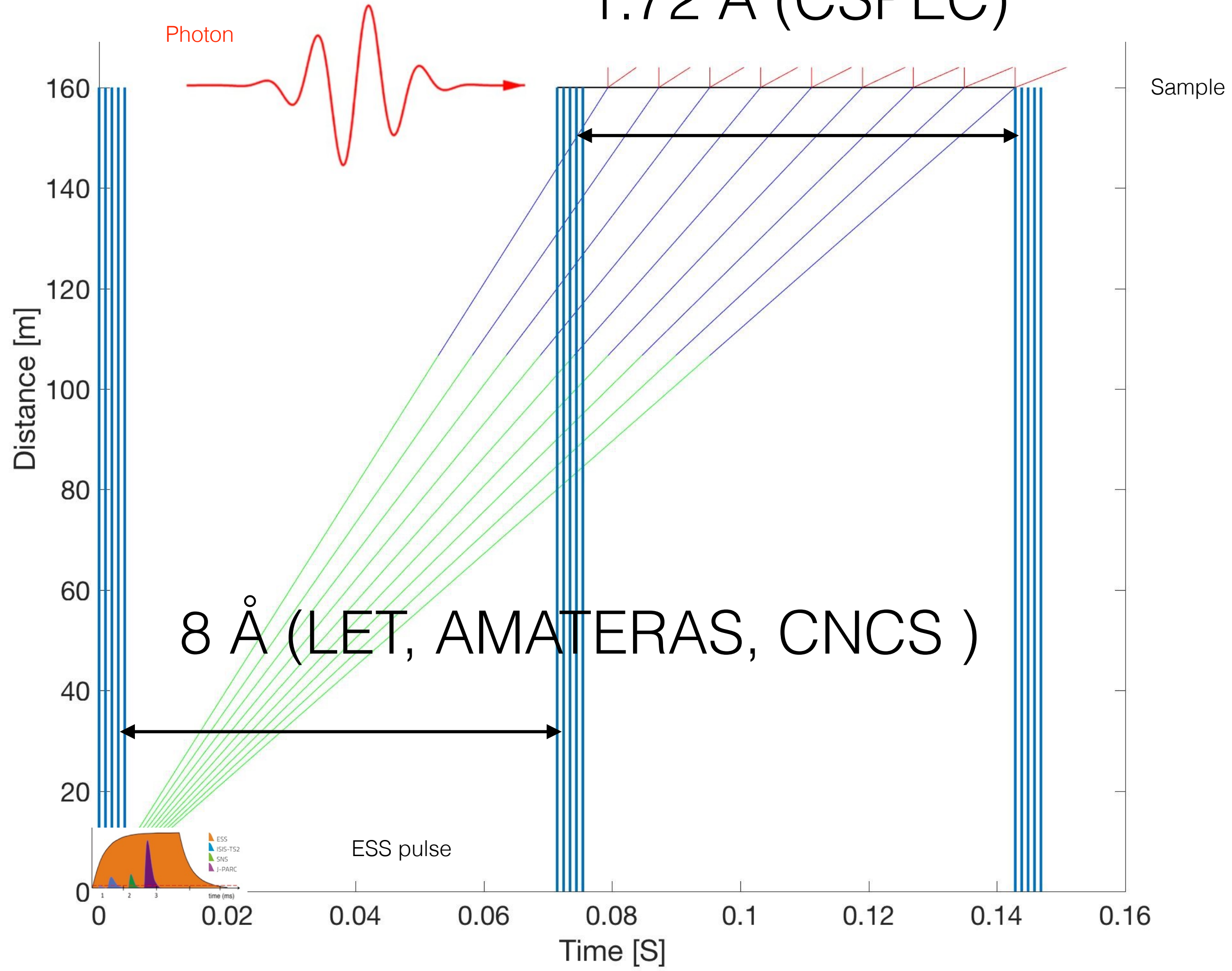
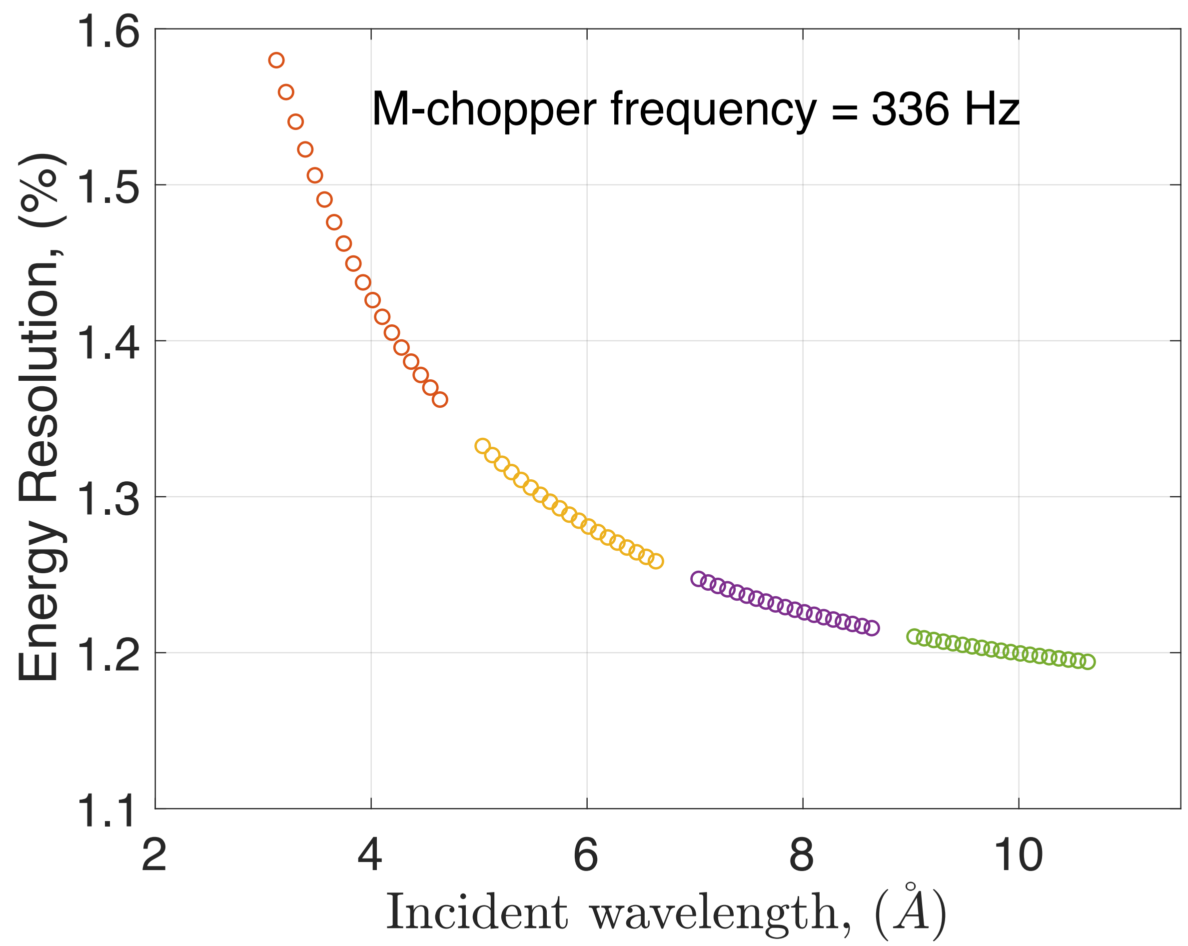
(1) 160 m = more flux.

In-situ/kinetic phenomena. 1 min resolution.



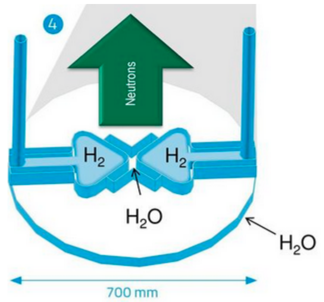


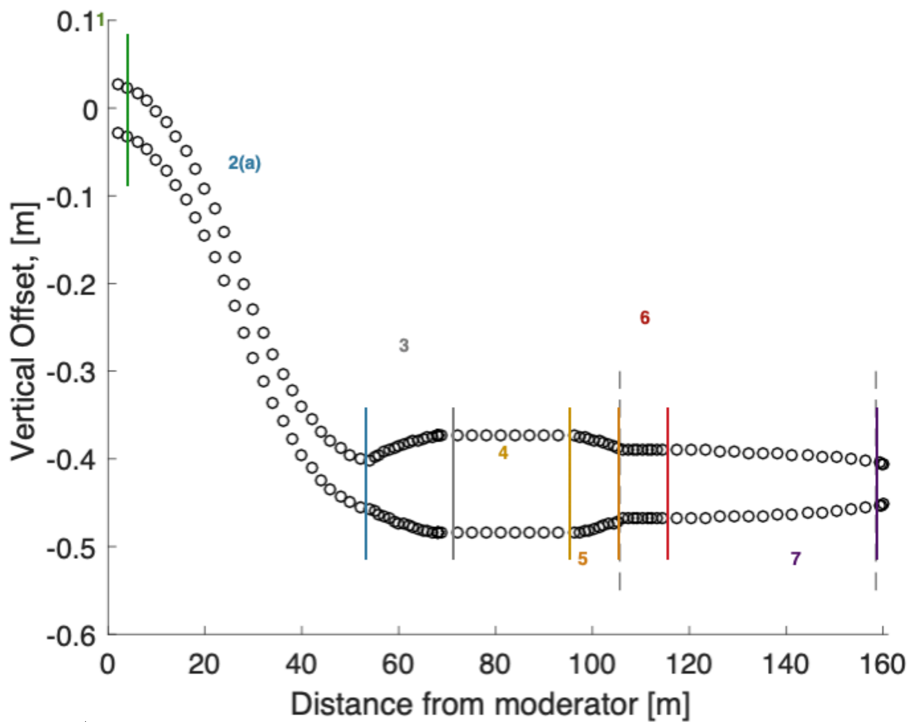
3 Å = E_{min} = 5.67, E_{max} = 16.9 meV

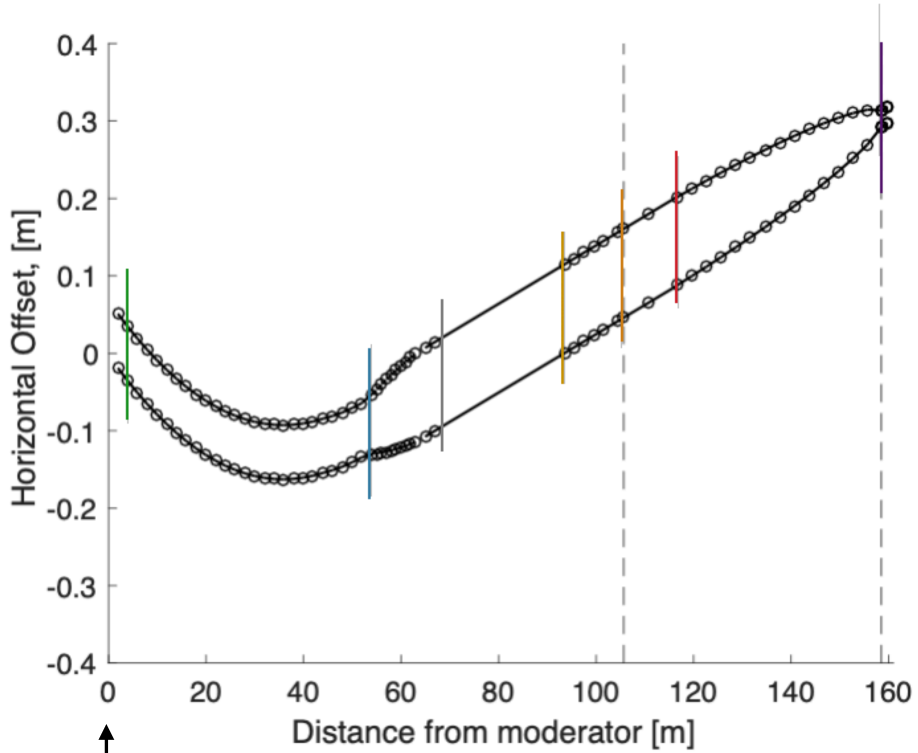
6 Å = E_{min} = 1.76, E_{max} = 3.02 meV

8 Å = E_{min} = 1.06, E_{max} = 1.58 meV - Add pulses when possible - gain in flux

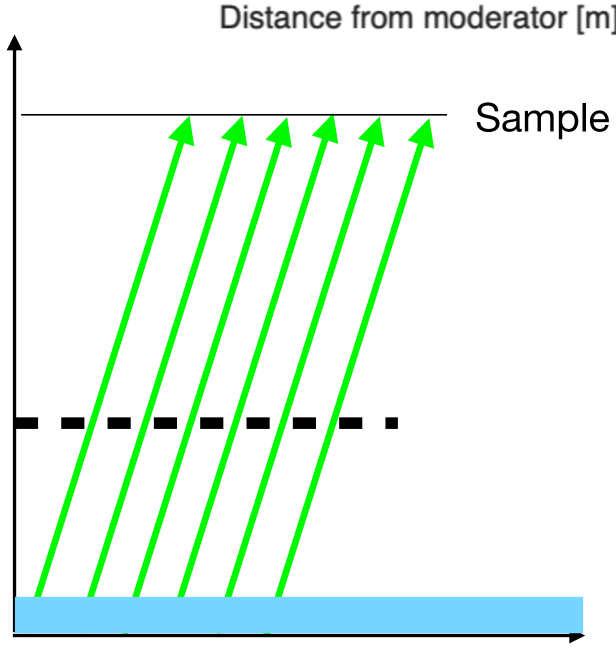
(2) 160 m & cold neutrons & spallation source = less noise . S/N 10^5.



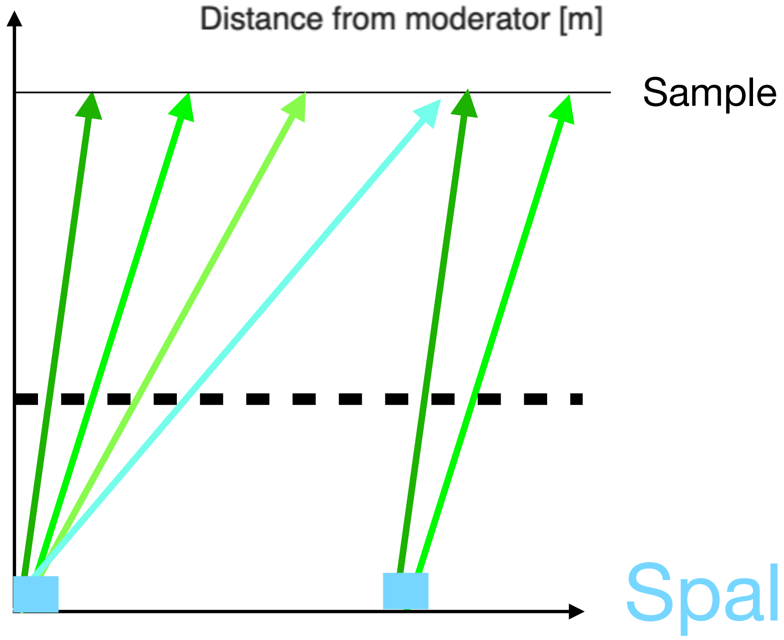




Cold neutrons: S-Bender



Reactor



Spallation

No ambient background

Fast and epithermal neutron dose rate (E > 1 eV) limited to within bunker

F. Grunauer : MCNP6 simulations

Assume 5 MW. All choppers and shutters open.

12.1.1. Region between bunker wall and cf wall

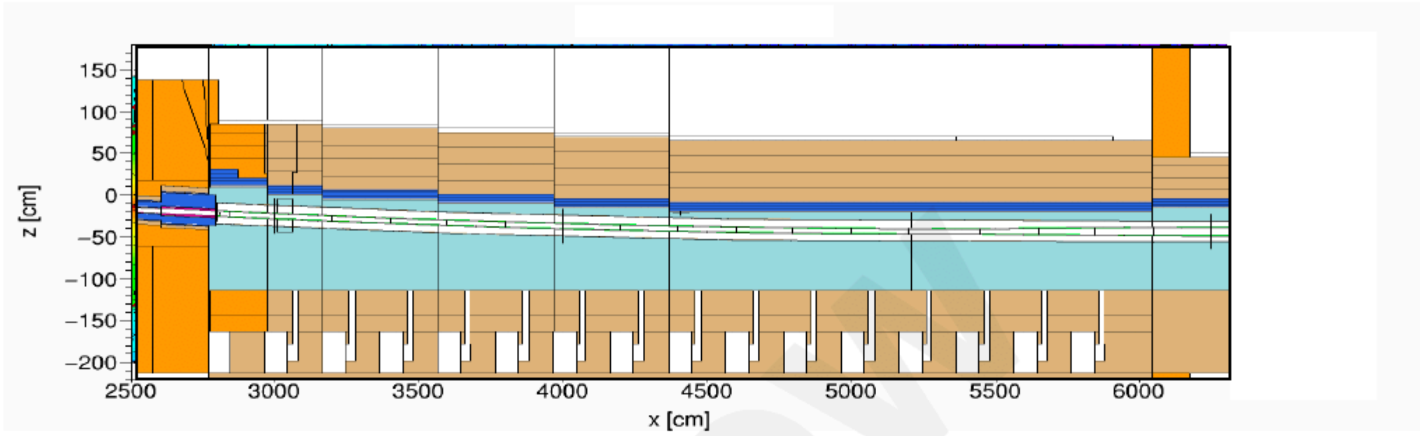


Fig. 130: Vertical area through the Monte Carlo model of the CSPEC guide shielding between the bunker-wall and the cf-wall for which the radiation distribution is shown in the figure below.

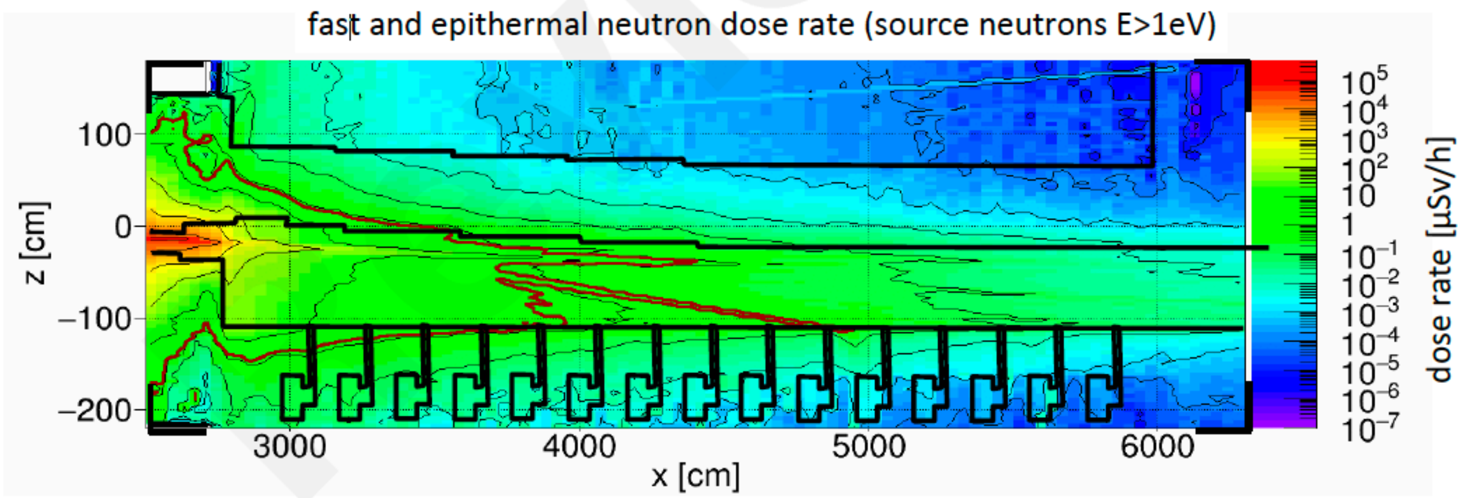


Fig. 131: Fast and epithermal neutron dose rate (source neutrons E>1eV). The red line is the 1.5µSv/h border.

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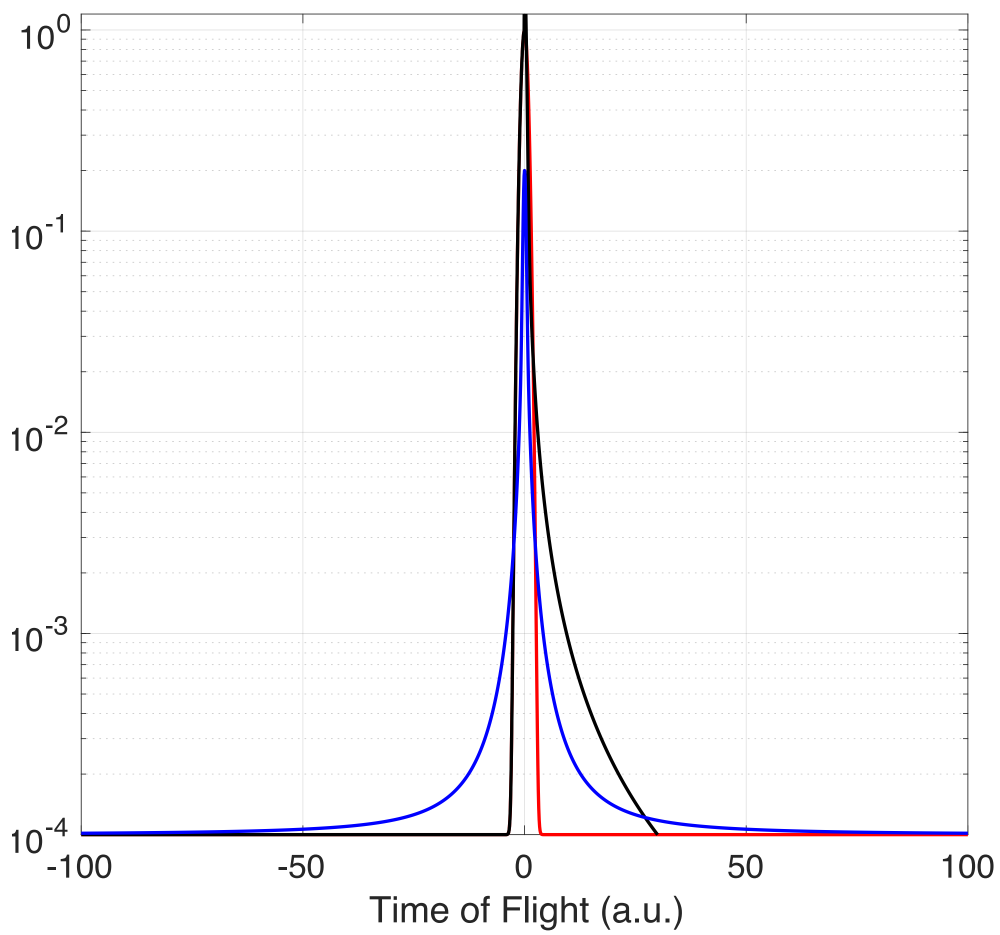
Advantages of Reactor and Spallation source chopper spectroscopy

(3) Cleantime of flight pulses.

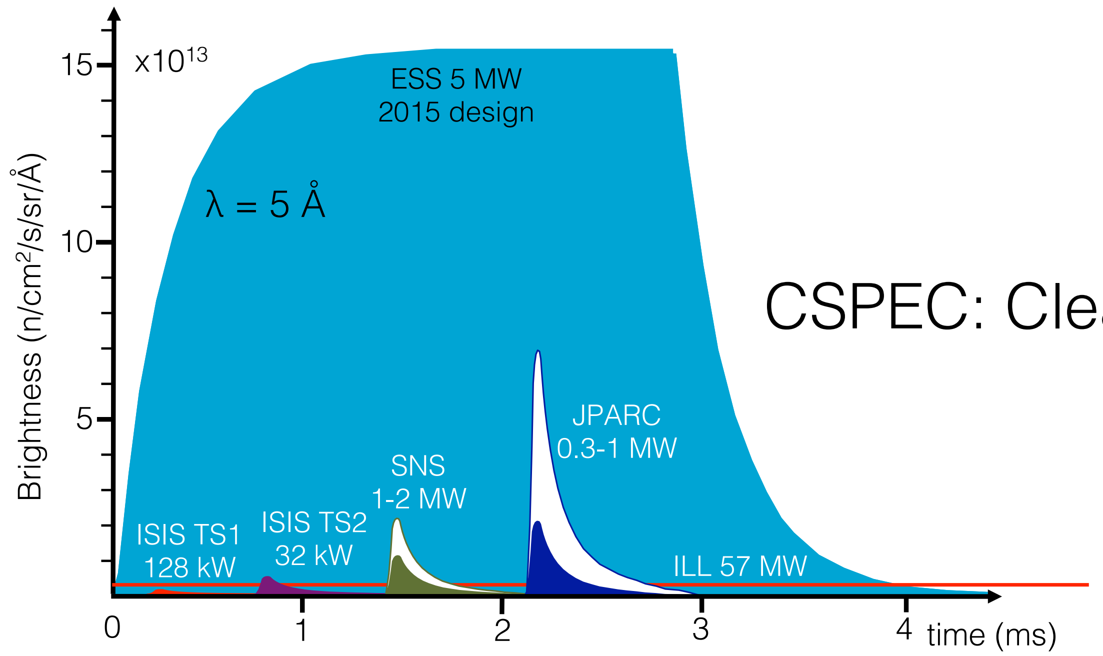
$\Delta E/E = 1.5\ \%$ @ 4 Å (Ei, $\Delta E = \infty < E_i < 0.2E_i$)

Linewidth extracted on a reactor source. (Chopper blades)



Linewidth extracted on a short pulse spallation source. Carpenter function

Information of interest. (QENS)



CSPEC: Clean symmetric pulses.

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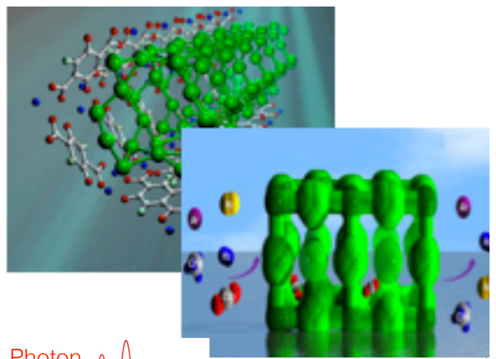
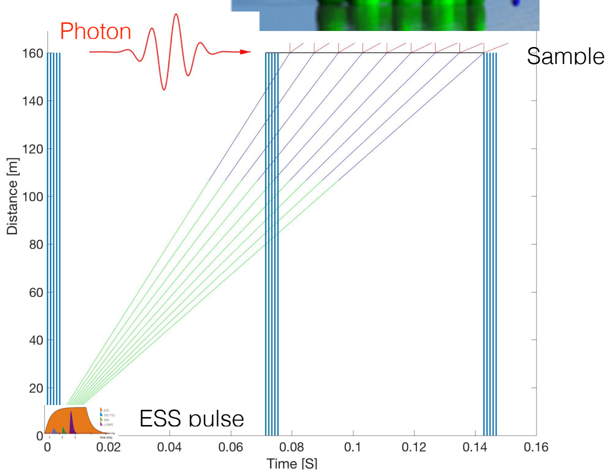
Perform in-operando studies on the < minute timeframe.
Probe time dependent phenomena

Ionic transport: determines the efficiency of fuel cells & batteries.
Improvement of ion conductivity imperative to improve efficiencies:

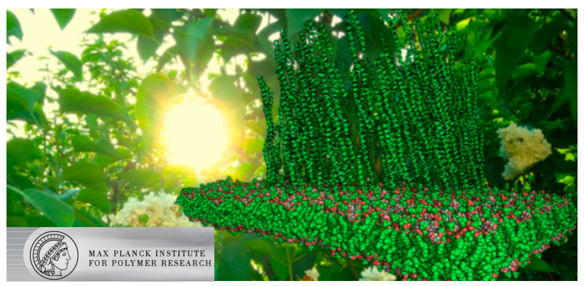
Batteries & fuel cells Ionic transport under real conditions
Next generation energy supplies.



Gas storage & catalysis Transient stages during hydrogen uptake and release, in a gas atmosphere, are difficult to address. In-operando kinetics:second - hour.
S. Yand, et al. Nature Chemistry, 2012, 4, 887-894



Life science & pump probe measurements:



Correlations between the light harvesting processes of a pigment/protein complex involved in photosynthesis and its internal dynamics.

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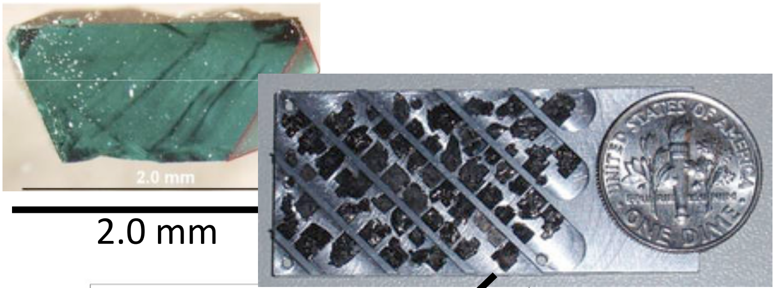
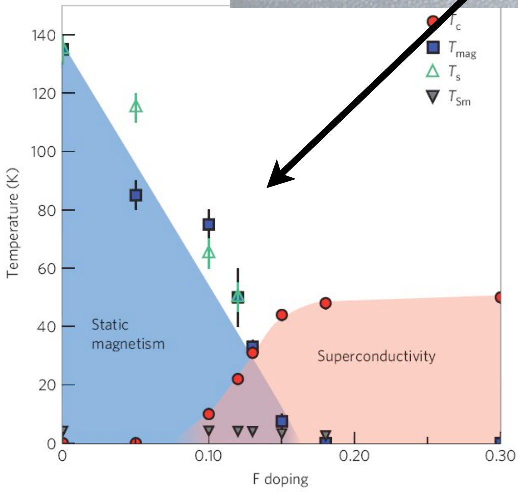
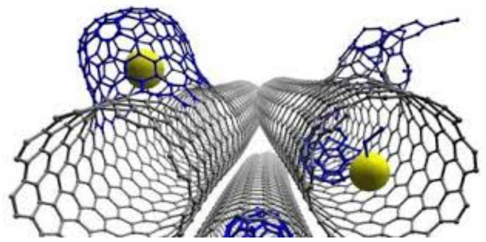
Current: Fe-arsenide single crystals



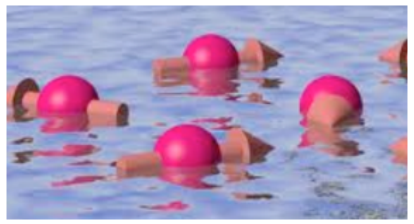


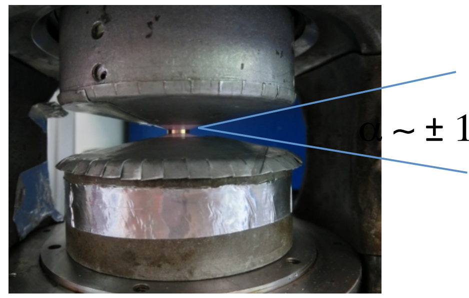
Nature Materials 8 (2009) 310

Small single crystals: High quality, few imperfections.
High pressure synthesis: not easily observed in nature.
Study many stoichiometries in a single experiment.
True global behaviour.



Functional materials:
Develop novel phases as a function of pressure (0 - 9 GPa)
Need samples as small as 1 mg (currently 500 mg is feasible).
Important energy implications





Strongly correlated physics:
High pressure, high magnetic field (at least 12 T) and low temperature (T < 0.1 K) simultaneously.
Out of equilibrium physics (Pulsed fields,)
Spintronics & Spin liquids ⇒ quantum computing

7 GPa : W.G. Marshall (ISIS) S. Klotz, High Press. Res. (2013)

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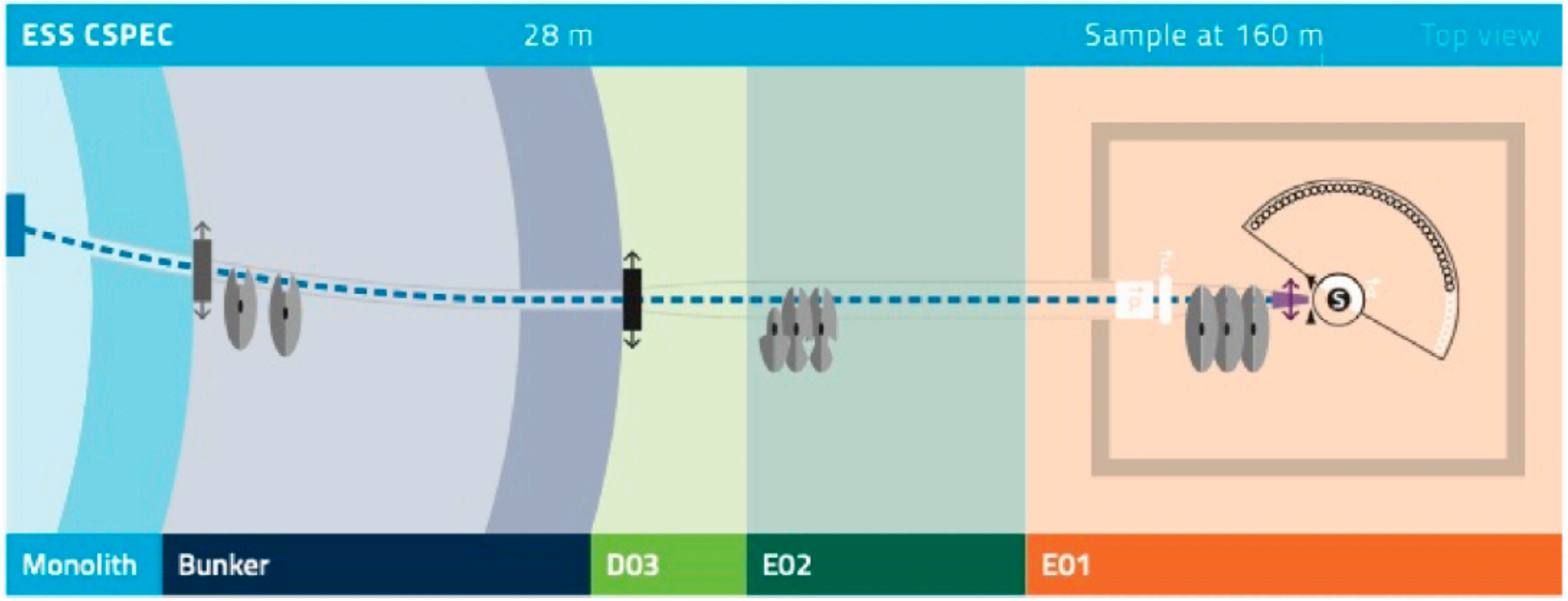

Large ticket items in-going/finalised:

- Guide : TUM in production, NBOA, BBG, Feedthrough under detailed design.
- Choppers: Tender out (LLB).
- Primary spectrometer shielding, TG3 complete.
- Vacuum housing: out of bunker, CTV - Vacuum housing: in bunker, CTV July 2020.
- Detector tank CTV: Tender process started (LLB).

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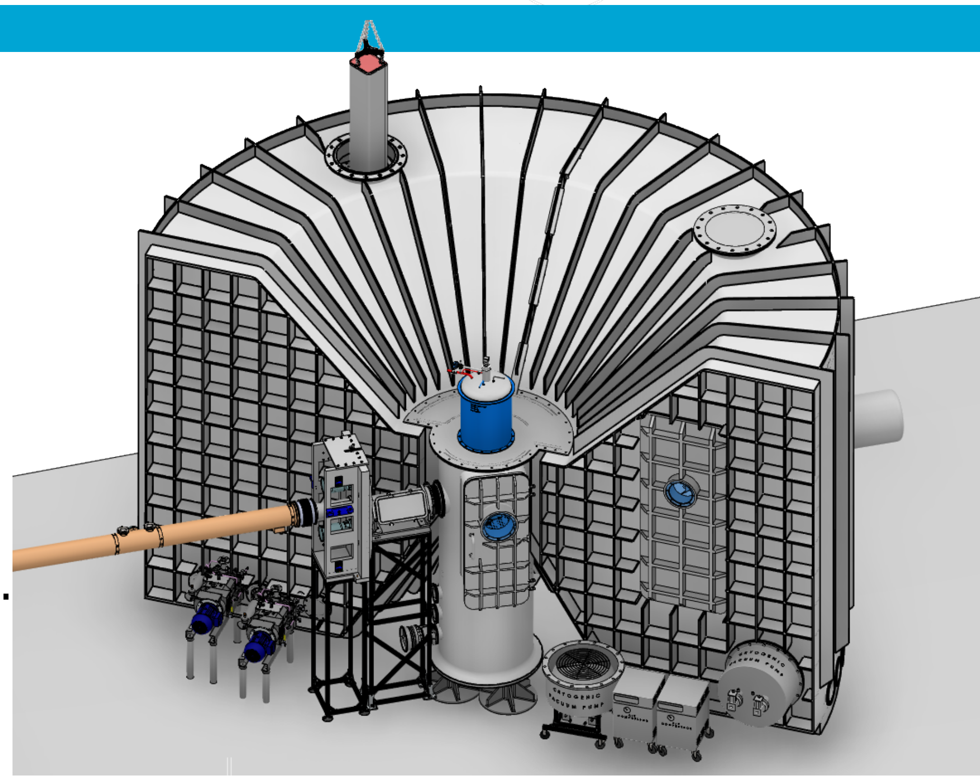
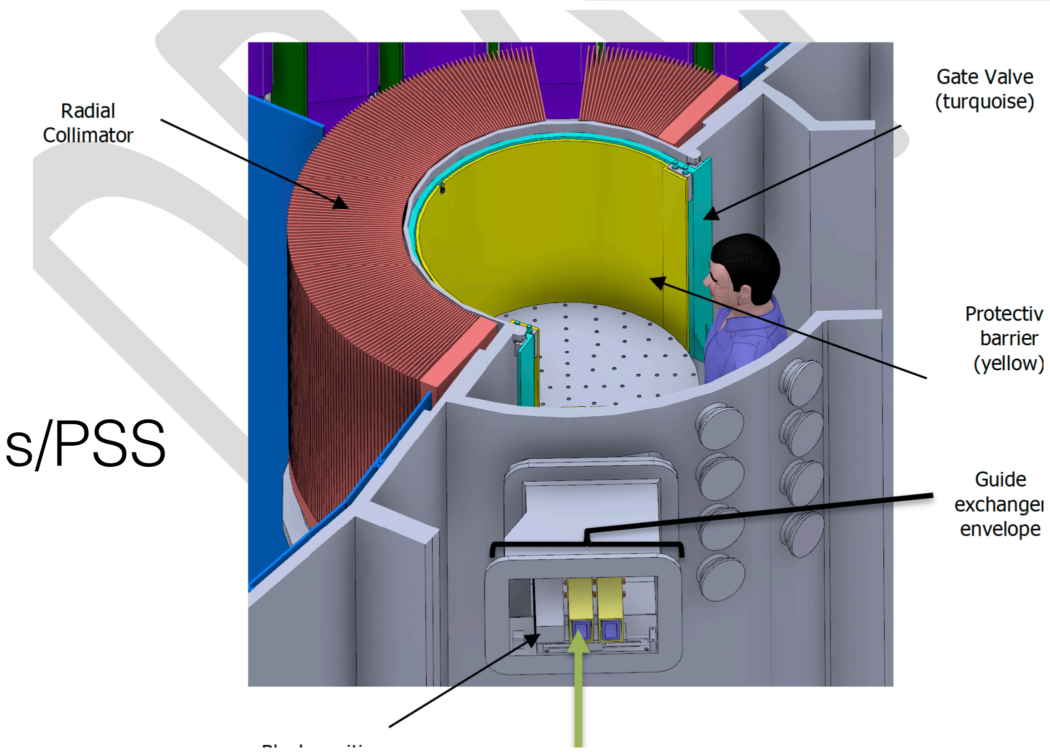
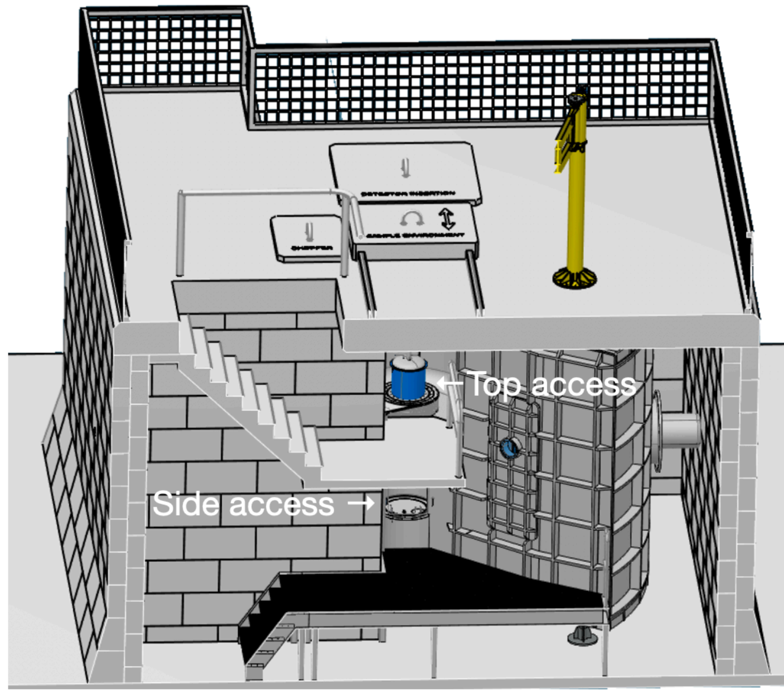
EUROPEAN SPALLATION SOURCE



Focus now:

- Radial collimator: design complete → tender.
- TOF chamber collimation
- Slits.
- Secondary spectrometer shielding (inclusive of beam stop).
- Monitors: ESS common project.
- Detectors: ESS/CSPEC project.
- Guide exchanger: on-going.
- Control Cabin.
- Sample environment (Daria): on-going.
- Data acquisition / DMSC: more focus.
- MCA/Vacuum/electrical/Hazard analysis/PSS





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CSPEC Detectors (day 1)

Contract between ESS / CSPEC signed: MG B^{10} detectors.

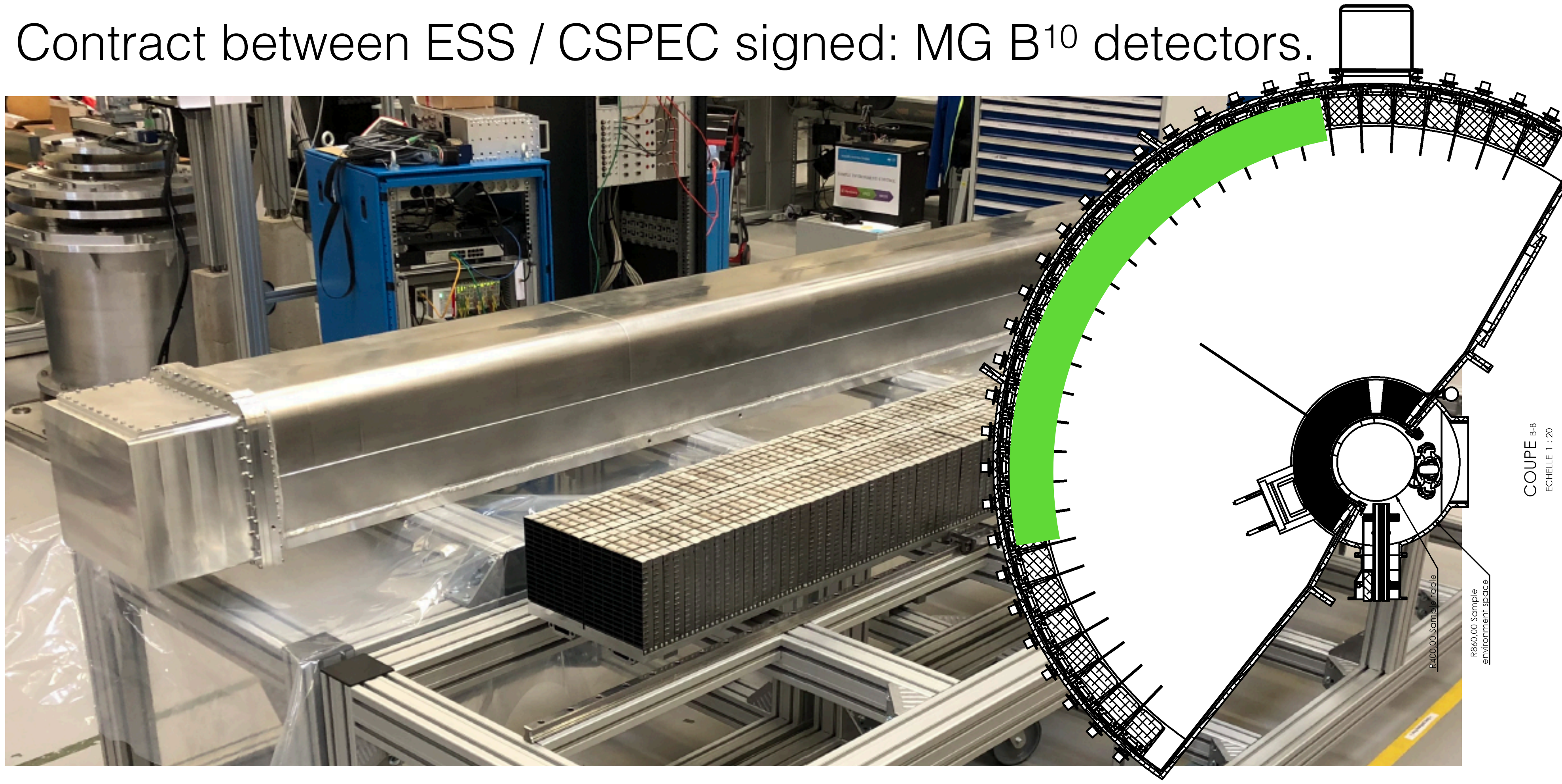


Table 1. Essential CSPEC detector performance requirements.

Specification Description	Requirements
Linewidth, intensity as a function of time-of-flight for an incoherent scatterer, measured at 2K, in the region 3σ < λ < 5σ	Shall be ≤ 2.5 times ^{3}He detectors (essential) Should be equivalent to ^{3}He detectors (desirable)
Detection Efficiency	Shall be ≥ 60% detection efficiency at 4Å
Geometrical/angular coverage 3.5m from the sample position	Shall be 5°≤ 2θ ≤ 97.7° in the horizontal plane Shall be ±26.5° in the vertical plane
Count rate capability	Shall be 50 times > ^{3}He detectors Should be 100 times > ^{3}He detectors
Dark noise across all detector	Shall be < 0.35 Hz/m^2 (essential) Should be < 0.14 Hz/m^2 (desirable)
Scattering signal to noise (total) The signal is defined as the peak neutron intensity on detectors by an incoherent scatterer, such as Vanadium, and compared to the noise defined as the neutron intensity at a time when the signal has decayed to background levels	Shall be 10^4 at 5Å (essential) Should be ~10^5 at 5Å (desirable)
Gamma efficiency	Shall be ≤ 10^{-6}

Milestone ID	Short description
#1	**Tenders/Requests For Quotations (RFQs) for key components submitted**
#2	**Sub-TG3: Grid design, Vessel design**
#3	**Key Components delivered to Suppliers**
#4	**Tender for Vessels submitted**
#5	**$^{10}B_4C$ Coating for MG.CSPEC Started**
#6	**Pilot Tests completed**
#7	**$^{10}B_4C$ coated blades for 1st Detector completed**
#8	**Construction of CSPEC Detectors started.**
#9	**1st Detector Vessel FAT**

18 detector modules at 100 % front end electronics grid.

Cost risk is transferred from CSPEC to NSS project. (4 277 753 euros)

Hand over of project is December 2022.

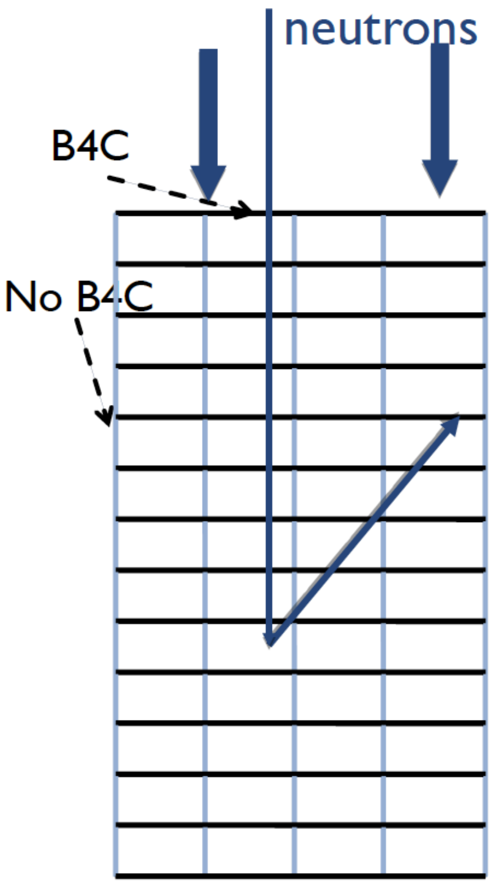
Project accountability / well defined milestones

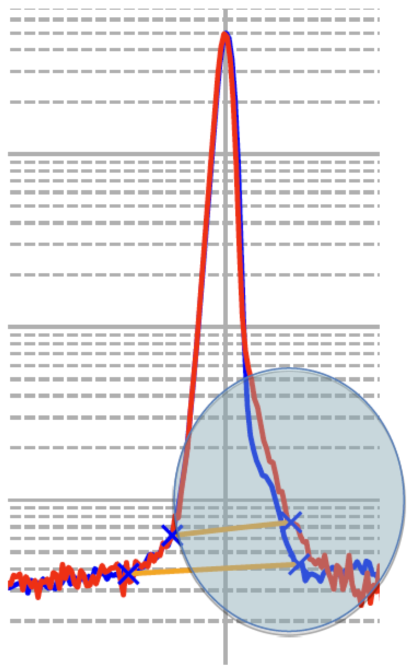
MG B10 Detectors: Pilot tests (LET/ISIS)

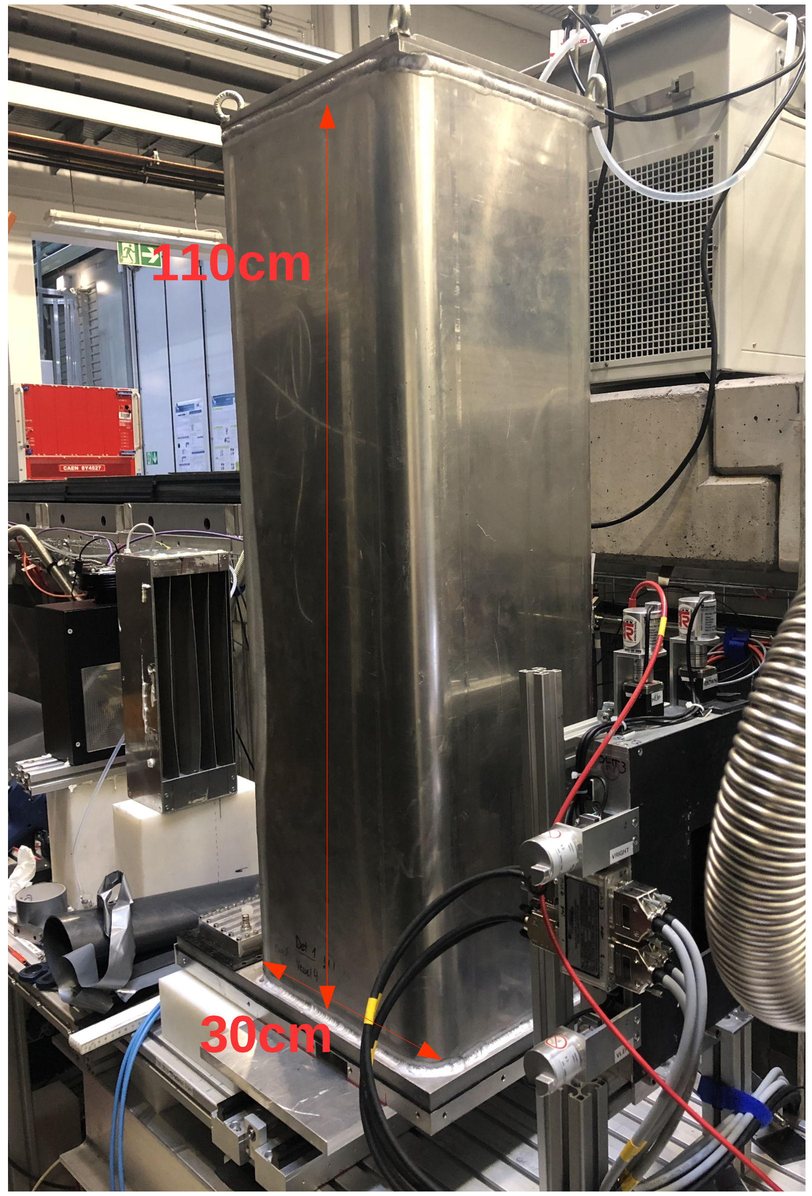
Pilot Tests completed	Nov 20	Subject to access to LET is granted in Sep 2020

Table 1. Essential CSPEC detector performance requirements.

Specification Description	Requirements
Linewidth, intensity as a function of time-of-flight for an incoherent scatterer, measured at 2K, in the region 3σ < λ < 5σ	Shall be ≤ 2.5 times ^{3}He detectors (essential) Should be equivalent to ^{3}He detectors (desirable)

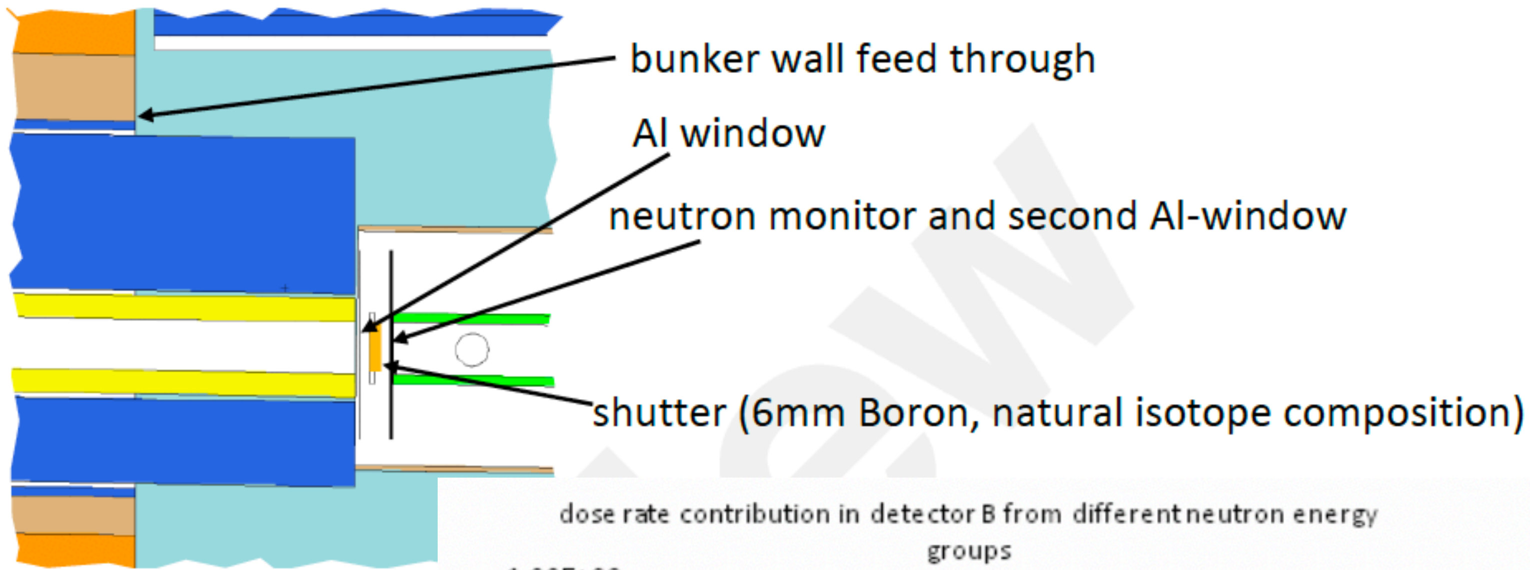


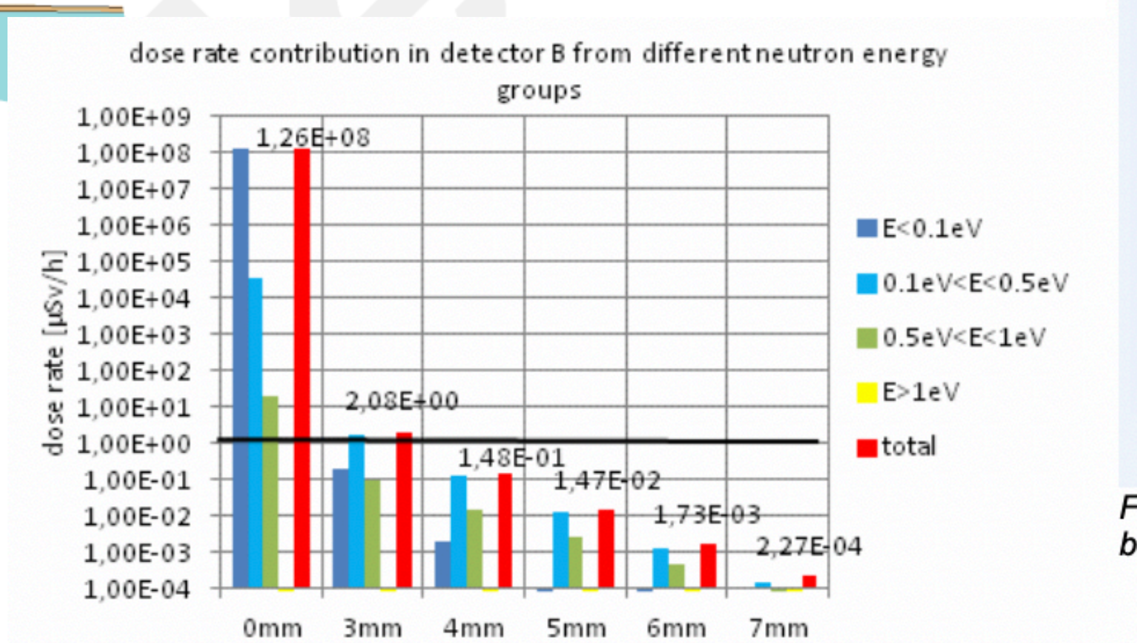


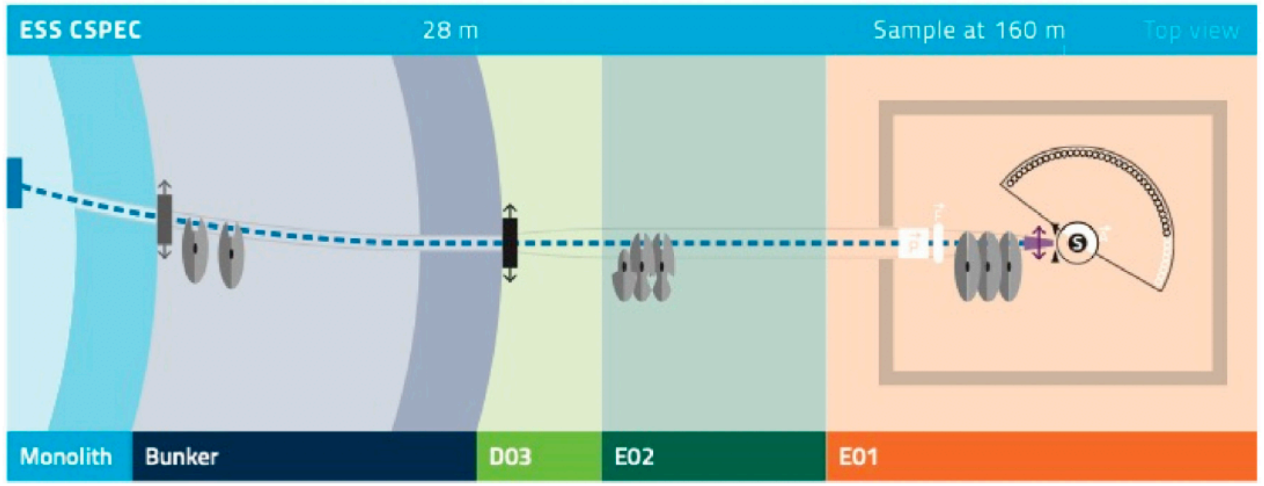


Shielding: F. Grunauer.

(1) Instrument shutter to access PS chopper & sample pot.







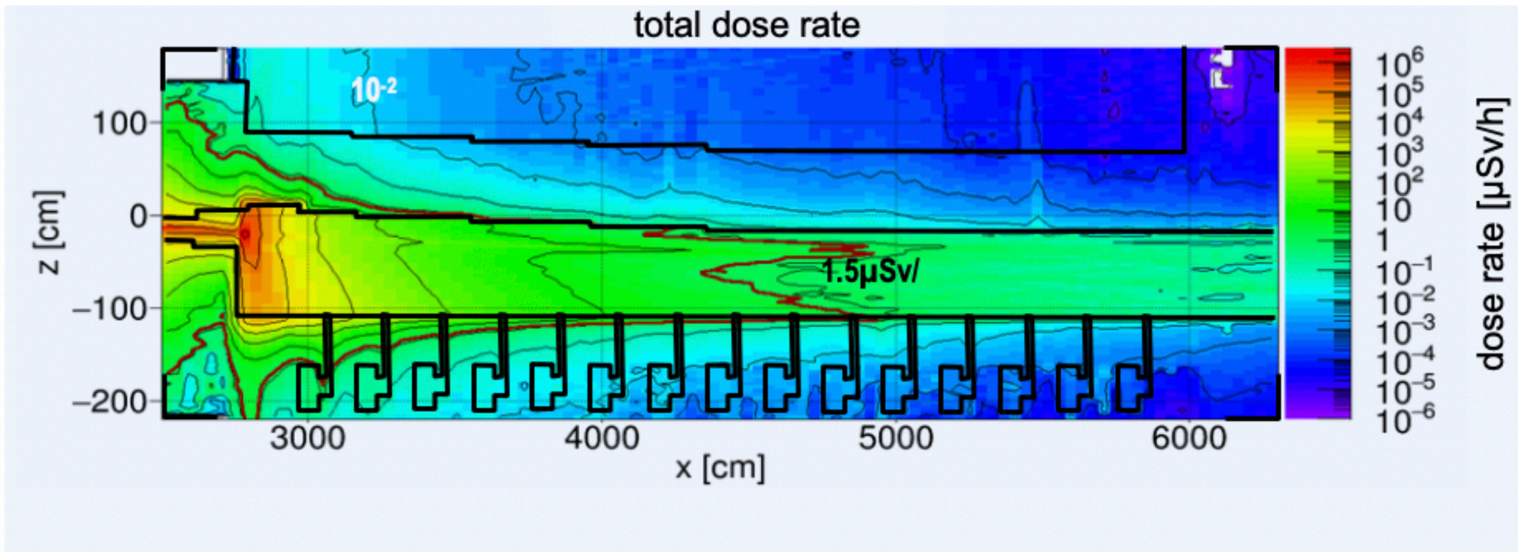


Fig. 7: Total dose rate distribution between bunker wall and cf-wall. The red line is the 1.5µSv/h border.

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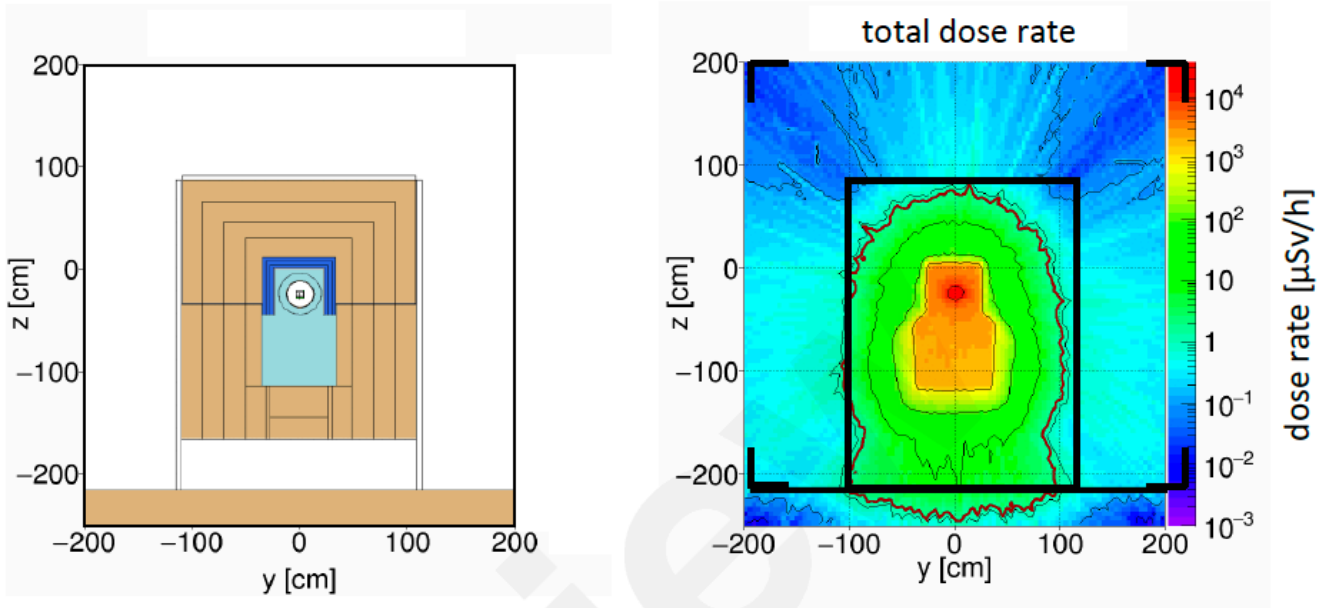
Shielding: F. Grunauer.

(2) Primary spectrometer

Assumptions
The spallation source is running at 5MW with 2GeV proton
All choppers and shutters are opened.

Steel (inner layer) & ordinary concrete
(166cm outside the bunker wall + heavy concrete).
Consider vacuum housing & guide realities.

@ 30 m from moderator



PS chopper pit: + 1.5 cm Jefferson Lab materials
: boron carbide + cement

PS Chopper pit @ 105.67 m

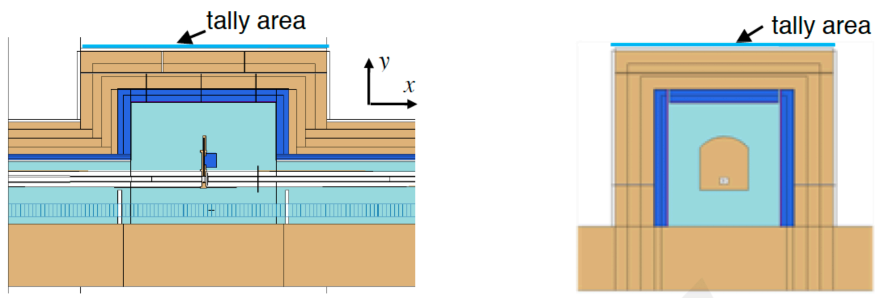
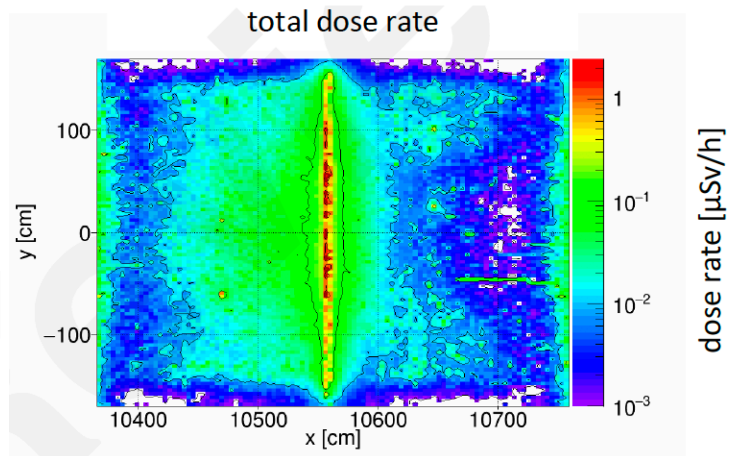
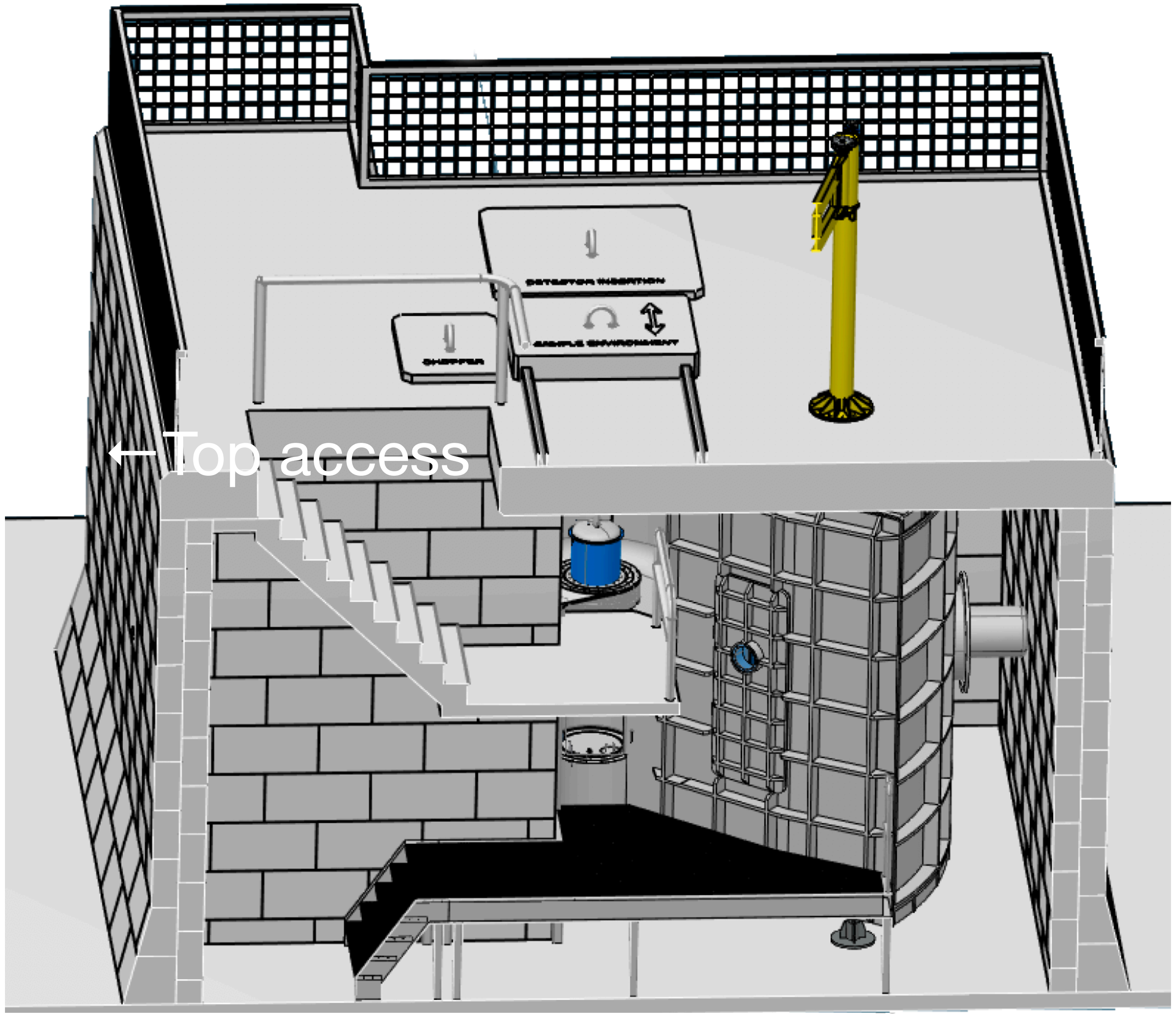


Fig. 115: Cuts through the tally area



Shielding: F. Grunauer.

(2) Secondary spectrometer
- Analytical calculations to date
- MCNPX Calculations shortly



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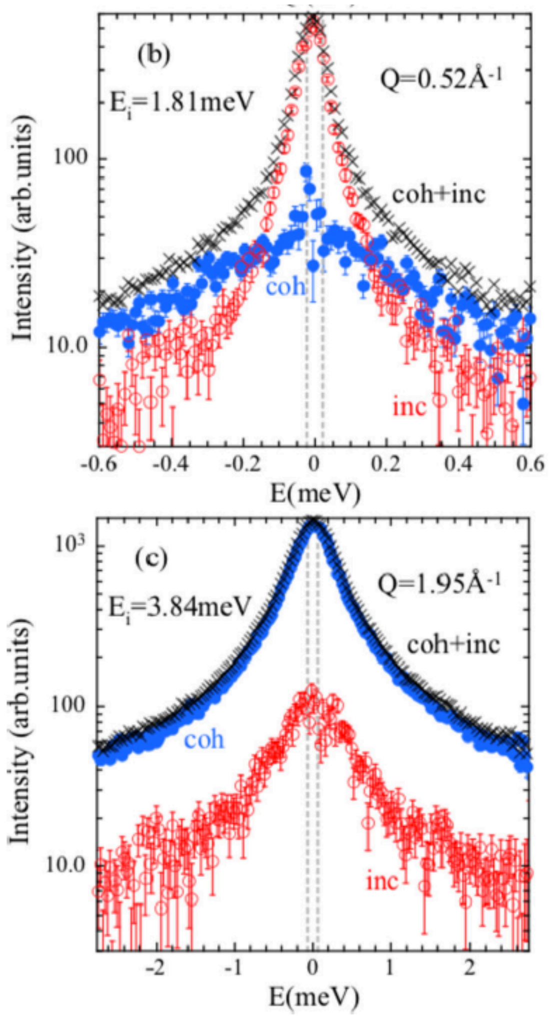
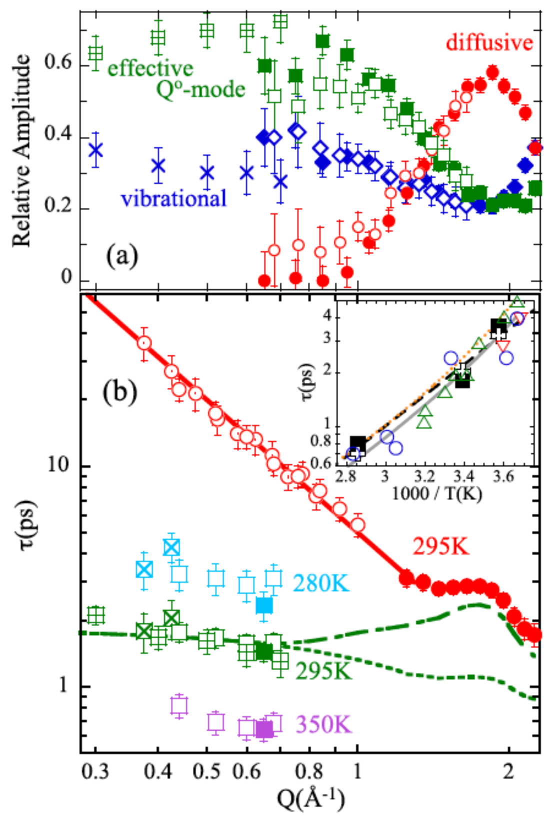
Polarisation Analysis (future)





PHYSICAL REVIEW RESEARCH **2**, 022015(R) (2020)

Rapid Communications

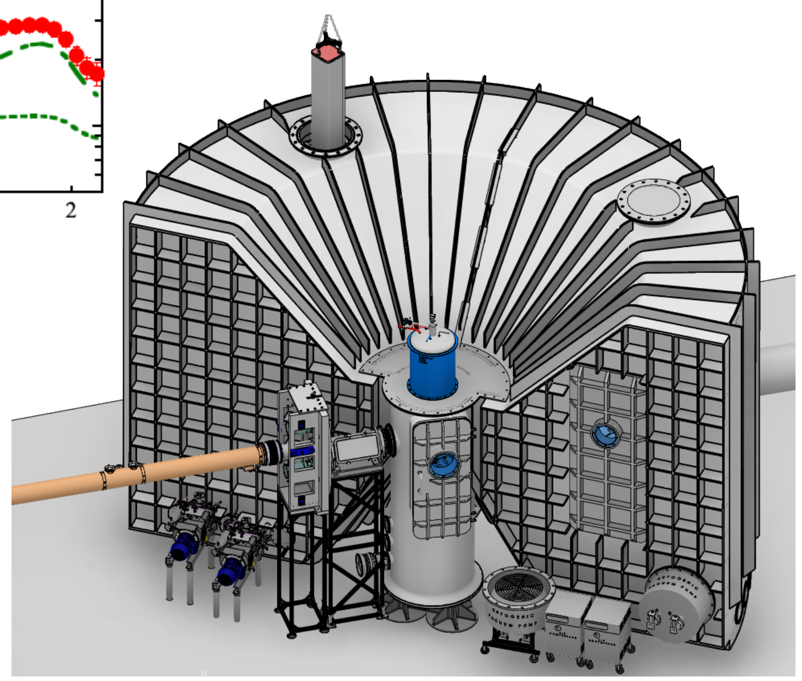
Coherent structural relaxation of water from meso- to intermolecular scales measured using neutron spectroscopy with polarization analysis

Arantxa Arbe,[1] Gøran J. Nilsen,[2] J. Ross Stewart,[2] Fernando Alvarez,[1,3]
Victoria García Sakai,[2] and Juan Colmenero[1,3,4,*]

[1] *Centro de Física de Materiales (CFM) (CSIC–UPV/EHU)–Materials Physics Center (MPC), Paseo Manuel de Lardizabal 5, 20018 San Sebastián, Spain*

PA provides an accurate description of S_{coh} (Q, ω) below Q_{max}

Study coherent scattering from meso- to intermolecular scales in H-bonded liquids, glass forming liquids, biological systems (water)



CSPEC; Future proof for PA

Exchangeable guide piece for Polariser/Flipper

Non-magnetic tank μr < 1.01, d > 1.45 m

Non magnetic guides post M chopper

He3 polarisation when possible.

Control, DAQ, reduction and a brief outline of analysis envisaged

Control (Cold commissioning - April 2022):
Control of choppers,focussing nose, gate valve, slits, collimator, rotation stage/s.
Control of Sample Environment when experiment is running/ not running
Time stamp essential (linked to ESS baseline timestamp)
Control by graphical user interface (GUI) and command line (CL)
Flippers for PA.

Monitoring (Cold commissioning - April 2022):
(not directly part of DMSC but some parameters will be required within dataset):
Choppers parameters (pressure, water flow, heat)
Detector tank pressure …

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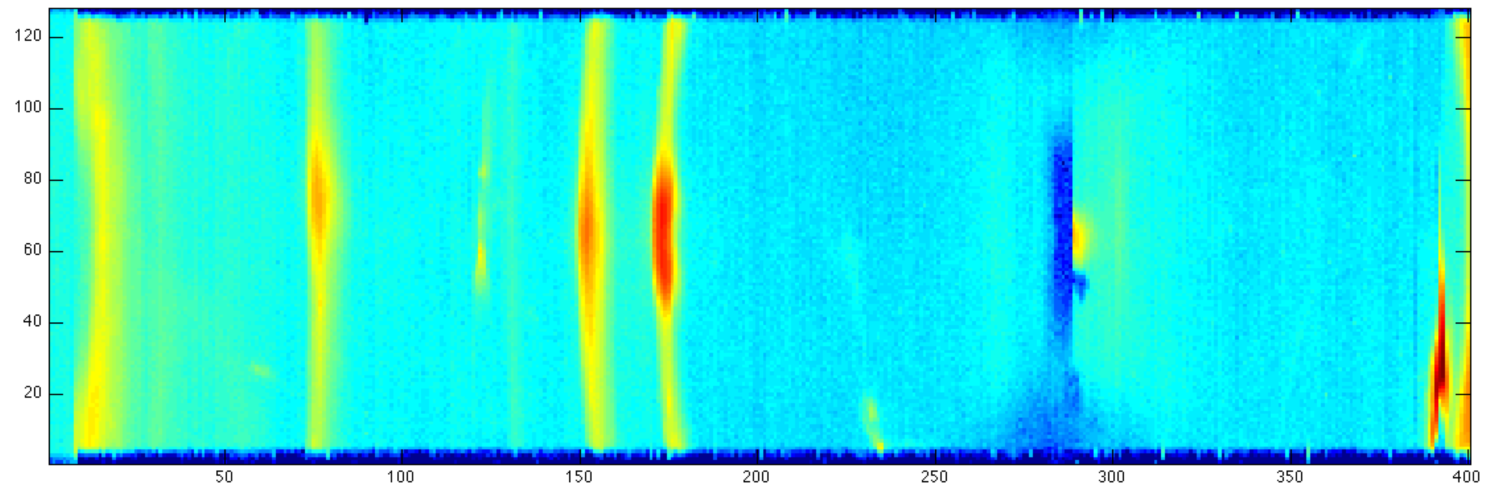
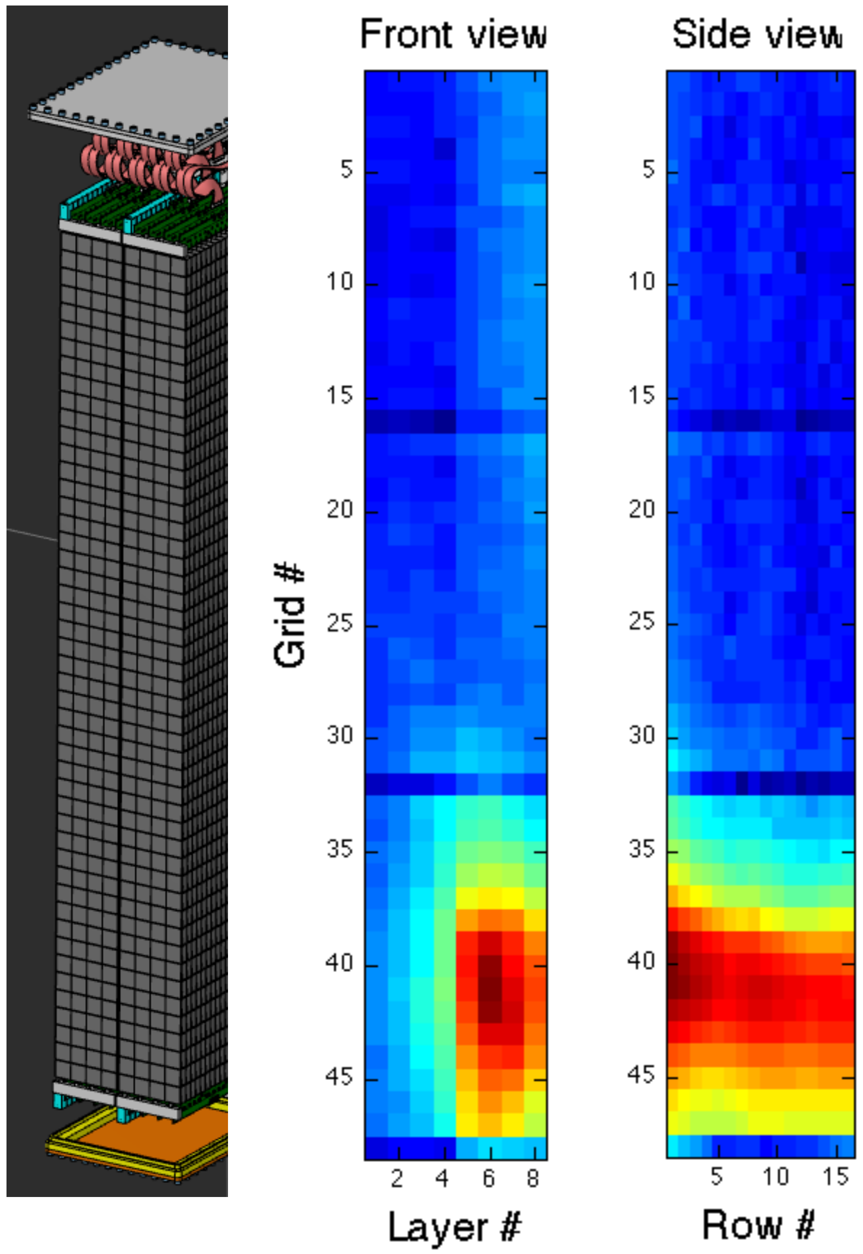
Data Acquisition (some in cold commissioning)

- Timestamp/position (event mode)
- Monitors (not event mode)
- Multigrid detector technology = (1.0x2.5x2.5 cm³)
- 3rd dimension can give further vital information.





LET tests

- Will test detector, not electronics
- Mesytec / not VMM

TECHNISCHE UNIVERSITÄT MÜNCHEN

Orphée Laboratoire Léon Brillouin

CSPEC

The Cold Chopper spectrometer of the ESS

EUROPEAN SPALLATION SOURCE

Reduction (Cold/Hot commisioning (June 2021)):

- Data live visualisation (< minute scale),
  ideally with a direct link to some initial theory.
- Quick transformation to determine E/Q resolution/ large data arrays (error prop)
- Understand background contributions
- Multiple scattering contributions
- From timestamp/position transformed to self and collective intermediate
- scattering functions I(Q, t) sand/or the self correlation function S(Q,w),
- transformed to ∑S(Q, w) for all RRM if possible.
- easy E/Q cuts

Mads Bertelsen McStas.

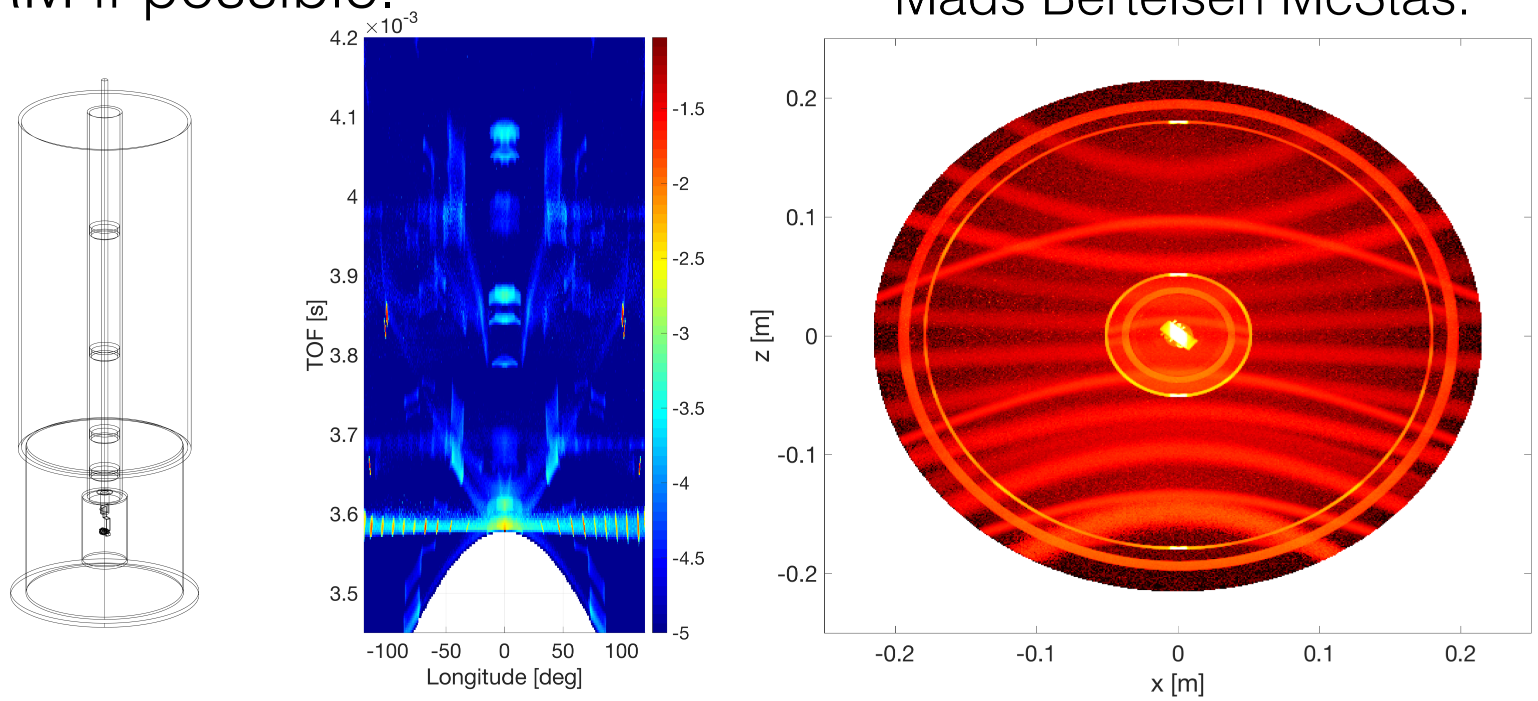


Figure 1: Left: Depiction of cryostat/sample model. Center: Time of flight banana monitor showing spurions. Right: Histogram over scattering locations in cryostat as seen from above.

Data analysis (Cold/Hot commissioning):

- Basic models for (e.g.) self-diffusion :

Ficks law
Chudley-Elloitt (CE) – jumps on a lattice
Singwi-Sjölander (SS)- alternation between oscillatory motion and directed motion
Hall-Ross (HR) – jump diffusion within a restricted volume

- Molecular Dynamics simulations i.e. VASP (DFT)
- SpinW
- McPhase
- SPINVERT
- Close collaborations with Lund/Stockholm University

- Ensure to incorporate instrumental resolution/ transmission profile
- McStas simulation of sample environment.

CSPEC

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EUROPEAN SPALLATION SOURCE

BUDGET

Proposal June 2018						
					Actual + guess Nov 2019	
Budget Proposal CSPEC		**TUM [kEUR]**	**LLB [kEUR]**	**Total [kEUR]**	**TUM [EUR]**	**LLB [EUR]**
Optics				**2614**		
	in-pile, NBOA	120			149 035,00 €	
	BBG	20			- €	
	in bunker guide	185			- €	
	bunker feedthrough	140			230 330,00 €	
	out-of bunker guide	1300			1 574 543,00 €	
	guide exchange	150			150 000,00 €	
	guide housing and piles	600			700 000,00 €	
	installation	99			- €	
Choppers				**1480**		
			1480			2 000 000,00 €
PSS				**100**		
		50	50		50 000,00 €	50 000,00 €
Shutter						
		20		**20**	20 000,00 €	
Beam Monitors				**70**		
		70			70 000,00 €	
Shielding				**1996**		
	Guide/ Halls		1129			1 181 000,00 €
	Detector Cave		867			625 000,00 €
Detector + Sample				**6147**		
	Detector Vaccum tank		1156			2 000 000,00 €
	Sample environement		375			375 000,00 €
	Radial collimator		200			100 000,00 €
	detectors	3474	942		3 914 420,00 €	363 333,00 €
Infrastructure				**100**		
	Instrument hutch		100			100 000,00 €
Manpower				**2323**		
		1197	1126		1 197 000,00 €	1 126 000,00 €
Contingency				**1650**		
		825	825		194 672,00 €	329 667,00 €
Total		**8250**	**8250**	**16500**	8 250 000,00 €	8 250 000,00 €

Lots of extra details not included.
Neglected: electrical work, MCA underestimated,
Vacuum housing cost underestimated
Cu guide housing underestimated. (20-30% more).

Agenda:
13:00 - 13:15 Aims of the ICEB. (PD)
13:15 - 13:30 CSPEC Overview and components reminder. In scope / future plans. (PD)
13:15 - 14:30 Project update: (Overview of project, schedule & budget)) (CSPEC/ESS) (FM)
14:20 - 15:40 Installation (FM)
15:40 - 16:00 Risks (FM)
14:30 - 15:00 DMSC, data management. (JT)
15:00 - 15:20 Sample environment (DN)
16:00 - 16:30 Discussion, actions, decision on risks, issues to follow up.

Aim:

Provide an overview of the project (inclusive risks) to partners.

Time decisions.

Costing decisions.