



ILL College 7 seminar

Grenoble, November 18th 2019

Progress in simulation software, shielding
methods and compact Larmor devices:
- A report from SINE2020 WP8

DTU Peter Willendrup,
Technical University of Denmark

1. Objectives

(and WP8 Structure)

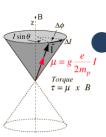
- Task 8.1: E-tools for integrated simulation using neutronics and Monte Carlo ray-tracing



- Task 8.2: Innovative Shielding Concepts and Materials



- Task 8.3: Compact Instrumentation for Larmor Labelling applications at the ESS



1. Objectives

(and WPs)

Improve

- Task 8.1: E-tools for integrated simulation using neutronics and Monte Carlo ray-tracing
- Task 8.2: Innovative Shielding Concepts and Materials
- Task 8.3: Compact Instrumentation for Larmor Labelling applications at the ESS

“cradle to grave” instrument-modeling capability beyond state of the art:

neutronics + ray-tracing → signal / noise



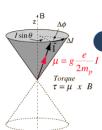
Measure

and understand (high-energy) background and utilise this to better shield our instruments using new shielding approaches (heavy concrete, laminar shielding)

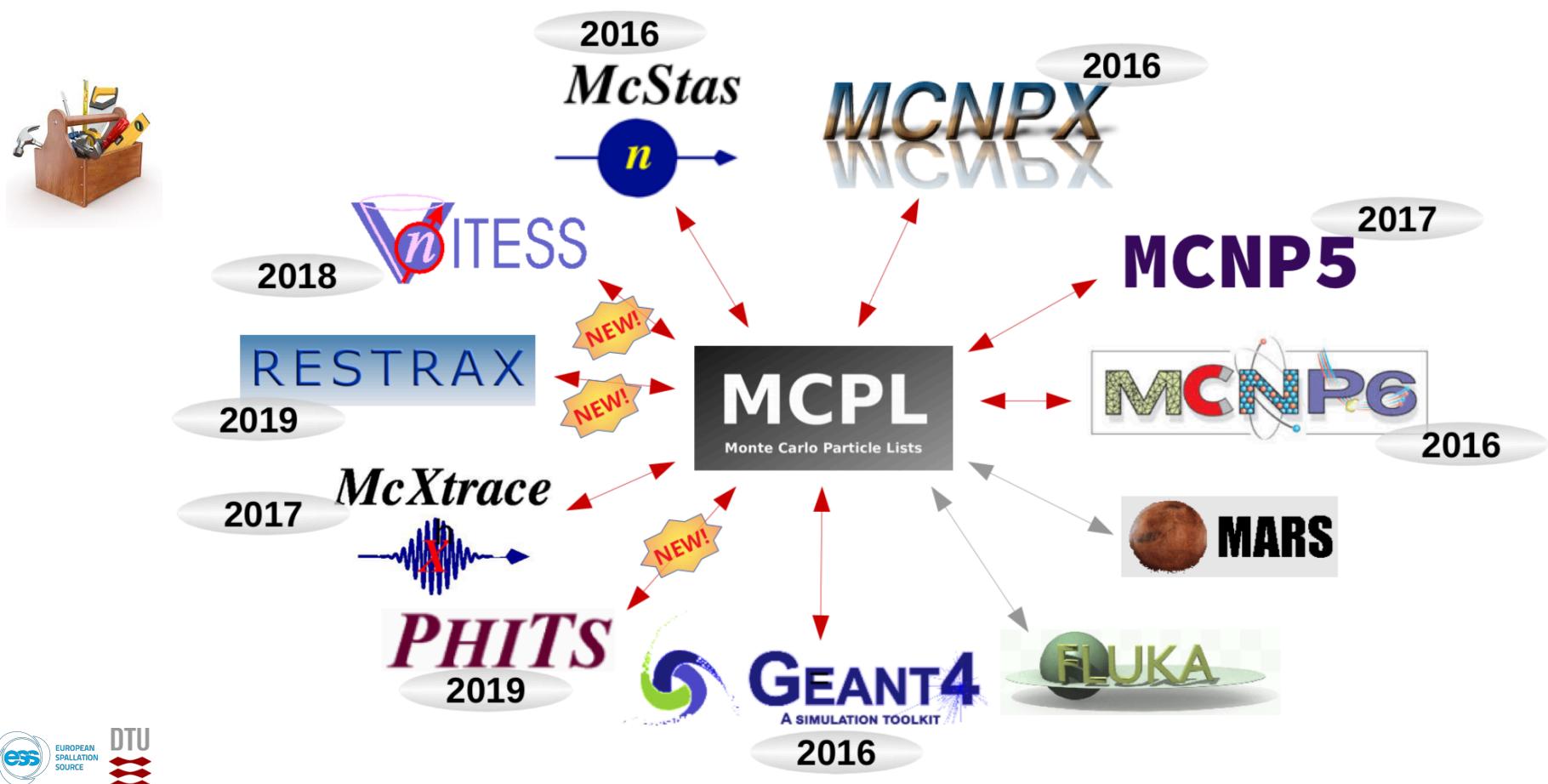


Investigate

the effect of the ESS pancake / butterfly moderator on the design of NSE and Larmor labelling instruments at this facility



Task 1 achievements 1: MCPL interchange format



T. Kittelmann, et al., Monte Carlo Particle Lists: MCPL, *Computer Physics Communications*, Volume 218, September 2017, Pages 17-42, ISSN 0010-4655, <https://doi.org/10.1016/j.cpc.2017.04.012>

Task 1 achievements 1: MCPL interchange format



```
pkwi-mbp2018:4_McStas pkwi$ mcpltool W3.mcpl.gz
Opened MCPL file W3.mcpl.gz:

Basic info
Format : MCPL-2
No. of particles : 174450495
Header storage : 171 bytes
Data storage : 6280217820 bytes

Custom meta data
Source : "MCNPX-2.7.0"
Number of comments : 2
-> comment 0 : "MCNP(X) SSW file converted to MCPL with ssw2mcpl"
-> comment 1 : "Title/description encoded in SSW file: 'Input File: ''"
Number of blobs : 0

Particle data format
User flags : no
Polarisation info : no
Fixed part. type : no
Fixed part. weight : no
FP precision : single
Endianness : little
Storage : 36 bytes/particle

index pdgcode ekin[MeV] x[cm] y[cm] z[cm] ux uy uz time[ms] weight
0 2112 0.018837 131.29 150.88 19.66 0.61947 0.77528 0.1233 0.0013887 7.7394e-27
1 2112 0.021846 139.8 143.02 14 0.66303 0.73946 0.11659 0.0012184 1.4012e-28
2 2112 0.34503 135.14 147.44 18.926 0.6868 0.7196 0.10242 0.0003827 3.361e-17
3 2112 0.39514 129.99 152 11.639 0.67837 0.73181 0.065348 0.00034582 2.1271e-28
4 2112 0.39995 134.82 147.73 11.244 0.69895 0.71234 0.063561 0.00034449 4.8273e-26
5 2112 0.43034 134.34 148.16 13.595 0.70471 0.706 0.070283 0.00032745 2.436e-23
6 2112 0.023844 137.39 145.34 18.262 0.74022 0.33843 -0.58098 0.00033134 1.1614e-20
7 2112 0.44336 130.45 151.6 12.905 0.67163 0.73335 0.10538 0.000306 4.6873e-26
8 2112 0.44692 136.01 146.63 15.649 0.69704 0.70795 0.11372 0.00030363 4.9599e-25
9 2112 0.46274 129.51 152.4 9.4062 0.68973 0.7206 0.070773 0.0002787 1.0161e-21
```

File properties & stats

Simulation metadata

Particle storage properties

Task 1 achievements 1: MCPL interchange format



```
McCode — pkwi@pkwi-mbp2018: ~/Projects — bash — 98x35
pkwi@pkwi-mbp2018:~/Projects$ pymcpltool --stats /Users/pkwi/Projects/SINE2020BIFROST/W3.mcpl.gz

-----
nparticles : 174450495
sum(weights) : 18527.8
-----

          :      mean        rms       min       max
-----
```

ekin	[MeV]	: 1.38306	9.65091	2.07568e-15	1990.84
x	[cm]	: 169.62	28.6837	97.6746	200
y	[cm]	: 3.42827	101.954	-174.527	174.527
z	[cm]	: 14.2431	3.27836	8.5598	19.9434
ux	:	0.815141	0.194949	-0.844703	1
uy	:	0.00809299	0.534939	-0.999928	1
uz	:	0.00137547	0.106366	-0.999943	0.999988
time	[ms]	: 0.485192	0.782116	2.36574e-05	993.475
weight	:	0.000106207	0.00949162	0	3.40407
polx	:	0	0	0	0
poly	:	0	0	0	0
polz	:	0	0	0	0

pdgcode	:	2112 (n)	11856.2 (63.99%)
		22 (gamma)	6667.51 (35.99%)
		2212 (p)	3.04239 (0.02%)
		1000010020 (D)	1.00065 (0.01%)
		-211 (pi-)	7.77578e-06 (0.00%)
		211 (pi+)	2.22455e-06 (0.00%)
		1000010030 (T)	3.87931e-10 (0.00%)
		1000020040 (alpha)	5.22881e-11 (0.00%)
		[values]	[weighted counts]

userflags	:	0 (0x00000000)	18527.8 (100.00%)
		[values]	[weighted counts]

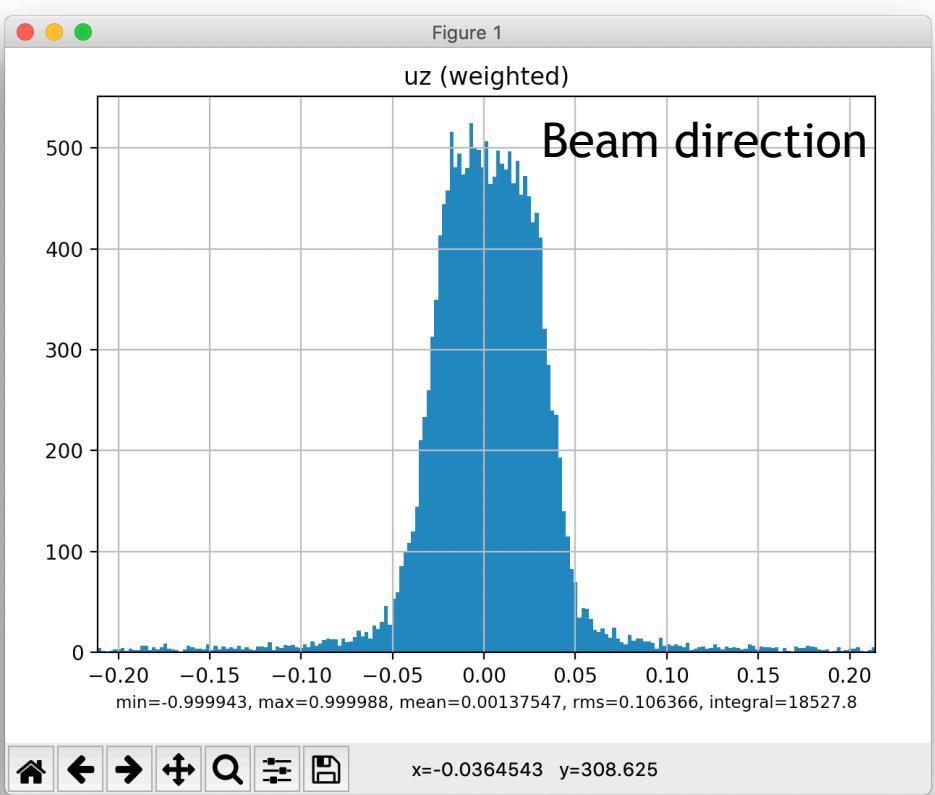
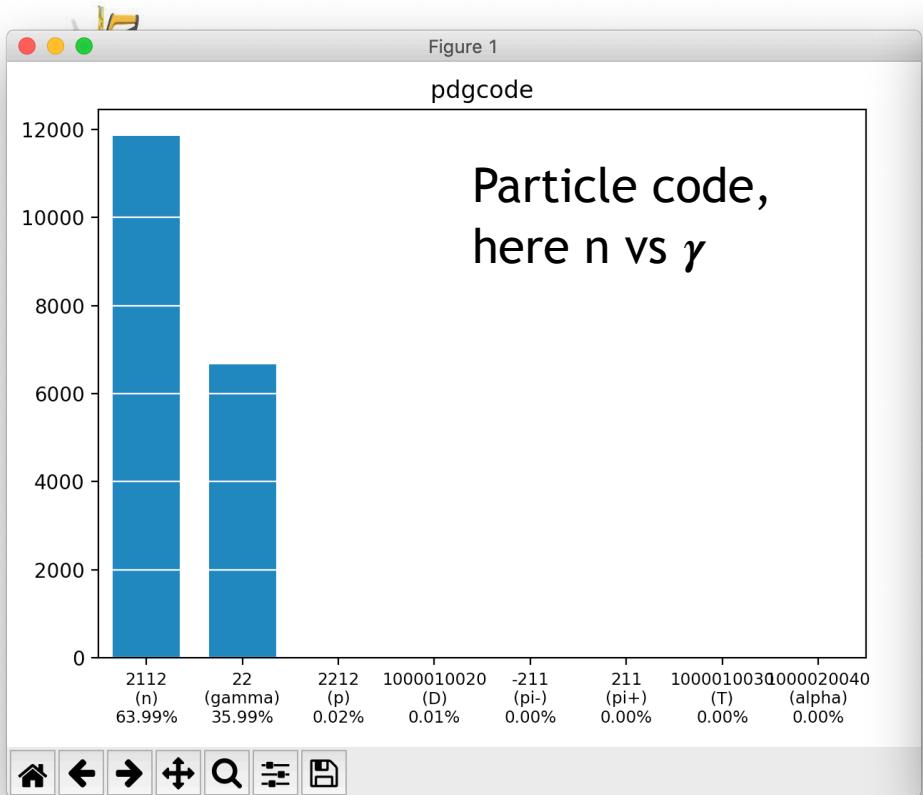
```
pkwi@pkwi-mbp2018:~/Projects$
```

Gaussian
stats
on particle
Properties

Particle
type stats

Includes command line
tools for stats...

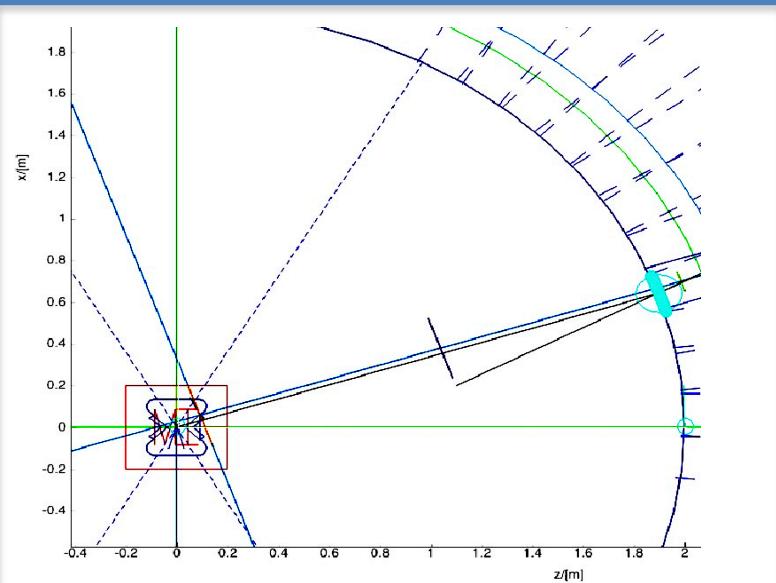
Task 1 achievements 1: MCPL interchange format



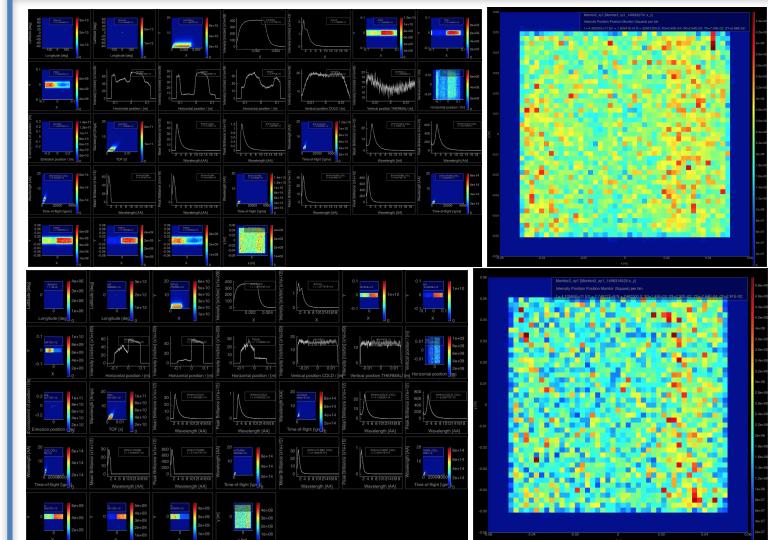
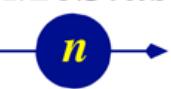
... plus gui tools for
stats...

Task 1 achievements 1: MCPL interchange format

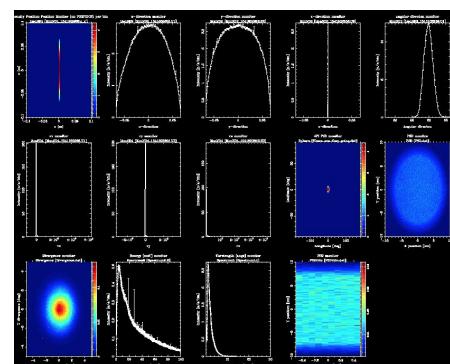
Used for bringing MCNP-based source-terms to McStas at multiple facilities: ESS, HIFR



Visualisation of events in the file W8.mcpl.gz within the ESS_butterfly_MCPL instrument. The coordinate system of choice is the TARGET coordinate system.



Output from MCPL-based and analytical ESS sources:
- overview plot and "end of curved guide" PSD for W8.



MCNP output from the ORNL HIFR source available for transport in McStas.



Task 1 achievements 2: (improved) Supermirror patch to MCNP-6



1. Initial implementation 2009 for MCNPX: 

F. X. Gallmeier et. al. (2009) Implementation of Neutron Mirror Modeling Capability into MCNPX and Its Demonstration in First Applications, *Nuclear Technology*, 168:3, 768-772, DOI: 10.13182/NT09-A9304

2. Improved implementation 2013, MCNPX and enabling MPI support:  

E. B. Klinkby, et. al. (2013) Interfacing MCNPX and McStas for simulation of neutron transport, *Nuclear Instruments and Methods A*, 700, 106-110 DOI: 10.1016/j.nima.2012.10.052

3. Current, MCNP6, MPI and standard variance reduction schemes:



Much improved implementation, allows standard variance reduction schemes and allows “deterministic propagation” in neutron guide volumes

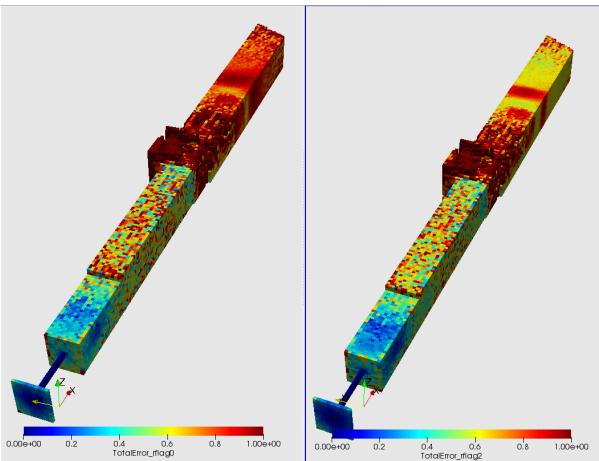
M. Magan & R. Bergmann, Supermirror physics with event biasing in MCNP6, NIMA-D-19-00551, submitted in October 2019.



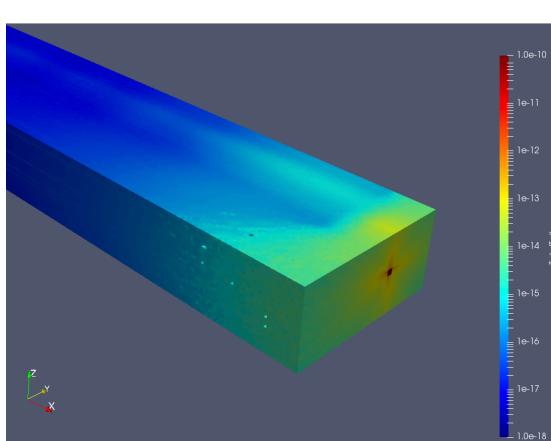
Task 1 achievements 2: (improved) Supermirror patch to MCNP-6



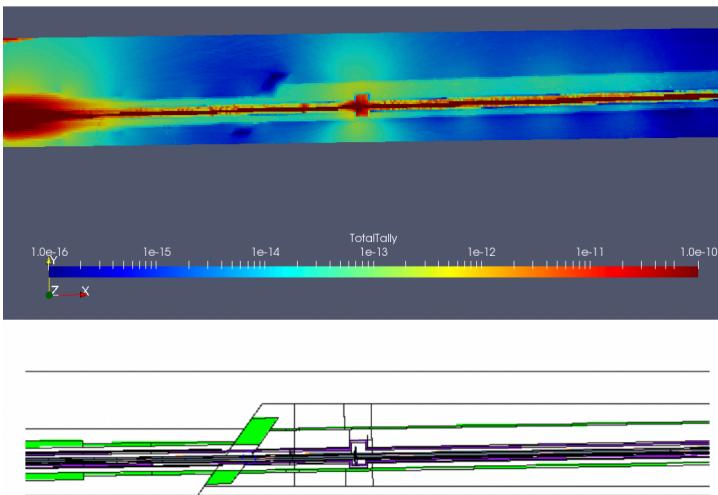
Prior to D8.3 work, the standard MCNP variance reduction tool of DXTRAN spheres was not possible together with the super mirror patch!



Comparison of stochastic (left) Vs deterministic guide reflection. Relative errors.

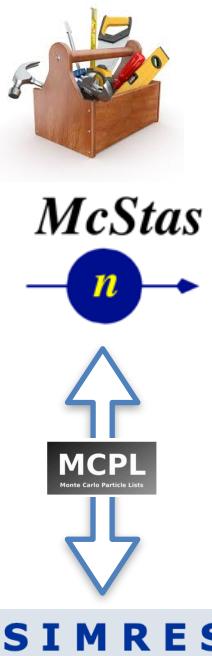


Neutron flux (per source particle) in the MIRACLES Geometry: detail at the end of the guide.



Radiation creation at features like neutron choppers is clearly visible and solved.

Task 1 achievements 3: McStas <-> SIMRES interchange



Why combine SIMRES + McStas?



- Independent code validation by performing inter-comparison tests
- Complementarity: Each package includes unique features and models not available in the other two.
- Performance options: For example, efficient sampling strategy allowing fast simulations at a single CPU in SIMRES, versus highly configurable programming environment which is paid off by slower simulations in McStas.

Task 1 achievements 3: McStas <-> SIMRES interchange

D8.11: Transport of sample models from McStas to SIMRES:

- Uses MCPL to “sandwich” e.g. the McStas Single_crystal in a SIMRES simulation workflow.
- Mechanism not limited to samples, but can expose any McStas component in SIMRES



McStas



SIMRES

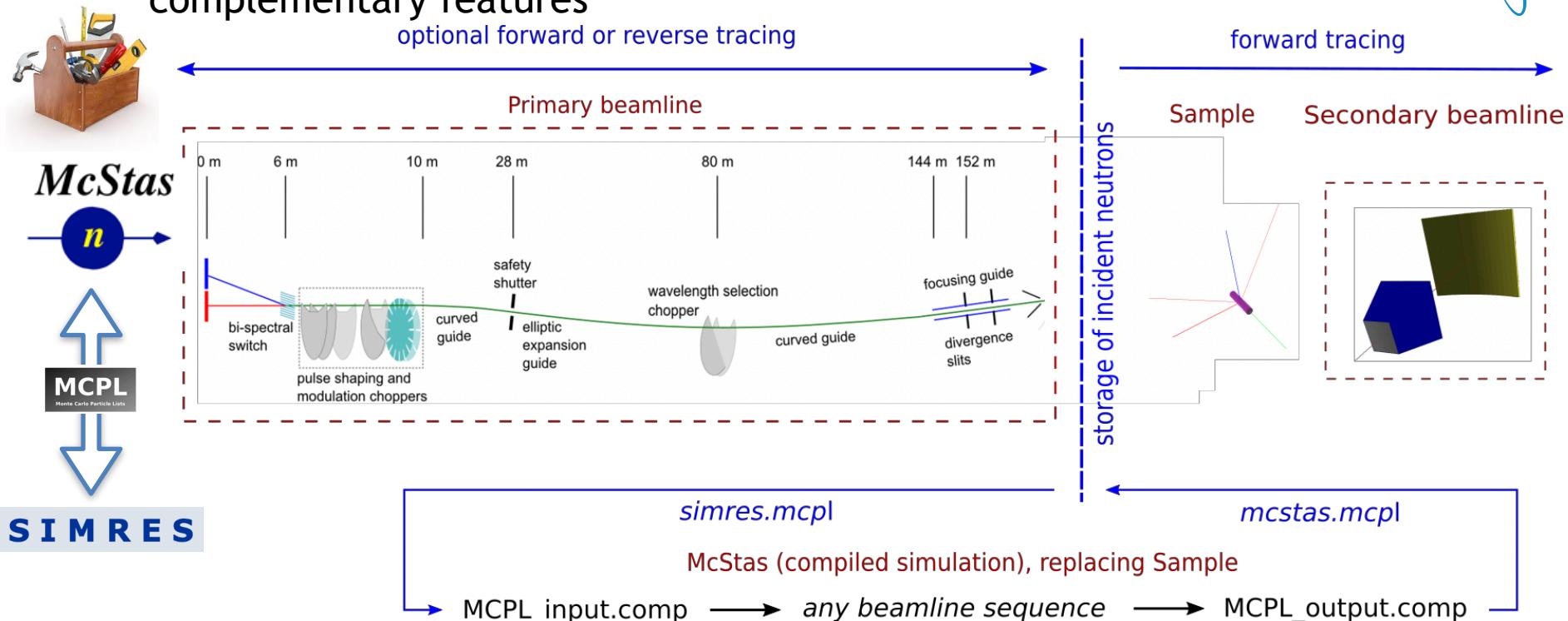


```
1 COMPONENT in = MCPL_input( repeat=1, filename="vin.mcpl")
2 AT(0,0,0) RELATIVE Origin
3
4 COMPONENT single_crystal = Single_crystal(
5   reflections="Al2O3-sapphire.lau",
6   yheight=0.05, radius=0.01, mosaic=1, delta_d_d=1e-4,
7   az=4.757, ay=0, az=0, bx=2.3785, by=0, bz=-3.364,
8   cx=0, cy=12.9877, cz=0,
9   p_transmit=0.1)
10 AT (0, 0, 0) RELATIVE PREVIOUS
11
12 COMPONENT out = MCPL_output( filename="vout.mcpl")
13 AT(0,0,0) RELATIVE PREVIOUS
```

Multiple examples of this were released with McStas 2.5

Task 1 achievements 3: McStas <-> SIMRES interchange

D8.12: Full ESS BEER beam line simulation combining McStas and SIMRES complementary features



A schematic showing the flow of neutrons in a simulation combining SIMRES and McStas. The sample component of SIMRES is replaced by a compiled McStas simulation executable. It uses primary beam neutrons from SIMRES monitor and returns back the result by using the MCPL input/output components. The 3rd step (secondary beam simulation by SIMRES) is optional, simulations can be finished already by the McStas part.

Task 1 achievements 3: McStas <-> SIMRES interchange

D8.12: Full ESS BEER beam line simulation combining McStas and SIMRES complementary features



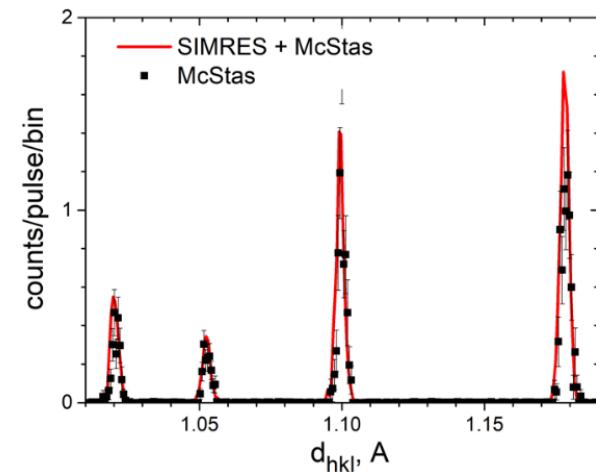
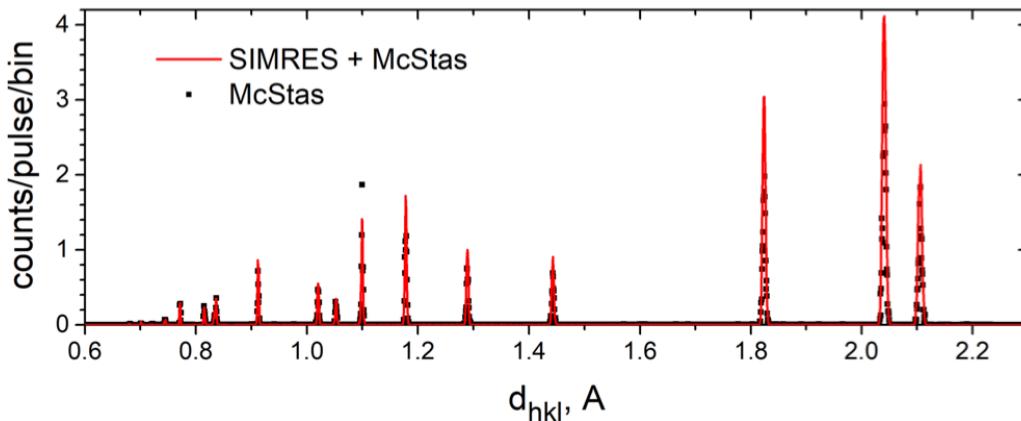
McStas



MCPL



SIMRES



Diffractograms simulated by the combined SIMRES+McStas ray-tracing (red line) and by McStas only (black points). The detail on the right permits to assess differences, which are within the statistical errors.

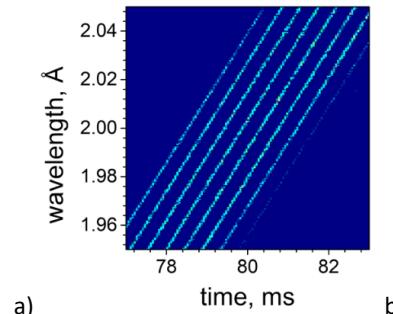
	Rel. error (primary beam)	Computing time
SIMRES + McStas	1.1 %	56 s
McStas	1.8 %	1110 s

!

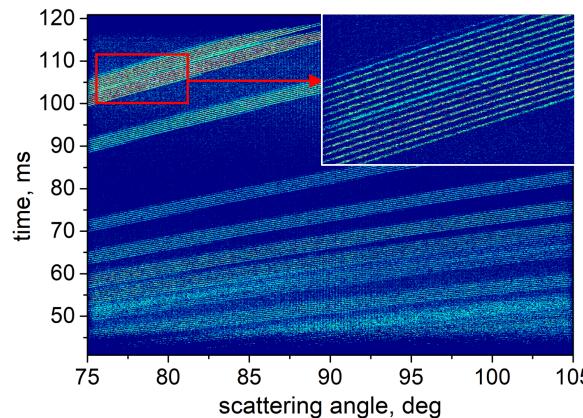
Task 1 achievements 3: McStas <-> SIMRES interchange



McStas



a)



b)

Figure 3. (a) Modulated beam structure at the primary slit – SIMRES MCPL output passed to McStas.
 (b) ToF – 2θ map of events registered by the detector component
`(NPI_tof_theta_monitor.comp)` in McStas; multiplexed diffraction lines from the duplex steel
 sample (`PowderN.comp`).



S I M R E S

Takes advantage of

- SIMRES for small gauge-volume in strain measurements
- Flexibility in McStas-based data-evaluation -> reconstructed peaks from modulation signals

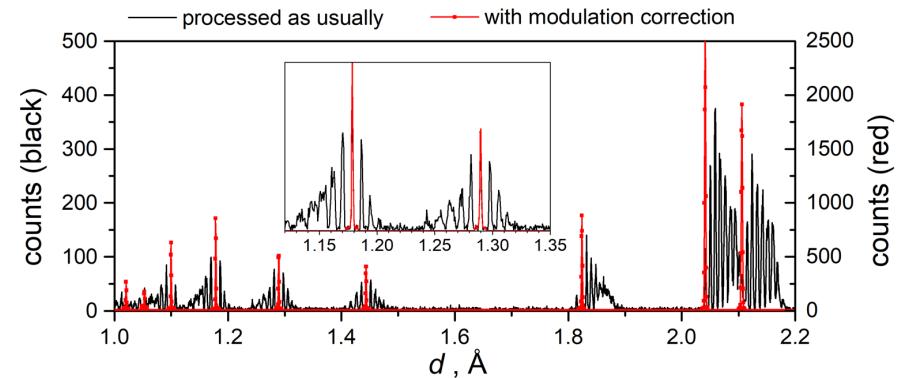
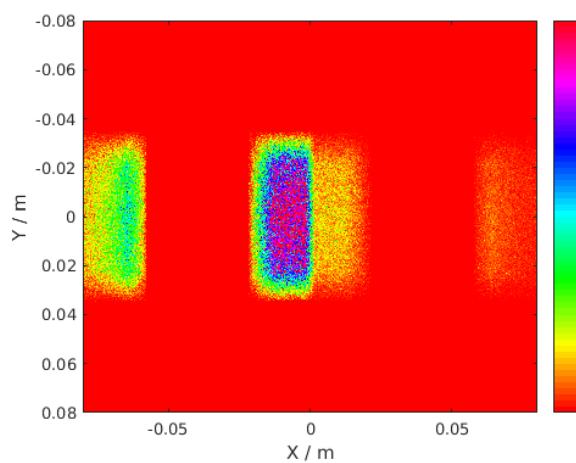
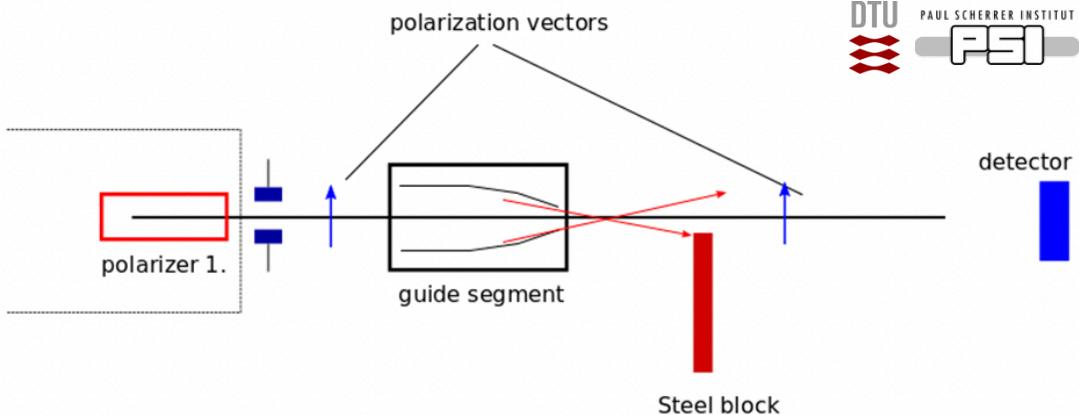


Figure 4. Diffractogram produced by the McStas component `NPI_tof_dhkl_detector` with the modulation analysis switched off (black, left scale) and on (red, right scale).

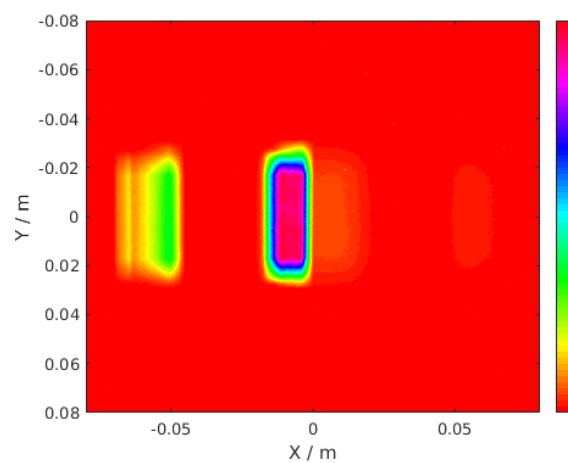
Task 1 achievements 4: experiments and benchmarks



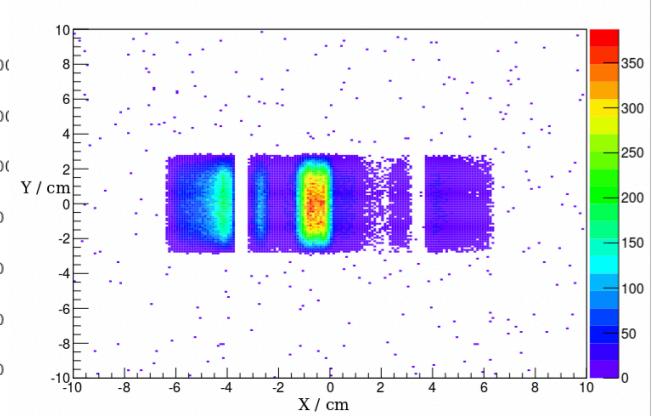
D8.4 experiments, McStas and MCNP calculations at the PSI BOA beam line



McStas

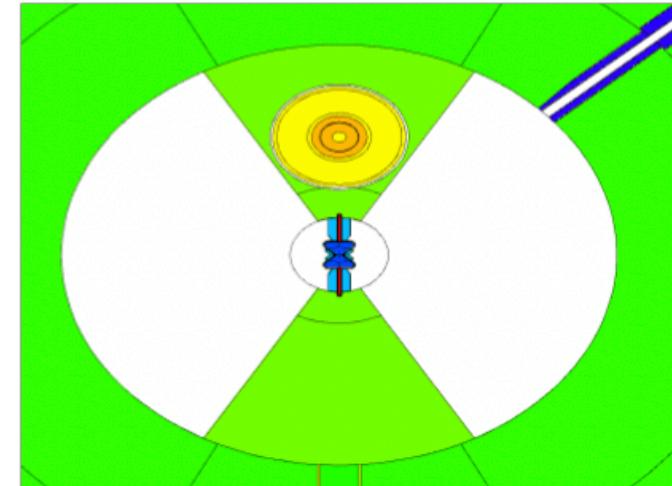
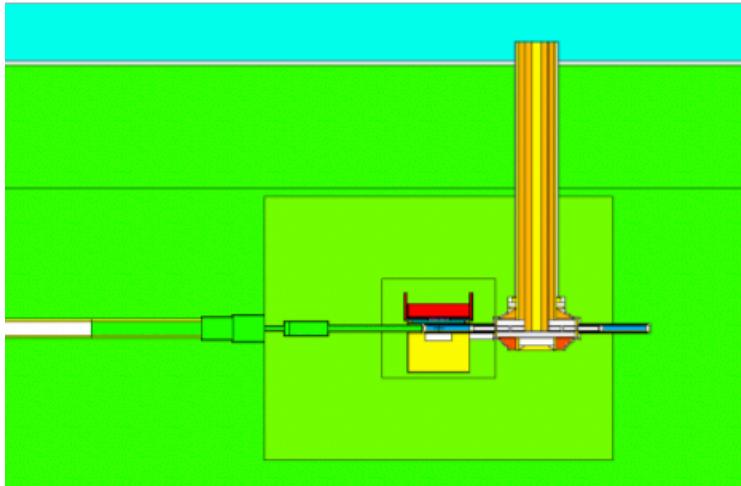
Experimental data



MCNP6

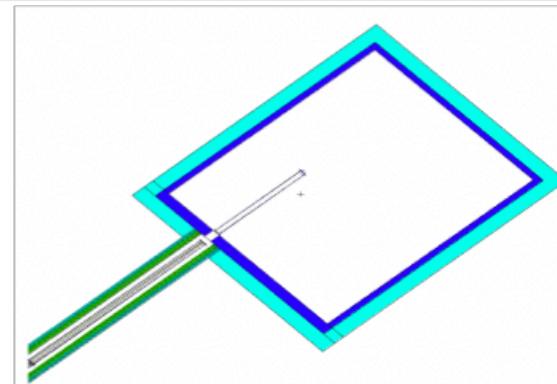
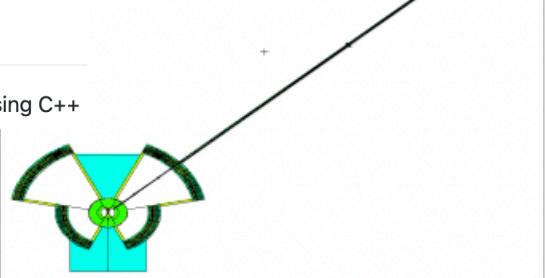
Task 1 achievements 5: illustrated example cases w/code

D8.13 Simulation tool-suite applied to BIFROST at ESS



CombLayer

MCNP(X) project builder using C++



CombLayer-driven MCNP6 model of ESS source and the BIFROST instrument up to sample pos

Ansell, Stuart (2016). CombLayer - A fast parametric MCNP(X) model constructor (JAEA-Conf--2015-002). Arai, MasatoshiYonemura, Masao, Yonemura, Masao, & Suzuki, Jun-ichi (Eds.). Japan

Task 1 achievements 5: illustrated example cases w/code

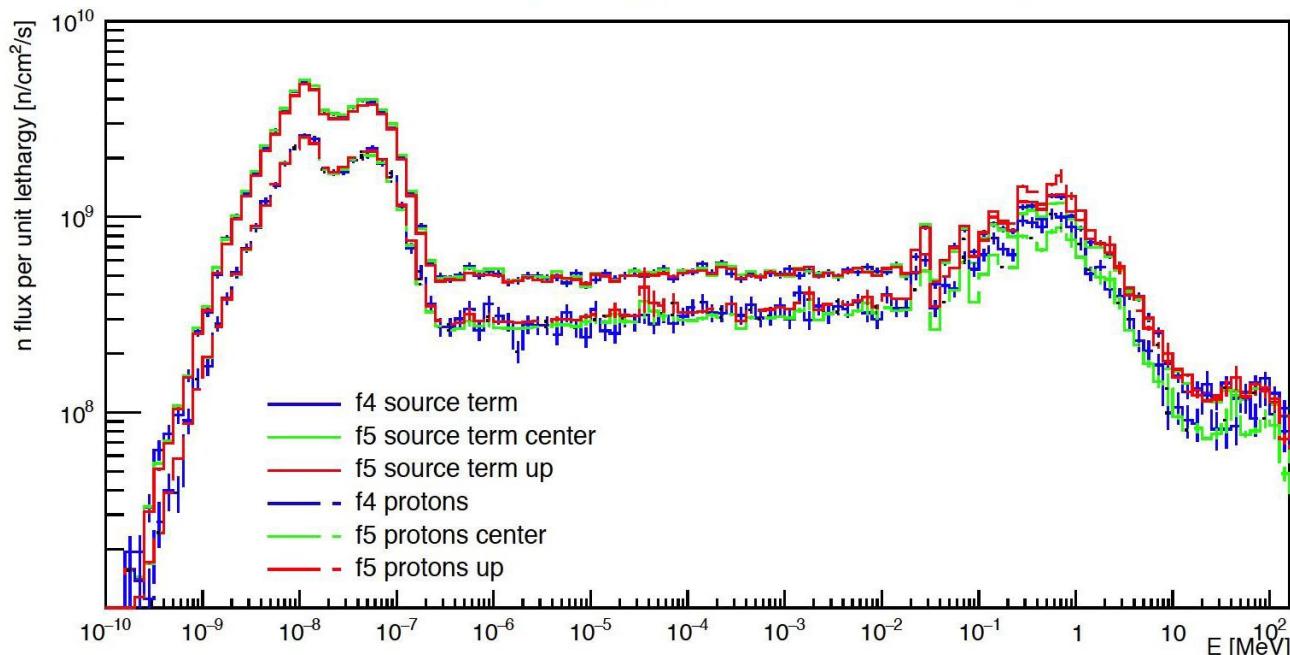
D8.13 Simulation tool-suite applied to BIFROST at ESS



Supermirror patch applied to

```
REFLE53 953 1 -4359
REFF1 0.99 2.19E-2 4 6.07 3E-3 $supermirror
RFLAG1 2
```

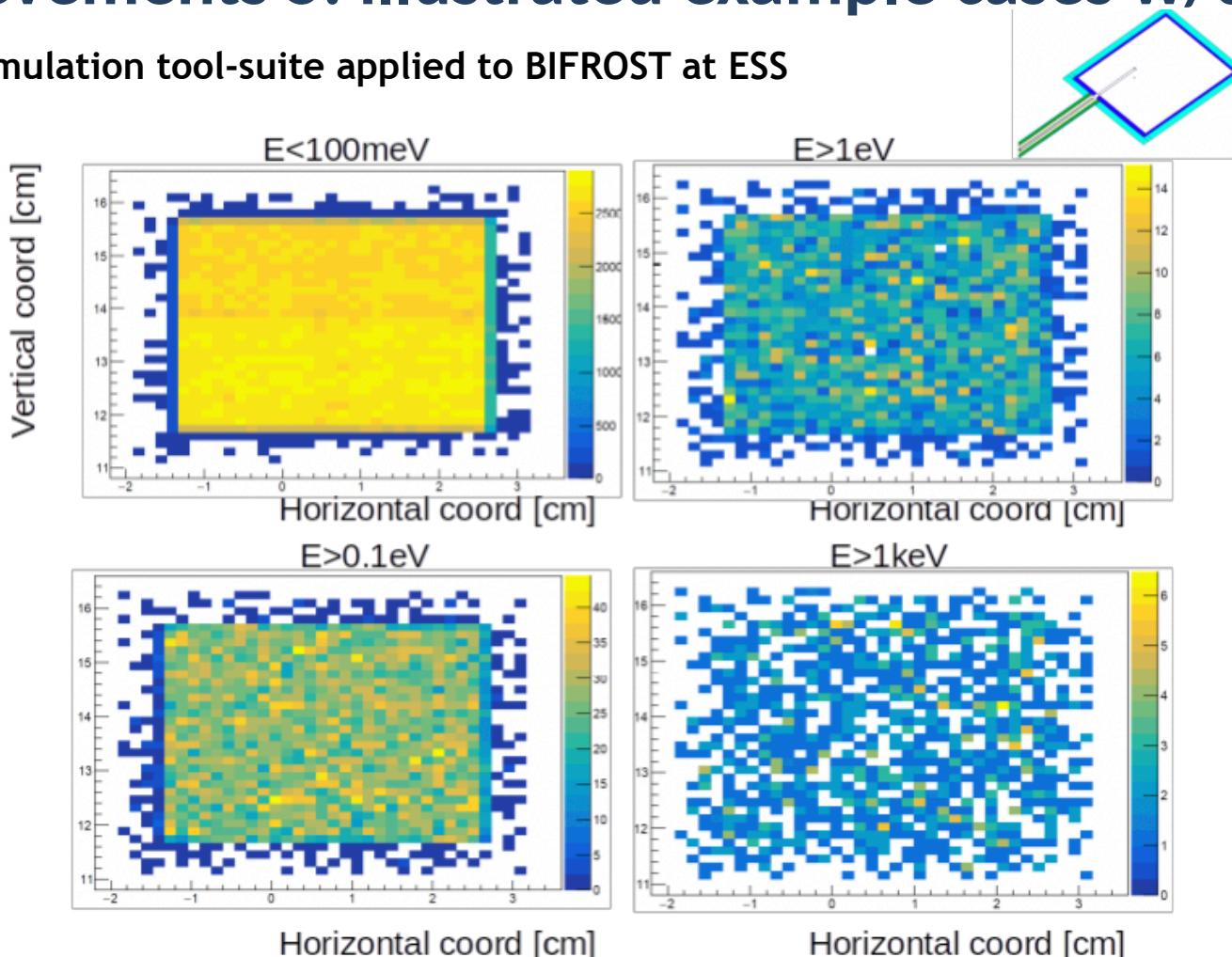
CSPEC 8X10 cm² opening, protons vs source term, corr=1.3



Synthesising neutron-source from proton source in

Task 1 achievements 5: illustrated example cases w/code

D8.13 Simulation tool-suite applied to BIFROST at ESS



Beam cross section at sample position, all transported by

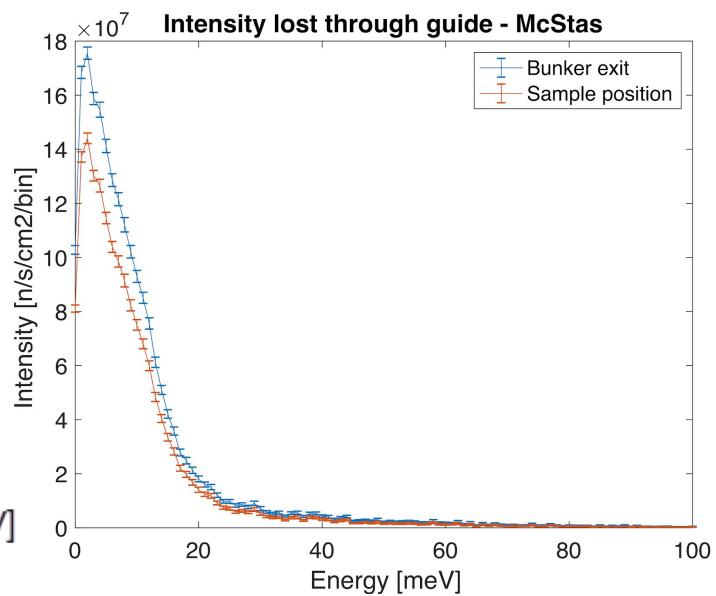
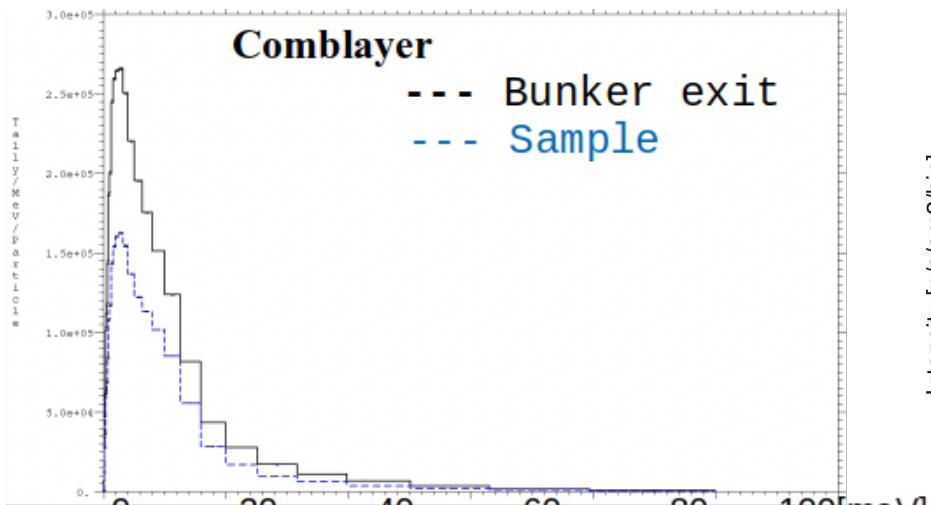


Task 1 achievements 5: illustrated example cases w/code

D8.13 Simulation tool-suite applied to BIFROST at ESS



Beam losses along beamline, +SM vs McStas

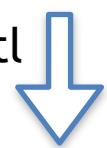


The intensity loss in the McStas simulation is **22%**, whereas the corresponding loss found in the SM MCNP simulations where **37%**. These differences are thought to be due to small differences in the guide geometry - in the SM MCNP case the geometry is inherited from its CombLayer implementation, whereas the McStas geometry originate from the instrument team directly.

Task 1 achievements 5: illustrated example cases w/code



DS CATia



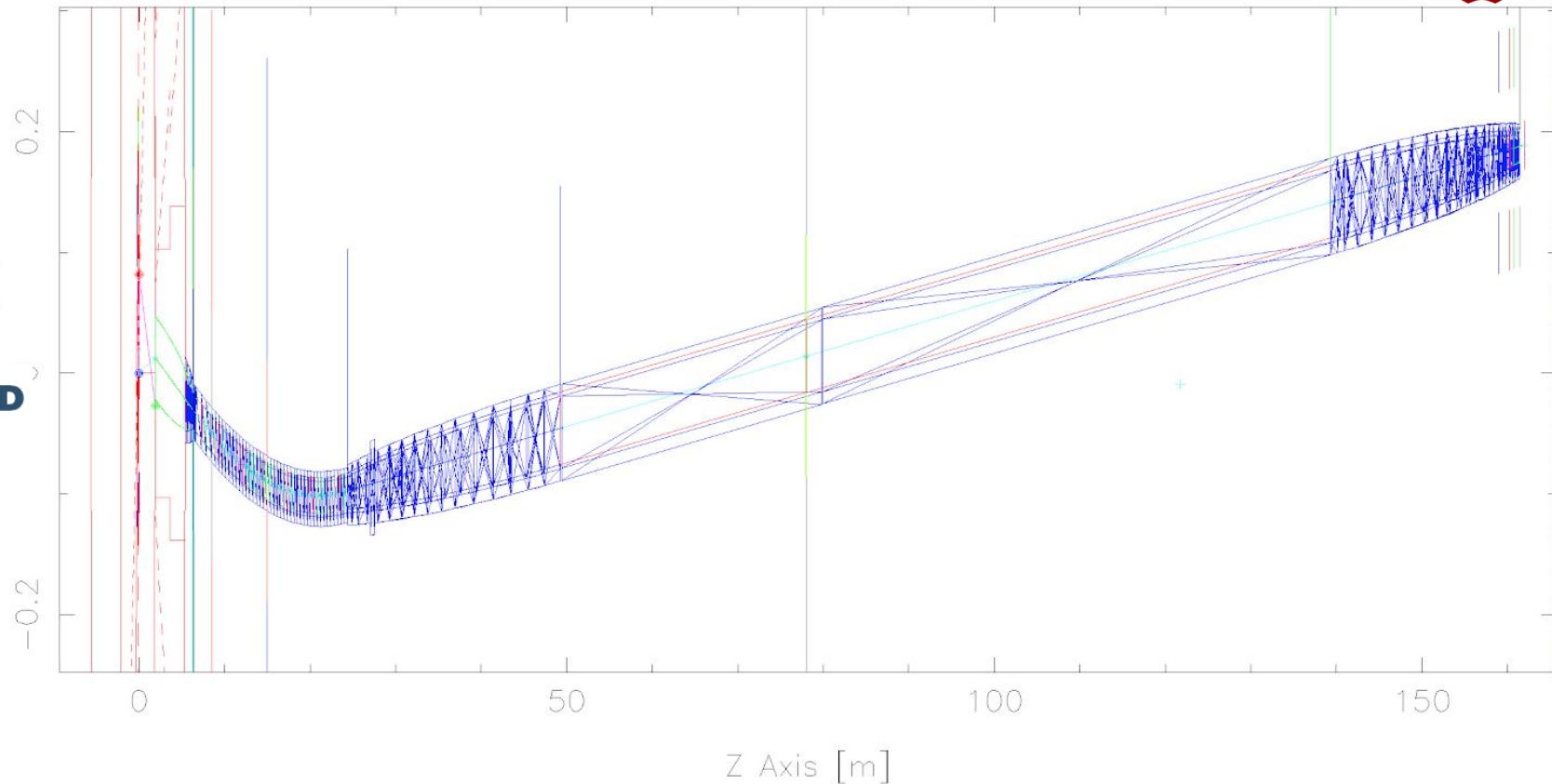
FreeCAD



McStas



D8.13 Simulation tool-suite applied to BIFROST at ESS



*CAD model (blue) overlayed with McStas instrument geometry. The precision in placement of the sample position is **of the order cm** over the 150 m instrument length.*

Task 1 achievements 5: illustrated example cases w/code

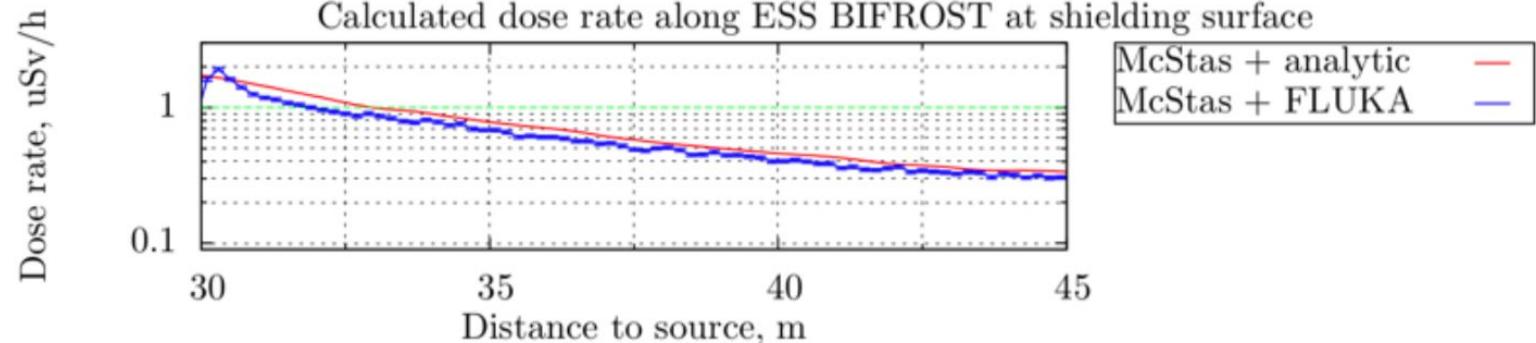
D8.13 Simulation tool-suite applied to BIFROST at ESS



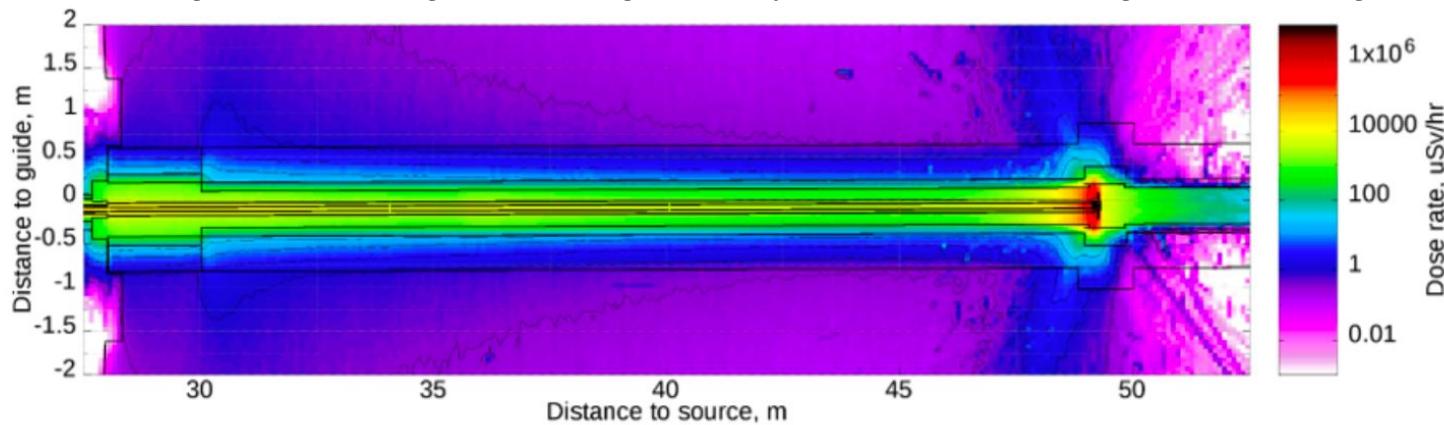
McStas



γ -dose rate
Estimates



Dose rate along ESS BIFROST guide shielding at the surface calculated according to [3] and using FLUKA



Dose rate distribution in the shielding around BIFROST guide, cut by horizontal plane at guide height.

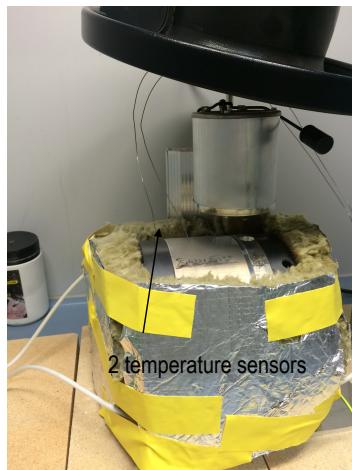
[3] R. Kolevatov et.al. Neutron absorption in supermirror coatings: Effects on shielding NIM. A 2019, **922**, pp. 98-107 <https://doi.org/10.1016/j.nima.2018.12.069>

[6] R. Kolevatov, McStas and Scatter Logger driven calculations of prompt gamma shielding for the neutron guides, submitted to JNR SINE 2020 ISTSI proceedings

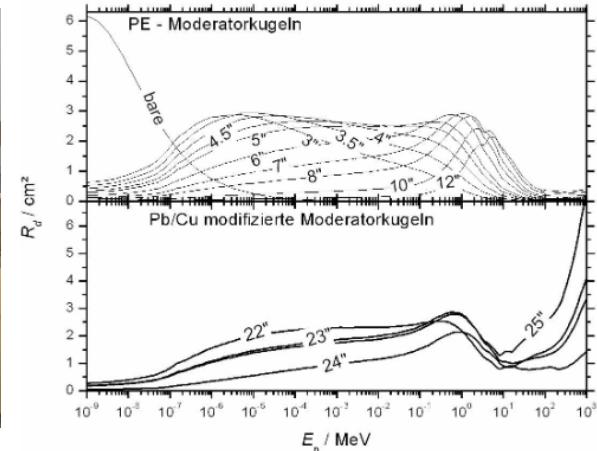
Task 2 achievements 1: Improved Bonner Sphere Spectrometer



SINE2020 WP8-developed
BSS-system with PE
moderators, Cu and Pb shells



Temperature controlled heating and cooling
(at least 3-4 times per sphere)



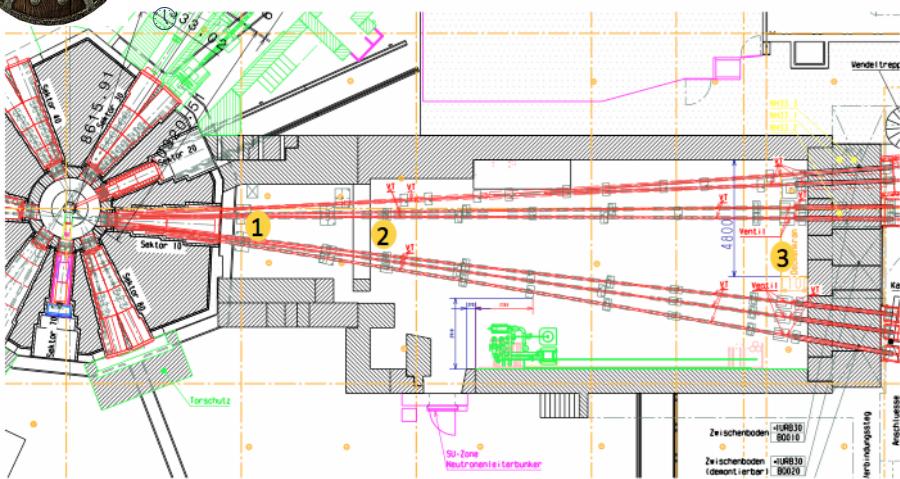
Range extension:

~20 MeV-> ~5 GeV!

Task 2 achievements 2: Understanding facility backgrounds - PSI



PSI measurements & simulations

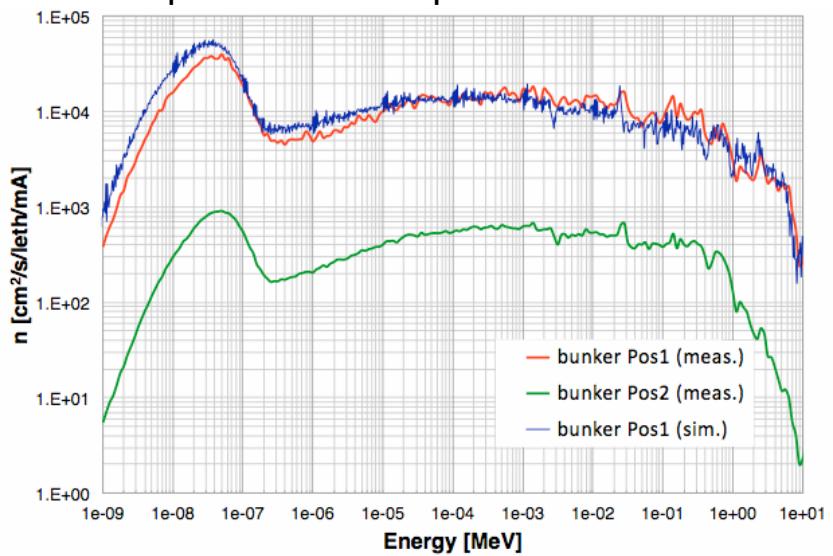


SINQ neutron guide bunker with the three measurement position

The agreement between simulations and measurement is very good. The small differences in the thermal region could be scattering effects which are not fully implemented in the MCNPX model.

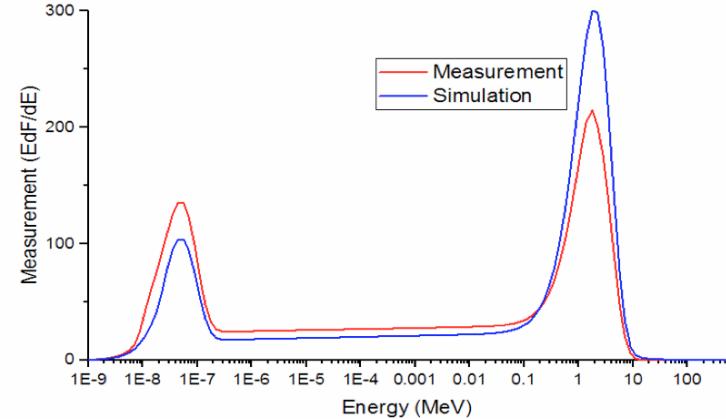
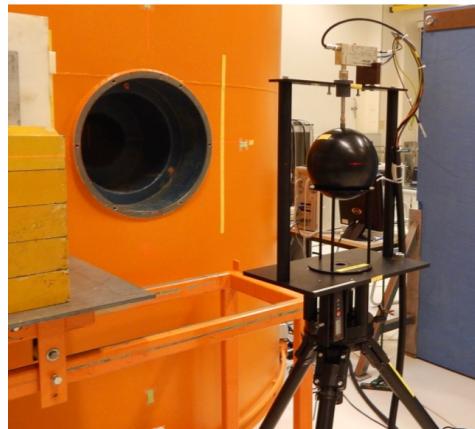
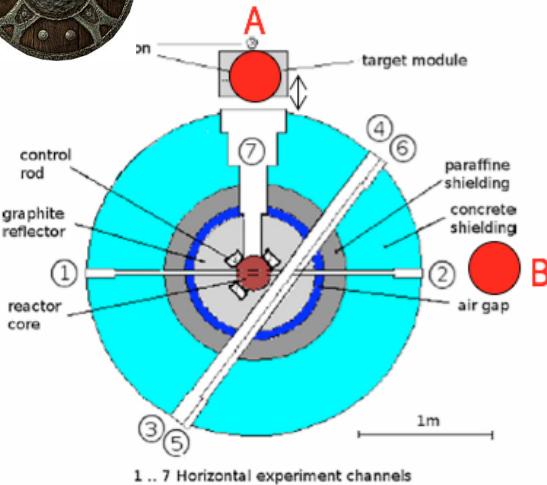


Setup in the middle position 2



Task 2 achievements 2: Understanding facility backgrounds - PSI

AKR-2 Dresden measurements & simulations

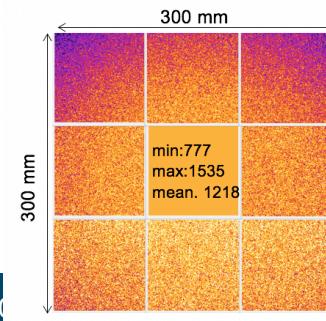


Cross section of the reactor setup and the two measurement positions

Data evaluation / modelling done for position A, as the spheres are not fully illuminated in position B which thus requires more complex data interpretation

Measurement setup at position A

Measurements and Simulations for Position A

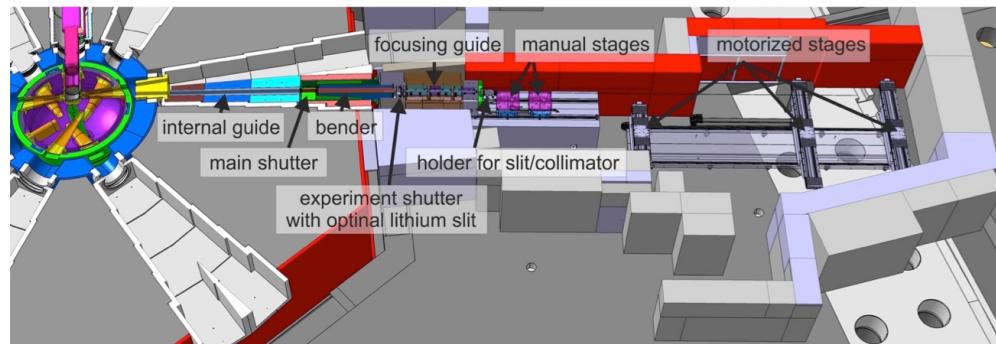


Thermal Neutron flux distribution of position A

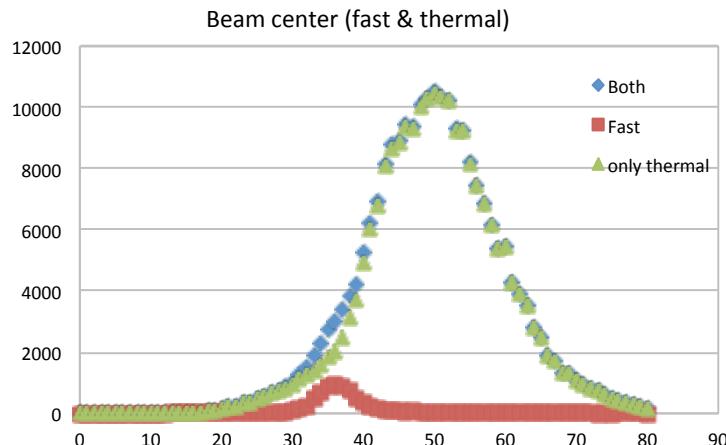
Task 2 achievements 2: Understanding facility backgrounds - PSI

SINE
2020

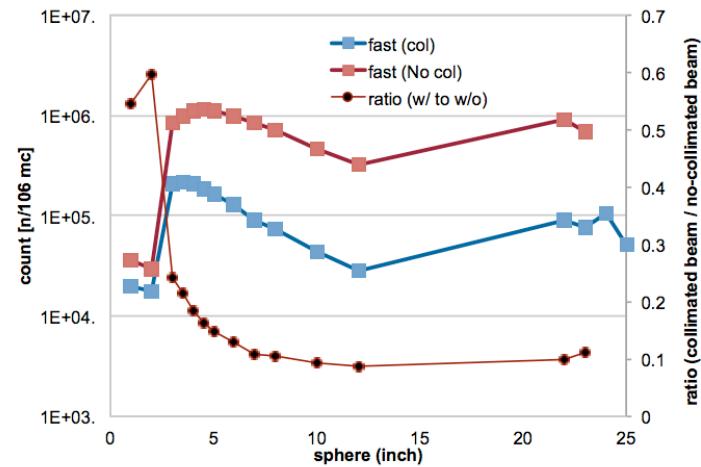
Use of the BSS spectrometer with BOA@PSI



BSS-system with PE moderators and Cu shells



Fast and thermal neutron flux distribution at the BOA beamline

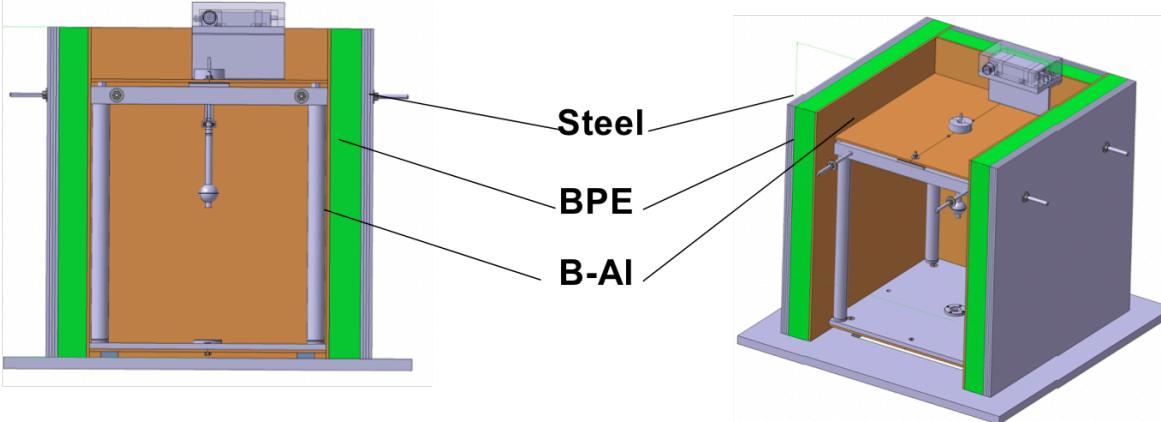


BOA – Fast neutron spectrum measured by the BSS system

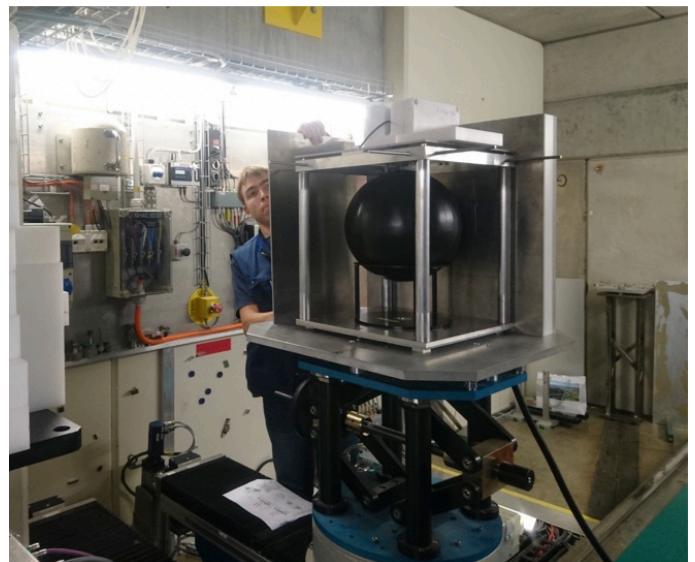
Task 2 achievements 2: Understanding facility backgrounds - PSI



Shielding-box setup



Shielding box for material investigations



Measurement setup at BOA beamline

Created for

- Easy decomposition of background from different directions, e.g. sky-shine vs. reflection from floor
- Easy setup/evaluation of laminar setups

Task 2 achievements 2: Understanding facility backgrounds - PSI

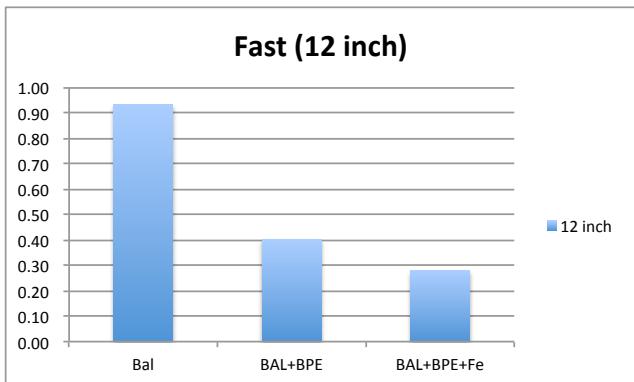


Figure 8a: Fast neutron transmission

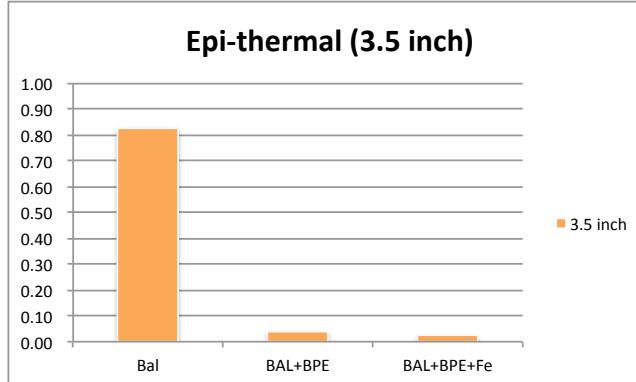


Figure 8b: Epi-thermal neutron transmission

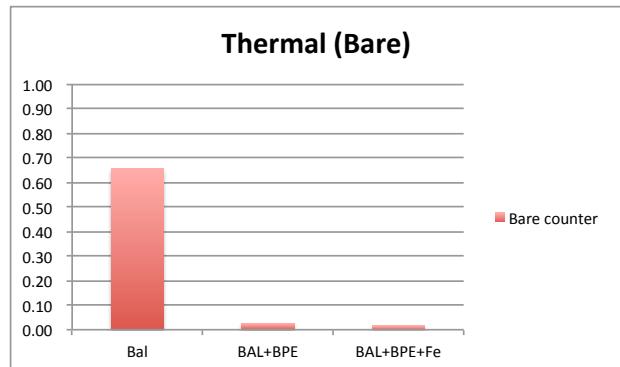
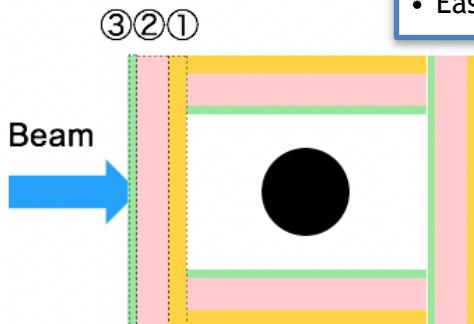


Figure 8c: Thermal neutron transmission

- Created for
- Easy decomposition of background from different directions, e.g. sky-shine vs. reflection from floor
 - Easy setup/evaluation of laminar setups

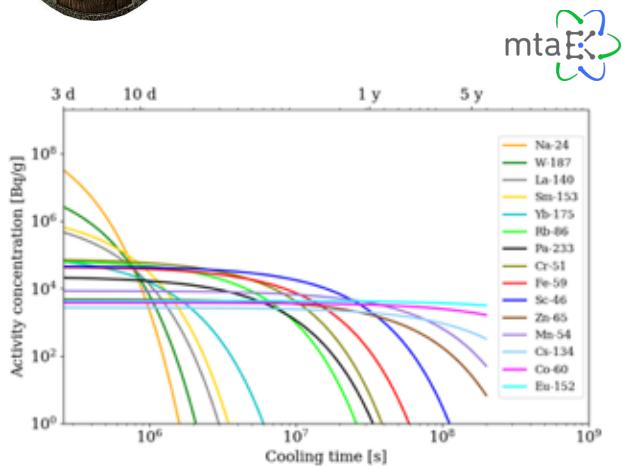


1 Yellow is steel

2 Pink layer is B-PE

3 Green layer is BAI

Task 2 achievements 3: New shielding concepts



- 14 different mineral cast samples were investigated.
- Epument 130 and Epument 145 are comparable to concrete
- Epustone 161 is specially made as a replacement for granite
- Epument is usually without Boron (test samples have 1 and 3 % B4C)



Probennummer	Bezeichnung	Basismineralguss	Modifizierung	Anzahl Prismen
1	171013_1	EPUMENT 130/3 A1	Standard	6
2	171013_2	EPUMENT 130/3 A1	+ 1% Borcarbid auf Komp. C	6
3	171013_3	EPUMENT 130/3 A1	+ 3% Borcarbid auf Komp. C	6
4	171017_1	EPUMENT 130/3 A1	ohne EFA (Opalia)	6
5	171017_2	EPUMENT 130/3 A1	ohne EFA (Opalia) + 1% Borcarbid auf Komp. C	6
6	171017_3	EPUMENT 130/3 A1	ohne EFA (Opalia) + 3% Borcarbid auf Komp. C	6
7	171023_1	EPUMENT 161L St2	Standard	6
8	171023_2	EPUMENT 161L St2	+ 1% Borcarbid auf Komp. C	6
9	171023_3	EPUMENT 161L St2	+ 3% Borcarbid auf Komp. C	6
10	171023_4	EPUMENT 161L St2	+ 1% Borcarbid auf Komp. C (- 1% Komp. C)	6
11	171024_1	EPUMENT 161L St2	+ 3% Borcarbid auf Komp. C (- 1% Komp. C)	6
12	171025_1	EPUMENT 145 B1	ohne EFA (Opalia), ohne Basalt 8-11	6
13	171025_2	EPUMENT 145 B1	ohne EFA (Opalia), ohne Basalt 8-11, + 1% Borcarbid auf Komp. C	6
14	171025_3	EPUMENT 145 B1	ohne EFA (Opalia), ohne Basalt 8-11, + 3% Borcarbid auf Komp. C	6
			Summe	84

Task 3 achievement: Feasibility of Larmor-tech at ESS instruments

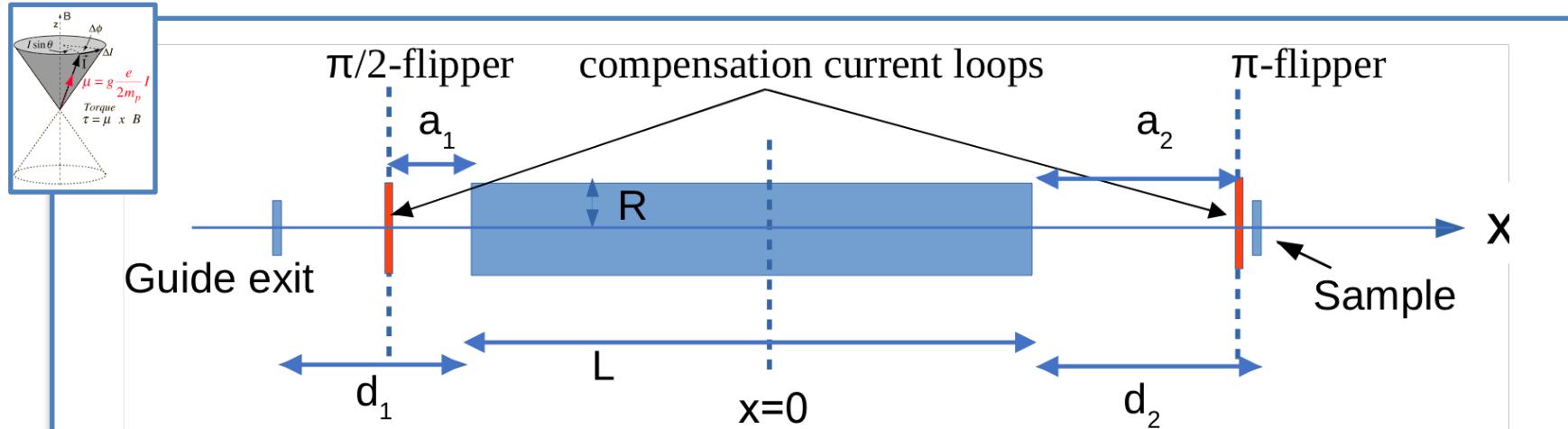


Fig. 1: Schematic representation of the configuration considered for the first arm of a NSE spectrometer. The layout is characterized by the lengths L, a_1, a_2 and R . The blue rectangular area represents the main precession coil.

Results show a clear gain with the “pancake moderator”.
Rectangular beam cross-sections height / width ratio $\sim 1:4$,
ala ESS “pancake moderator” beams lead improved the
homogeneity of the magnetic field integrals by at least 30 %.
Relative inhomogeneities become worse for shorter coils,
in order to reach high resolution, the length of the instruments
cannot be reduced, i.e. not be more compact than e.g. at the ILL.

An IN15-like instrument will have
gain in resolution at the ESS

Task 3 achievement: Feasibility of Larmor-tech at ESS instruments

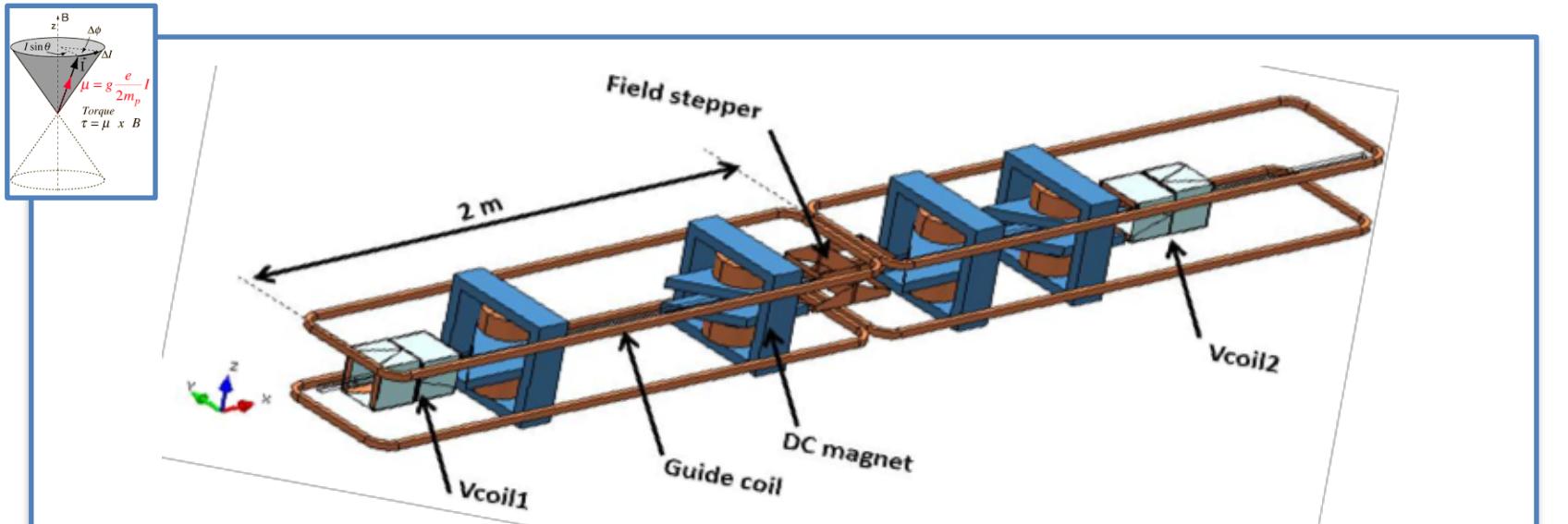


Figure 2: Schematic drawing of SEMSANS arrangement considered for the magnetic field calculations. The white boxes illustrate the Vcoils, which act as $\pi/2$ flippers, the blue components are DC magnets with parallelogram shaped pole shoes, the central coil is a field stepper. The long upper and lower create a homogenous magnetic field, which guides the beam polarisation.

Compact design could be easily implemented as an add-on. Could be installed and removed, according to the experimental requirements and would substantially extend the capabilities of the ESS. Instrument candidate SKADI, would allow simultaneous SANS and SEMSANS. Another candidate is ODIN, add-on to be used for high resolution dark field imaging.

Only practically applicable dark-field method for ESS, by synchronising the fields with the source pulse



Neutrons: Cradle to Grave workshop, Coimbra, Portugal, September 6th 2016

- Requirements/Developments for a (bidirectional) Monte Carlo variance reduction method applied to **neutron beamline transport systems**.

Speaker	Presentation topics	Video link
Peter Willendrup, DTU/ESS	Welcome, agenda, setup (No slides)	(no video)
Erik B Knudsen, DTU	McStas-MCNP interface solutions	Video #1 (partial)
Thomas Kittelmann, ESS	MCPL "Monte Carlo Particle List" interchange format	Video #1
Xiao Xiao Cai, DTU/ESS	NCrystal, coherent scattering library for Geant4	Video #1
Emmanouela Rantsiou, PSI	Code, simulations and experiments including guides at BOA, PSI	Video #2
Douglas Di Julio, ESS	Metaheuristics for Vitess, simulation of laminar shielding problems (Talk cancelled)	(no video)
Phil Bentley, ESS	Neutron acceptance diagram methods	Video #2
Steven Lilley, STFC	Initial experiences using Advantg in fusion and spallation	Video #2
Stuart Ansell, ESS	"MCNP model builder / CombLayer, "fast" beamline constructor, variance reduction. Instrument background calculations for long beamlines at the ESS."	Video #3
Jan Saroun, NPI	RESTRAX/SIMRES reverse tracing, optimisation, McStas <i>reverse tracing</i> prototype	Video #3



Website with talks and videos available at
<http://coimbra2016.essworkshop.org>

(Videos also on [McStas YouTube channel](#))



Workshop 2:



Innovative Simulation Tools, Shielding and Instrumentation 2019 (ISTSI2019) ECNS satellite

Talk title	Speaker
Welcome and SINE2020 / WP8 introduction	Peter Willendrup, DTU/ESS
News from the RESTRAX/SIMRES project, including MCPL support and McStas bindings for SIMRES	Jan Šaroun, NPI
News from the Vitess project including MCPL support	Egor Vezhlev, FZJ
News from the McStas project, including interoperability solutions for SIMRES, Vitess and MCNP	Peter Willendrup, DTU/ESS
Developments in the MCPL software framework	Thomas Kittelmann, ESS
An optimised neutron super mirror patch for MCNP, with applications (ESS-Bilbao)	Esben Klinkby, DTU/ESS
CombLayer-driven MCNP-McStas simulations for simulating instrument signal to noise	Esben Klinkby, DTU/ESS
McStas and Scatter-logger driven calculations of prompt gamma shielding for neutron guides	Rodion Kolevatov, IFE
Studies of relevant design-parameters to enable compact Larmor devices in ESS designs	Katia Pappas, TU Delft
Magnetic field calculations for compact Larmor devices in ESS designs	Michel Thijs, TU Delft
Simulation benchmarks for experiments at the PSI BOA beamline	Erik Knudsen, DTU
Extensions to the Bonner Sphere Spectrometer at PSI, plus experiments and simulation benchmarking for newly developed concrete	Masako Yamada, PSI
Studies of material composition and neutron activation, plus related simulations	Eszter Dian, MTA-EK and Esben Klinkby, DTU/ESS

Holiday Inn St. Petersburg, Russia, June 29th 2019

- a [SINE2020 WP8 "e-tools" satellite event of ECNS2019](#).

The workshop is held as a dissemination activity of the [WP8 workpackage](#) in the [EU SINE2020 Project](#) and is open to all [ECNS2019](#) participants



Website with talks available at
<http://istsi2019.essworkshop.org>



Access to the code, reports, results and examples

<https://github.com/McStasMcXtrace/SINE2020WP8>

README.md



SINE2020WP8

Repository for software and methods developed in WP8 under the EU SINE2020 project



This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 654000

For more information, please visit the SINE2020 website at <https://www.sine2020.eu>

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Questions?