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Abstract

This document entitled "Optimization study of a selected instrument using CombLayer and McStas-MCNPX" presents simulations to assess the expected **sample-position** signal-to-noise for the future BIFROST instrument at the European Spallation Source. For these simulations, we compare a palette of software and solutions developed in SINE2020 WP8.

To the extent possible, the used codes and models have been made available through the SINE2020WP8 GitHub repository at https://github.com/McStasMcXtrace/SINE2020WP8

The instrument and selected tools:

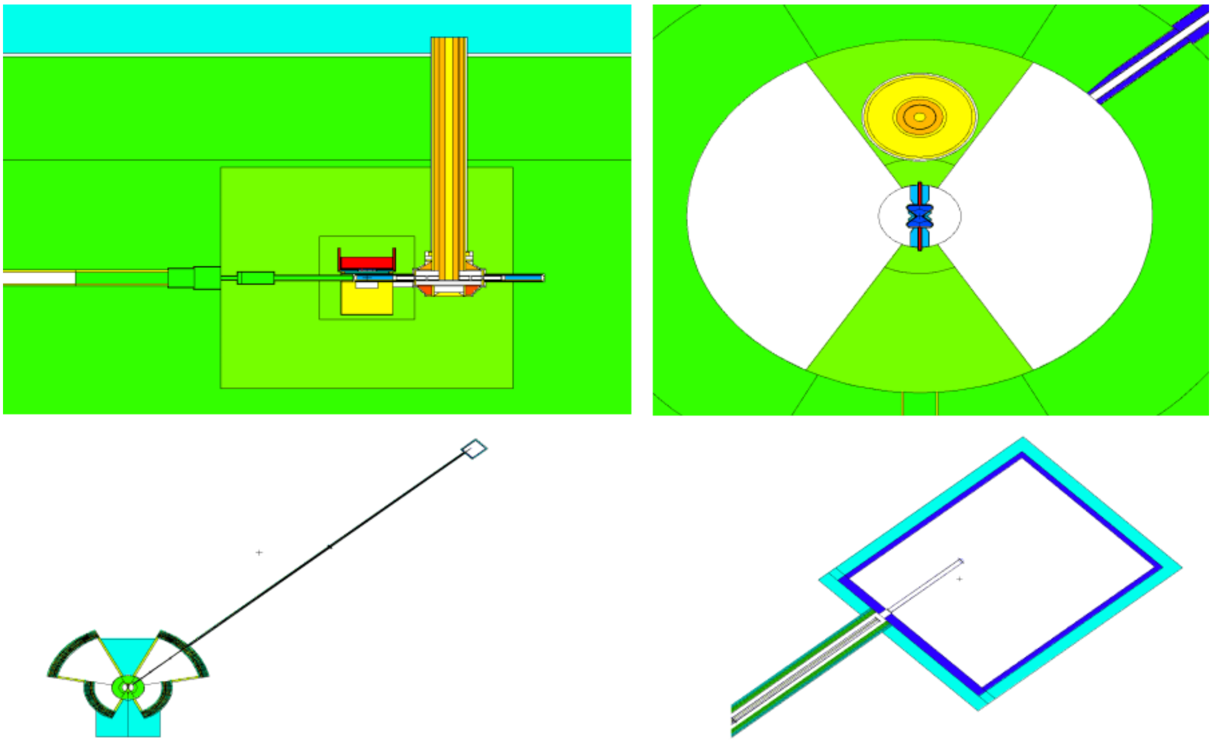
To assess the capabilities of the various coupling schemes developed, the BIFROST instrument at ESS is chosen. The reasoning behind this choice is that BIFROST is a long instrument (150m) and makes use of elliptical guides and therefore ranks among the most challenging instruments to model at the ESS.

The main tools applied in this study are

- Comblayer to drive the generation of the main BIFROST MCNP deck
- MCNP-variants
  - MCNP6.2 including the latest supermirror-patch (see also D8.3)
  - Standard MCNPX/CINDER for activation-induced gamma production
- McStas v. 2.5
- MCPL for transfer events between MCNP variants and McStas
- Geometrical validation through co-visualisation of engineering CAD-drawing and McStas model
- McStas-based shielding logger from Rodion Kolevatov (IFE) to estimate neutron capture along the BIFROST optics

Super-Mirror enabled MCNP (SM-MCNP)

Based on the Comblayer (http://coimbra2016.essworkshop.org/slides/CombLayer_Ansell.pdf) implementation of the BIFROST instrument an MCNP inputfile is prepared as illustrated below



Comblayer derived MCNP model of the BIFROST instrument.

Top left: protons arriving from left - the illustration shows the target (horizontal disk) and target shaft (vertical, orange) as well as the moderator-reflector plug (central, red+yellow). All is encapsulated in steel (green) for shielding purposes.

Top right: cross-section through the central parts of the ESS, showing the (blue) butterfly shaped moderator).

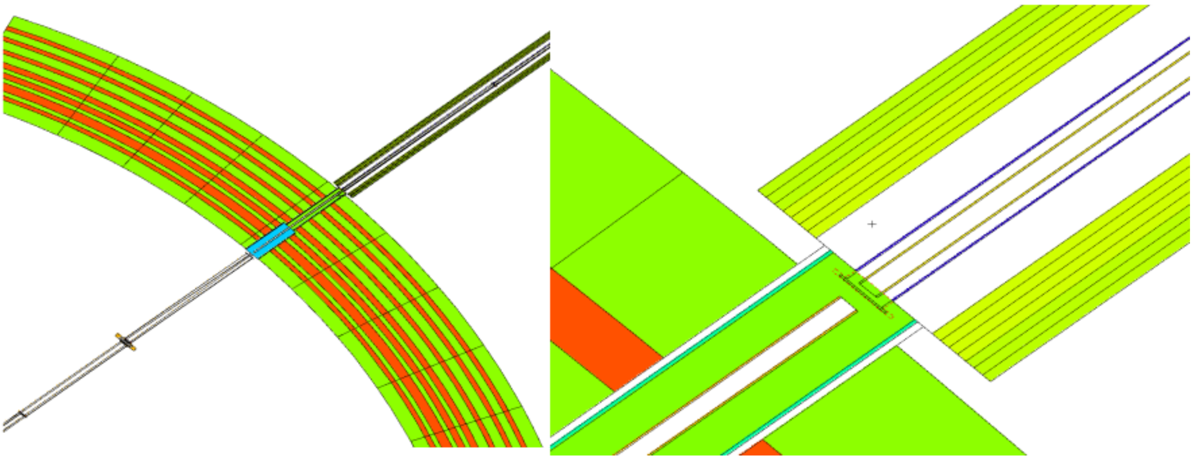
Lower left: birds perspective of the facility, showing the target building and bunker as well as the BIFROST guide and instrument cave.

Lower right: BIFROST Instrument cave

1 Model post-processing

1.1 Remove geometry clashes

Before a functional MCNP model was at hand, several shortcomings of the Comblayer model had to be resolved. In several locations, as shown below, the model exhibit geometry clashes (i.e. areas where objects collide), which must be fixed before the MCNP model can be used to run simulations of the BIFROST instrument.



The penetration of the BIFROST guide through the bunker wall. As seen more clearly on the right-hand zoom, there is a geometry clash (red dotted line) at the location of the start of the first guide section outside the bunker.

1.2 Define supermirror surfaces

Modelling cold/thermal neutron transport in guides using MCNP, is not available in the baseline version of the software. Instead, the work reported here, makes use of the software development reported elsewhere (D8.3) within the SINE2020 scope.

Comblayer does not (yet) include capability to define neutron optics in the code generation stage. Thus, the reflectivity of certain surfaces constituting the neutron supermirrors must be defined by hand in the model post-processing.

To define supermirrors in the MCNP model, the relevant surfaces are identified as well as the cells constituting the interior of the neutron guide. With these, reflectivity of a given guide segment is defined as shown in the below figure insert:

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

Surface 953 uses reflectivity card 1 (second line), for neutrons arriving from cell=4359. Reflectivity card 1 is defined by the parameters: R0=0.99, Qc=2.19E-2, m=4, alpha=6.07 and W=3E-3 (see eg. McStas manual)

1.3 Improving simulation efficiency

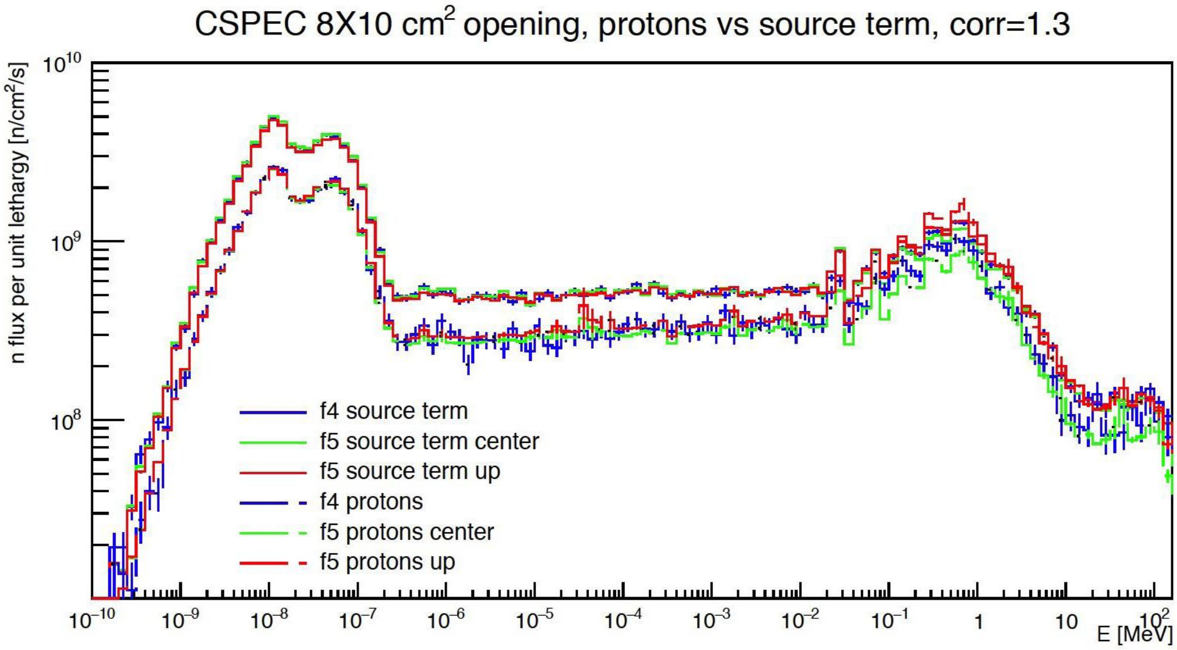
With the above steps, a functioning MCNP model is derived, which models:

- Protons interacting the tungsten target and subsequent creating of spallation neutrons
- Moderating of the neutrons to the thermal/cold regime
- Emission of neutrons through the beam extraction

- Transport of neutrons to the BIFROST cave

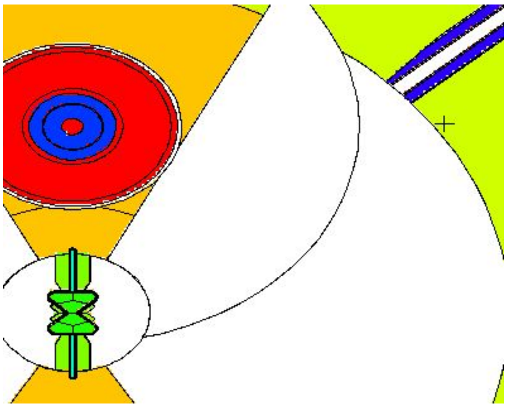
But, the above modelling scheme is exceedingly inefficient, to the extent where it is impossible to gather statistics at the sample position.

Similar challenges are encountered in numerous other modelling tasks at the ESS, and thus a general solution has been developed. Rather than modelling protons on target, dedicated neutron source terms are derived for each instrument-beamport, i.e. describing the neutron phase-space at the neutron guide entrance, 2m from the moderator. The source-term describes the full neutron spectrum (0-2000MeV) making it suitable for the present study, which include both signal and background - see figure below

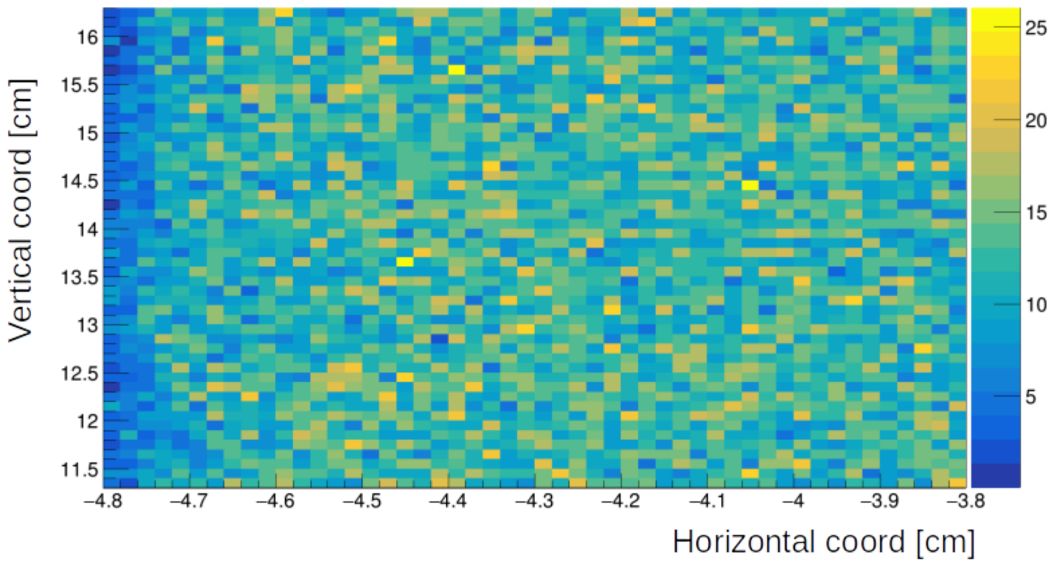


Comparison of neutron flux at the entrance of the CSPEC instruments between proton and neutron based source definitions as explained in the text.

To allow for cross-validation with alternative modeling schemes, below is shown the initial neutron distribution as it appears at the position of the source surface (small insert below).

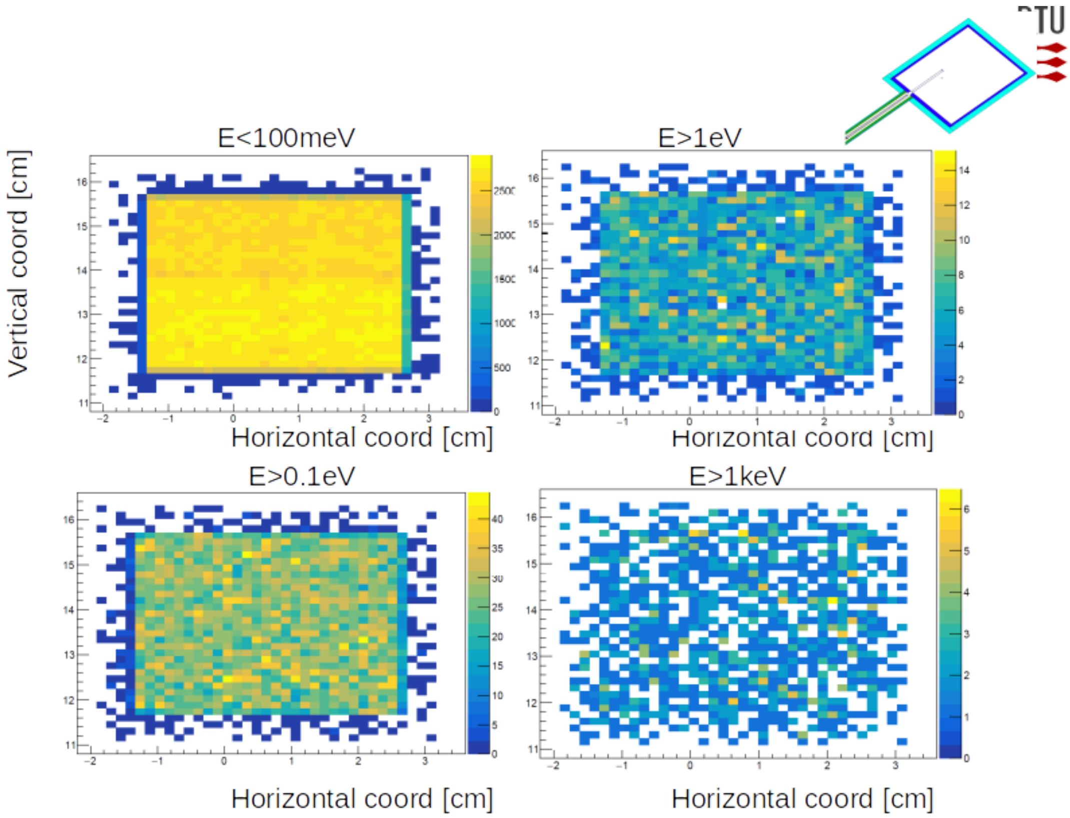


Emission surface at the entrance of the guide (blue, upper right)

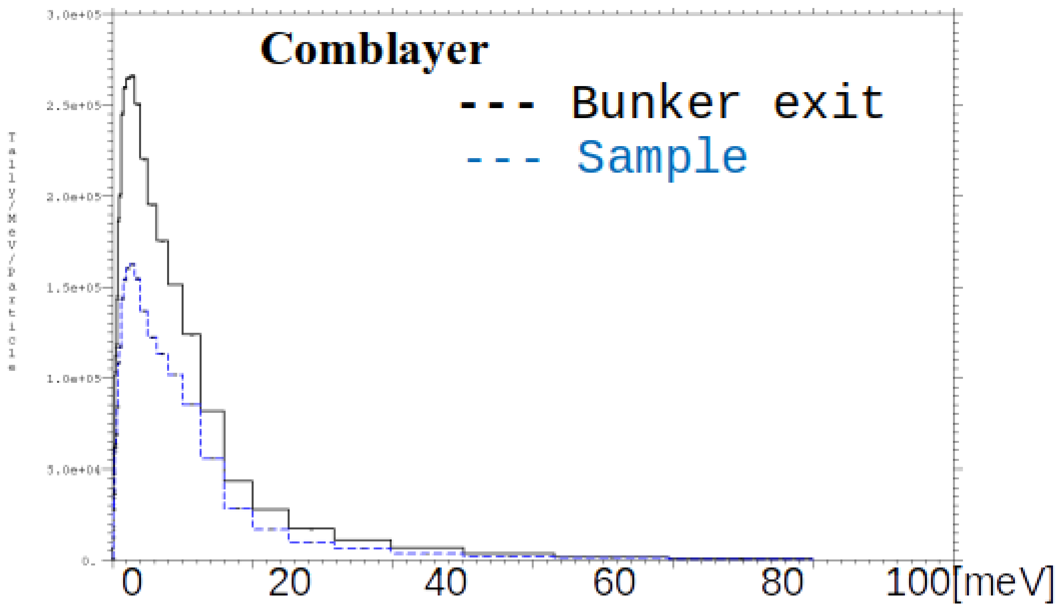


Spatial distribution of neutrons at the emission surface. The integrated flux (0-100meV) is: 1.1E11 n/cm2/s - which is directly comparable to other simulation schemes, as reported below.

After transport in the 150m guide, the corresponding spatial distribution is shown below in the upper left hand corner. The remaining inserts shows corresponding background distributions, for various choices of energy range.



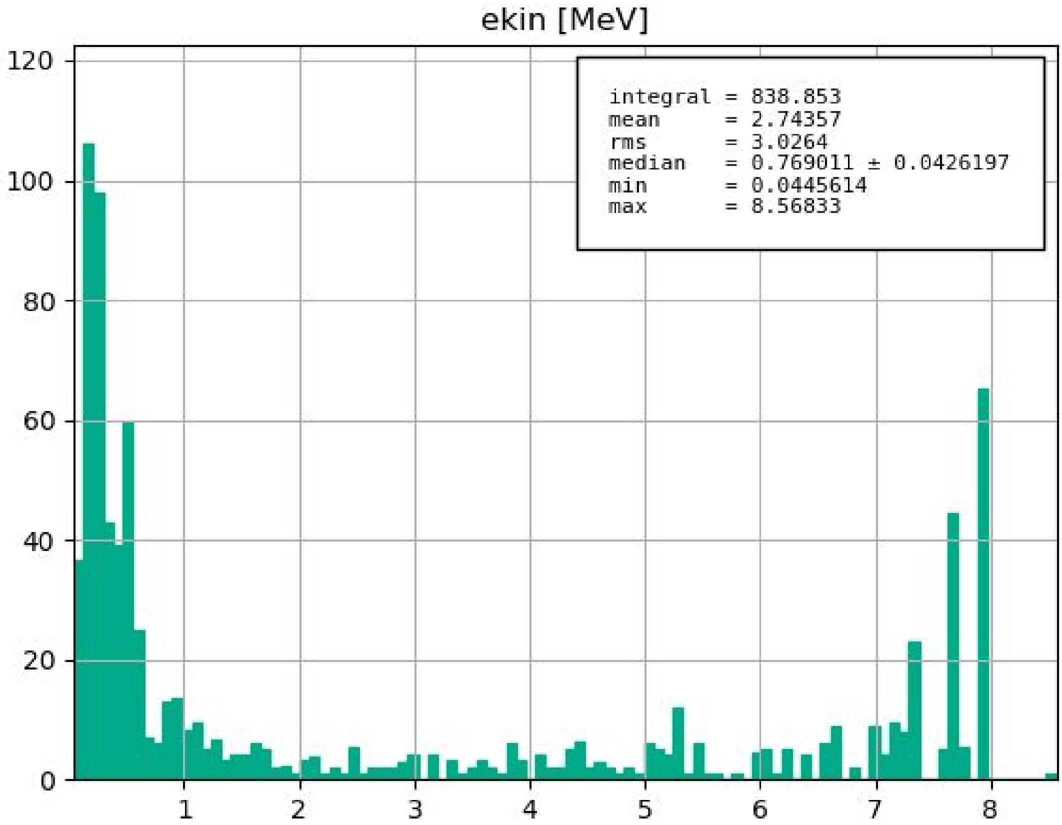
Finally, the below figure shows the spectrum at the sample position, as well as at the bunker exit. The intensity loss during the 150m transport amounts to 37% (0-100meV).



Gamma background

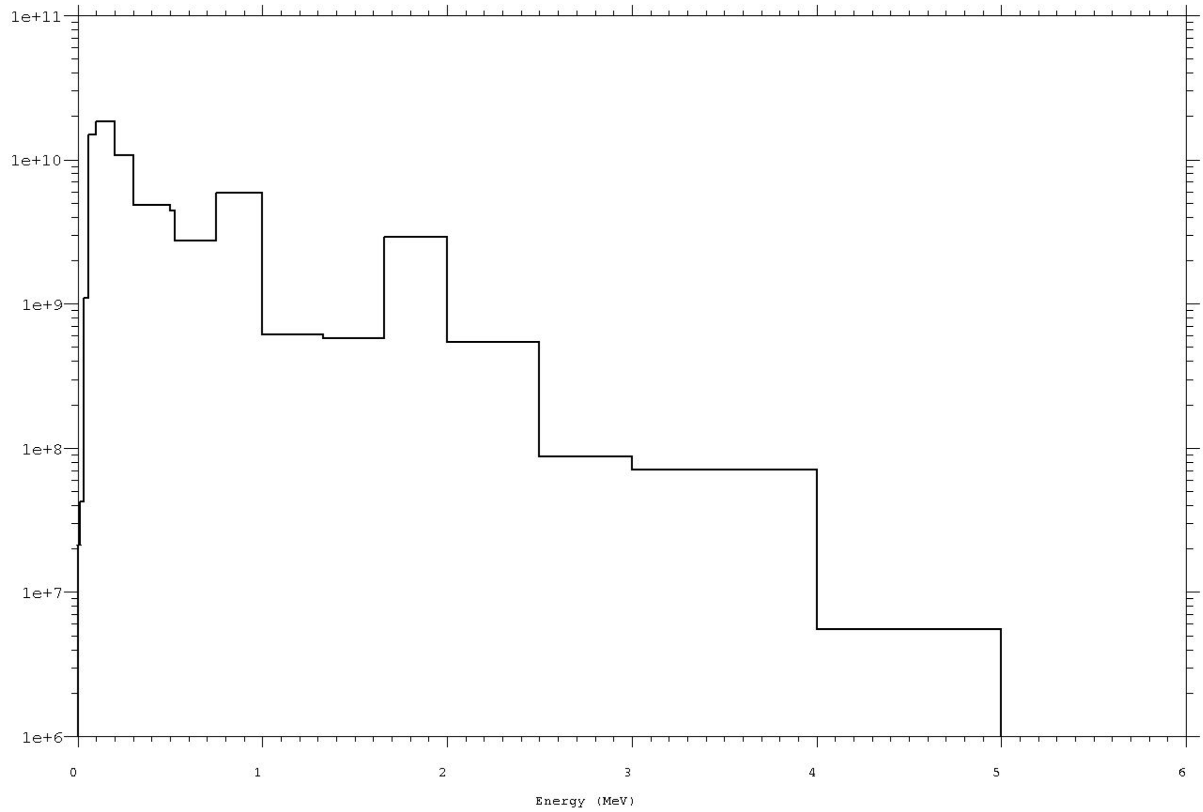
In addition to neutron signal and background that the sample position, also the presence of gamma radiation if of interest.

Gamma radiation can be created by neutron interacting with e.g. structural materials, and are traditionally considered in two groups: prompt gammas and gammas from activation. Simulation-wise, the prompt gamma comes directly with MCNP modeling, and for the present simulations, the gamma spectrum at the sample position is shown here



Prompt gamma spectrum [MeV] at the sample position.

Activation modelling is typically performed using dedicated activation codes, based on input from monte carlo simulations. For the present analysis, neutrons arriving in the instrument cave of bifrost are exported using the SSW functionality of MCNP6. Next the neutron-state file is converted to MCPL and exported to MCNPX where they are used as a neutron source. The MCNPX output in terms of neutron flux in the structural materials of the BIFROST cave is handed to Cinder'90 for an activation calculation. Finally, Cinder'90 tools convert the activation results to a gamma source based on an assumed irradiation and cooling scenario, and a MCNPX simulation is performed to estimate the decay gamma spectrum at the detector position. The resulting spectrum is shown below (arbitrary nomalization).

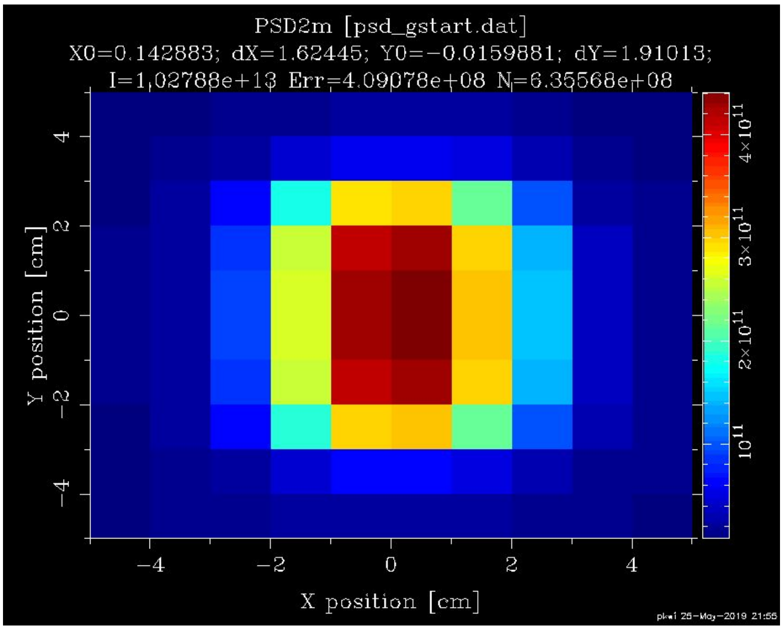


Spectrum of activation gamma's at the detector position in the instrumental cave of BIFROST during operations (i.e. no cooling time applied).

MCNP-McStas coupling.

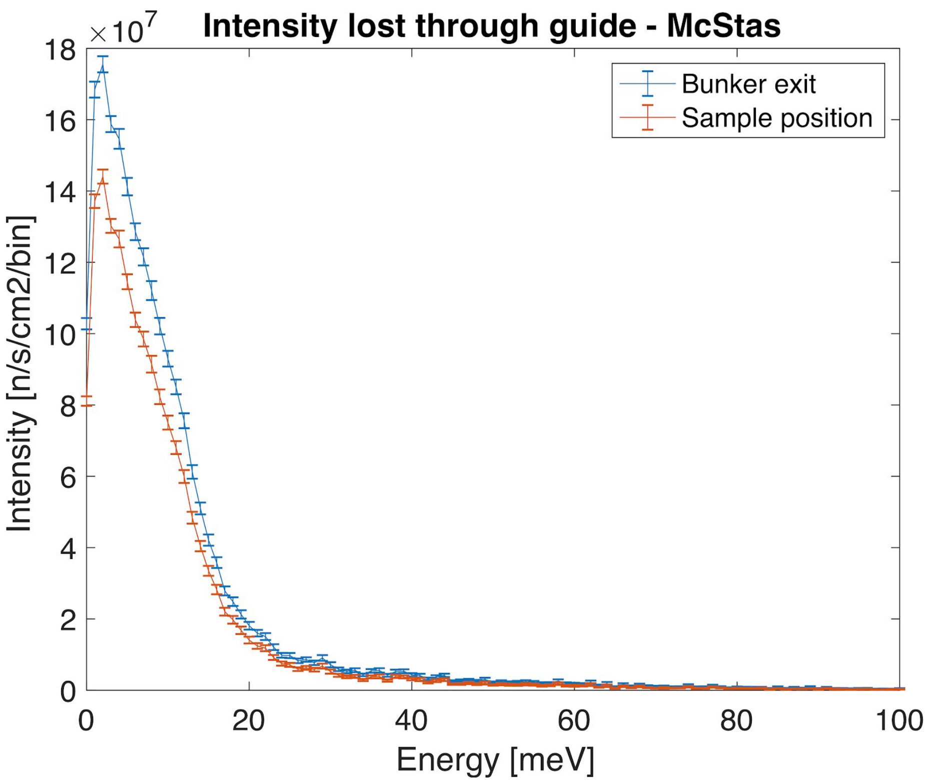
As an alternative modelling approach to the MCNP-only described above, a coupled MCNP McStas simulation was carried out. As in the above, MCNP proton on target simulations constitute the first step. Rather than deriving a dedikated beamline specific MCNP source at the guide entrance, the neutrons are simply handed to McStas, through the recently developed MCPL interface [1]. This coupling allow the individual neutron state parameters as determined at a given surface in MCNP to be stored on disk and used as a source in a subsequent McStas simulation.

For validation purposes, it is useful to visualize the location of the source neutrons at the guide entrance as reported by McStas.



The intensity recorded is 1.0E11 n/cm2/s (0-100meV) - to be compared to the 1.1E11n/cm2/s found using MCNP (see above).

After transport through the Bifrost guide system, the spectrum at the sample position is compared to the spectrum at the bunker wall below, in the same manner as for the 'pure' MCNP calculation.

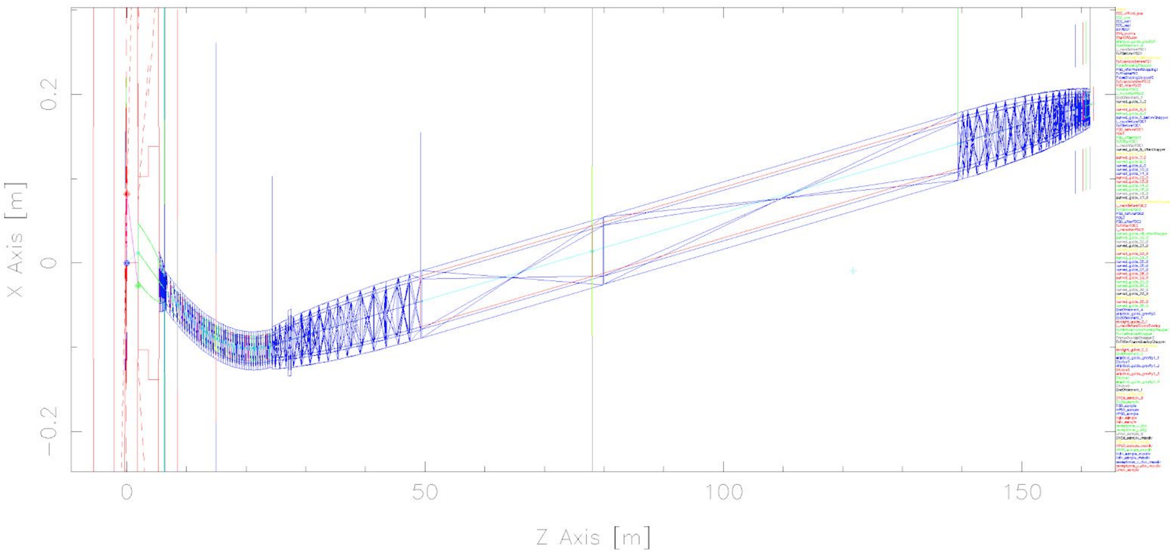


Neutron energy spectrum at the bunker exit (blue) and at the sample position (red) using the MCNP-McStas coupled simulation described in the text.

The spectrum observed in the MCNP-McStas coupled simulation is similar to that of the SM MCNP simulation shown above. 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 geometri - in the SM MCNP case the geometry is inherited from its Comblayer implementation, whereas the McStas geometry originate from the instrument team directly.

Geometrical model-validation.

The Comblayer/MCNP model was based on engineering drawings from the ESS. The McStas model however originated from a GuideBot[2] model, which as manually adjusted and gave input to the engineering mode. Hence it was necessary to ensure geometrical agreement between e.g. the engineering model and the McStas model. Thus, the engineering CAD drawing in CATIA format was first converted to STL[1] and finally to OFF[2] format which can be read and visualised in McStas. The figure below shows a good agreement (of order a few cm over the 150 m) between engineering CAD model and McStas model.



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.

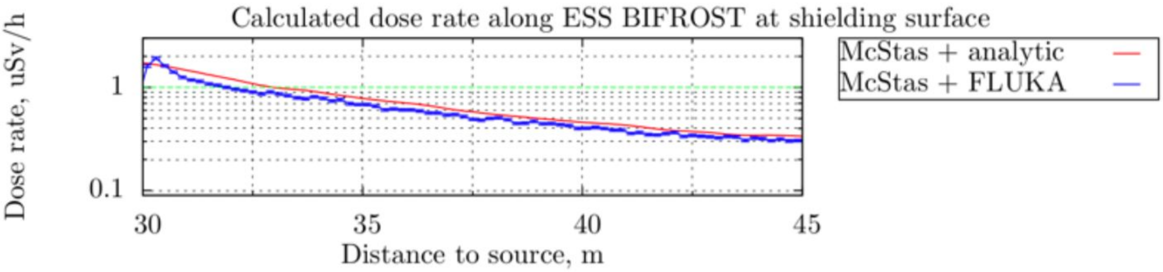
Gamma-production estimates through Shielding logger

Dr. Rodion Kolevatov from IFE has not been directly involved with the SINE2020 WP8 work, but has been working on shielding aspects of BIFROST as part of the Norwegian in-kind involvement with ESS. In connection with this work, Dr. Kolevatov has devised a method[3] to estimate gamma-production in supermirror-coatings, resulting radiation dose-rates and needed shielding. The method is based on processing the 'lost' intensity in McStas, that is

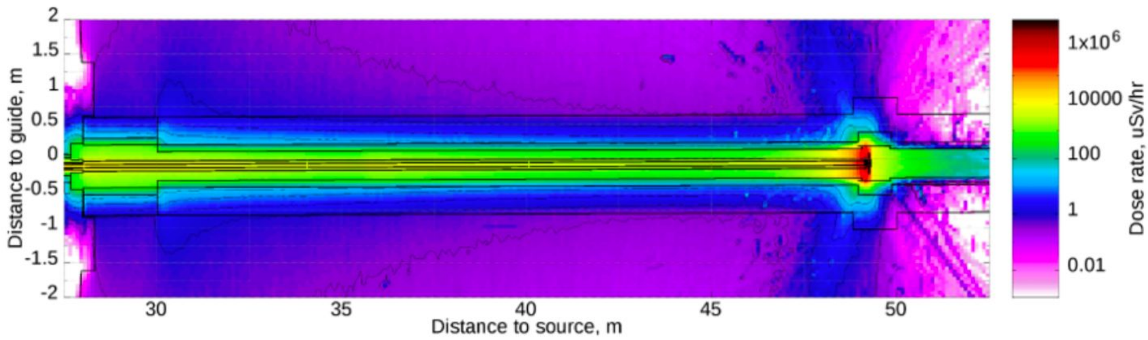
[1] STL conversion was performed within CATIA
[2] STL to OFF conversion was performed in FreeCAD

the non-reflected portion of the neutron beam, and uses the principle of the so-called scatter logger[4] by the authors of this deliverable report.

Recently Dr. Kolevatov contributed to the SIN2020 WP8 workshop *ISTSI2019*[5],[6] and announced the availability of easy-to-use McStas-based components implementing the abovementioned method, and we hence found it natural to mention this development in the context of our related deliverable report. The figures below are reproduced from [6].



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.

References

[1] 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

[2] Bertelsen, M 2017, 'The automatic neutron guide optimizer guide_bot', Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment, vol. 867, pp. 195-203. https://doi.org/10.1016/j.nima.2017.06.012

[3] R. Kolevatov, C. Schanzer, P. Böni., Neutron absorption in supermirror coatings: Effects on shielding, Nuclear Instruments and Methods in Physics Research, Section A: Accelerators, Spectrometers, Detectors and Associated Equipment — 2019, Volume 922, pp. 98-107 https://doi.org/10.1016/j.nima.2018.12.069

[4] E. B. Knudsen, P. K. Willendrup, E. B. Klinkby, McStas event logger : Definition and applications, Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment — 2014, Volume 738, pp. 20-24 https://doi.org/10.1016/j.nima.2013.11.071

[5] See the workshop website at http://istsi.essworkshop.org

[6] R. Kolevatov, McStas and Scatter Logger driven calculations of prompt gamma shielding for the neutron guides, submitted, to appear in Journal of Neutron Research

Acknowledgements

The development and use of the software in WP8 spans beyond the WP partners, and we would thus like to express our gratitude toward

- Thomas Kittelmann, ESS who is the main developer of the MCPL software.(MCPL was jointly supported by the BrightnESS (GA No 676548) and SINE2020 (GA 654000) Horizon 2020 projects.
- Rodion Kolevatov, IFE has developed a set of easy-to-use McStas models for estimating dose rates and shielding requirements which is now available together with the WP8 developments.