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Abstract

The title of this deliverable report is "Improved user interface", but should not be taken too literally - we are not as such developing user interfaces to the expert codes that the work in WP8 is based on. Rather, we have focused on:

a) providing worked and documented examples and use-cases and examples of expert codes.
b) developing interfaces between expert codes.

This way we maximize output from the work package and provide long term maintainable tools for users. In practice we are providing the users with an interface to all of our developed software solutions and methods to date, facilitated by a new GitHub repository with example datasets and thorough documentation at https://github.com/McStasMcXtrace/SINE2020WP8.

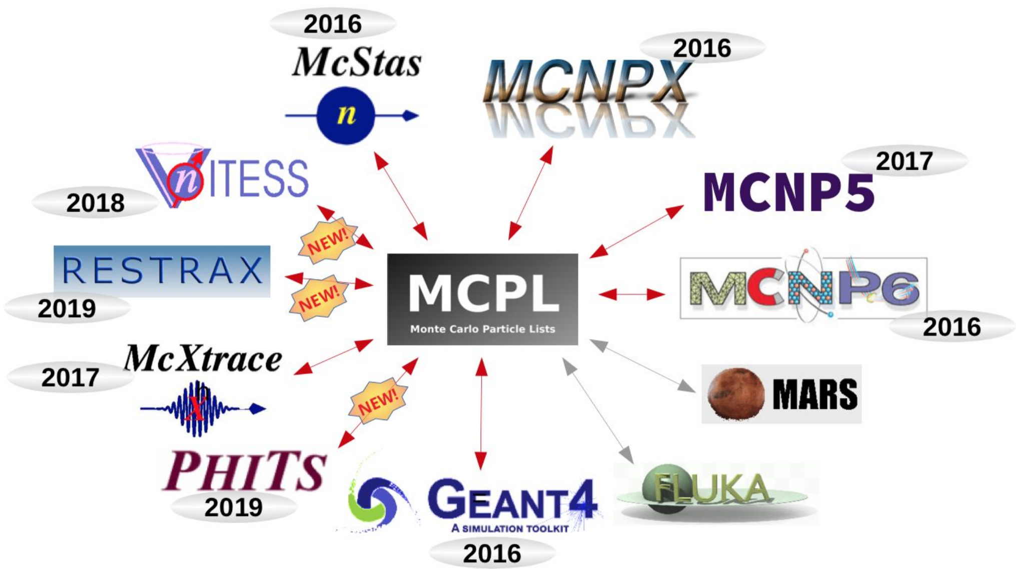
The developed solutions

The most easily applicable product of our WP is the MCPL event interchange software (see D8.2), for which support has been implemented in several softwares (see D8.2, D8.8 and D8.18) and used to solve a number of WP tasks (see D8.4, D8.1 and D8.13).

Supplementing the nice documentation readily available for MCPL (see https://mctools.github.io/mcpl/ and the related open access publication[1]), we have decided to make a number of practical examples of the use of MCPL available through our WP GitHub repository at https://github.com/McStasMcXtrace/SINE2020WP8.

Softwares supporting MCPL usage

Since the 2016 release of MCPL, a number of softwares currently support event exchange, see Fig. 1 taken from the ISTSI2019 presentation by Thomas Kittelmann, ESS.



MCPL usage examples

In the deliverable report at hand we will show a number of MCPL usage examples, to illustrate the flexibility and versatility of the MCPL solutions:

1) MCNP-based ESS source terms for use with McStas.
In connection with the assessment of the effect of new ESS source characteristics on instrument performance, a series of MCNP calculations were done for most of the ESS beamlines. The output in each case was an MCPL file containing individual neutron (and gamma etc.) events reaching a given beamport (as illustrated in Figure 1). These beamport-files have been made available through a dedicated website at the ESS DMSC: http://public.esss.dk/users/willend/MCPL/. Together with the McStas template instrument ESS_butterfly_MCPL_test.instr which has been distributed with McStas since release 2.4.1 (2016), the simulated MCNP neutron events can be transported along neutron guides in the McStas software.

The filenames of the event files reflect ESS instrument sector and beamport number, e.g. the BIFROST instrument will be placed in the West sector on beamport 4 and should thus use W4.mcpl.gz. Each of the event files are around 3-6Gb in size, are based on 1e5 protons on target. (The corresponding neutron production is a Dirac deltafunction in time, and thea actual ESS pulse timing and correct normalisation is generated in the McStas code.)

To be as realistic as possible and to allow multiple usage applications, the files Include multiple particle types, i.e. neutrons, gammas, protons and muons etc., and particles can have "any" physical energy, i.e. up to the linac proton energy. Further the particles originate from "anywhere" within the ESS target monolith, but of course mainly from the target, moderators and their surroundings. For a full description of the model and its use, please refer to the dedicated ESS Confluence webpage[2].

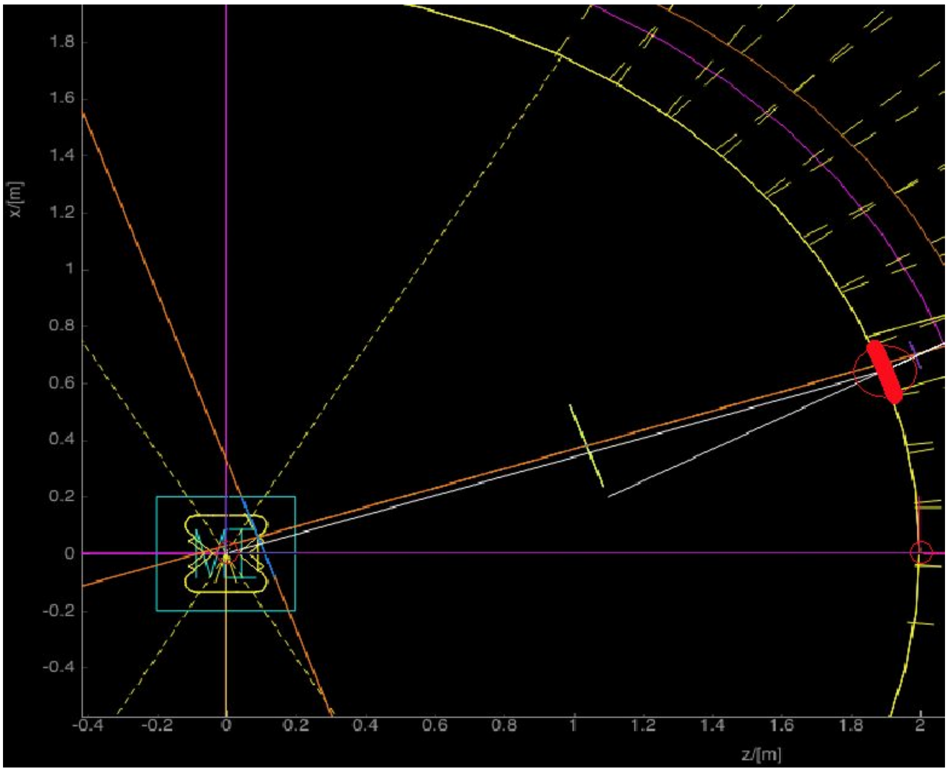


Figure 1: Visualisation of events in the file W8.mcpl.gz within the ESS_butterfly_MCPL instrument. The coordinate system of choice is the TARGET coordinate system.

To ensure agreement with analytical models of the ESS moderators available in McStas, neutrons transported through a simple curved neutron guide on beamport W8, using both the analytical and MCPL-based ESS source models. As can be seen in Figures 2 and 3, the agreement is very good.

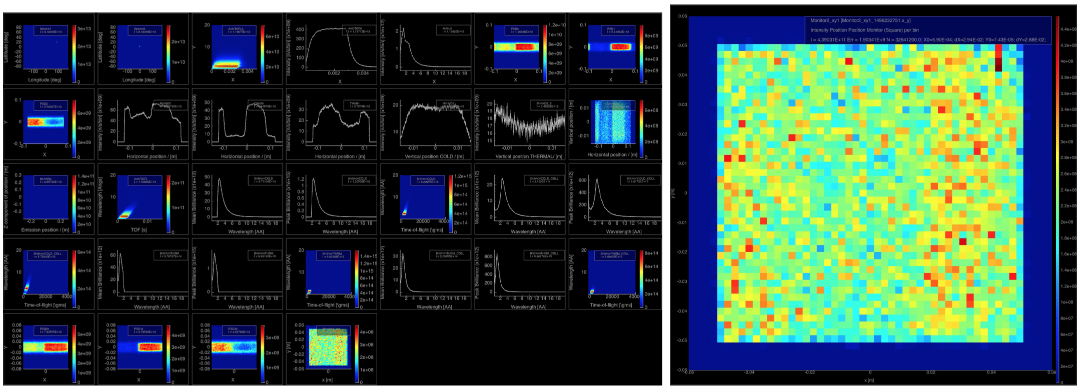


Figure 2: Output from the MCPL source: - overview plot and "end of curved guide" PSD for the W8 beamline.

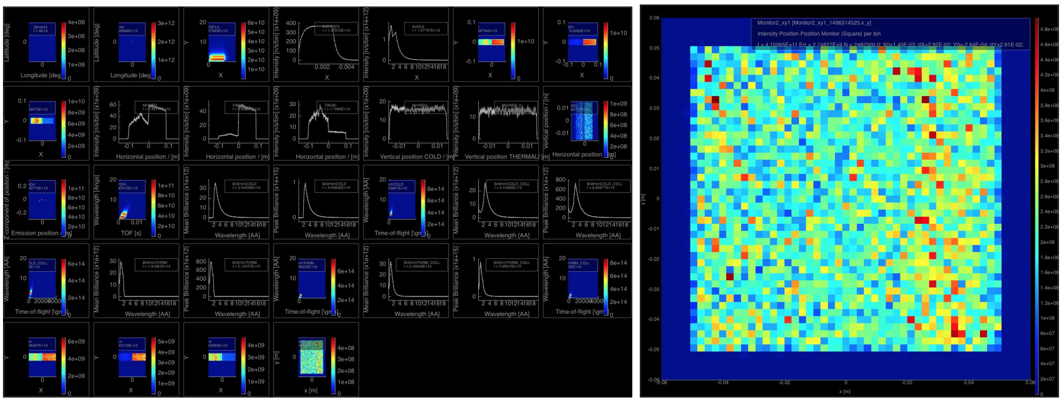


Figure 3: Output from the analytical ESS source: - overview plot and "end of curved guide" PSD for the W8 beamline.

2) MCNP-based HIFR source terms for use with McStas.

In collaboration with Igor Remec from the neutronics group at ORNL in the US, a set of MCPL-based beamport files were produced for the HIFR reactor upgrade. Figure 4 below, shows various beam properties as visualised when the events are transported in McStas.

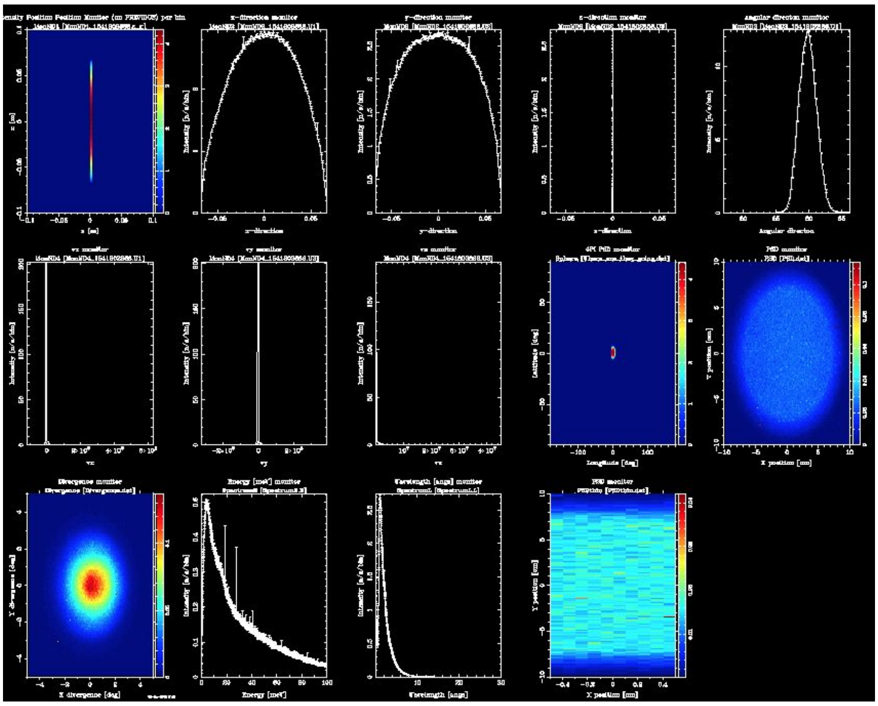


Figure 4: MCNP output from the HIFR source available for transport in McStas.

3) Geant4-based detector model used with McStas input data.

In connection with detector developments for the LoKI SANS beamline at ESS, MCPL files were used for transferring output from a McStas model of the beamline, including a simulated sample to a realistic Geant4 model of the detector. Figure 5 contains figures reproduced from [1] which is referred to for further details.

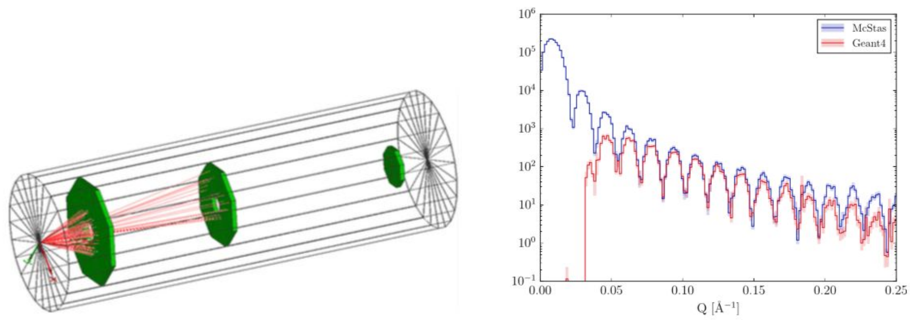


Figure 5: Left: Geant4 model of a complex, hexagonal detector originally envisioned for the LoKI instrument. Neutrons from the sample hitting the active detector area appear in red. Right: Raw Q distribution for a subset of the LoKI detectors (middle detector bank shown right). The McStas post-sample output appears in blue, while the distribution calculated from the simulated measurements in Geant4 appears in red.

4) Transfer of functionality from McStas to Vitess.

MCPL was further applied in to enable users of the Vitess software[3] to work with updated models of the ESS source from McStas, as Vitess was at the time (2017) not considered actively developed. In this solution, the general mcstas2vitess script was used to create Vitess modules containing MCPL_input.comp, MCPL_output.comp and ESS_butterfly.comp from McStas. Full details of the solution can be found at a dedicated ESS Confluence page[4].

Luckily Vitess has now been revitalised by the employment of Klaus Lieutenant at FZ Jülich, and since v. 3.4 of Vitess, the software now readily includes all of the above functionality.

5) SIMRES-McStas Simulations of the BEER instrument.

An advanced example is included with the newly released SIMRES version 6.4.0[5] based on the proposed BEER instrument at ESS. IN this example:

1. The primary spectrometer is simulated using a reverse Monte Carlo procedure in SIMRES.
2. The sample (a powder) in simulated with McStas
3. The secondary spectrometer using a forward Monte Carlo process in SIMRES.

In between steps 1,2, and 3 is an interface layer of simple intermediary MCPL-files. This advanced example is striking for several reasons: 1 for its use of reverse Monte Carlo which in cases like this may speed calculations up by O(3). 2. for its automated interfacing to McStas, through the mechanism developed in D 8.8? . Lastly the combination is completely automated to run within the SIMRES regular user interface as shown below.

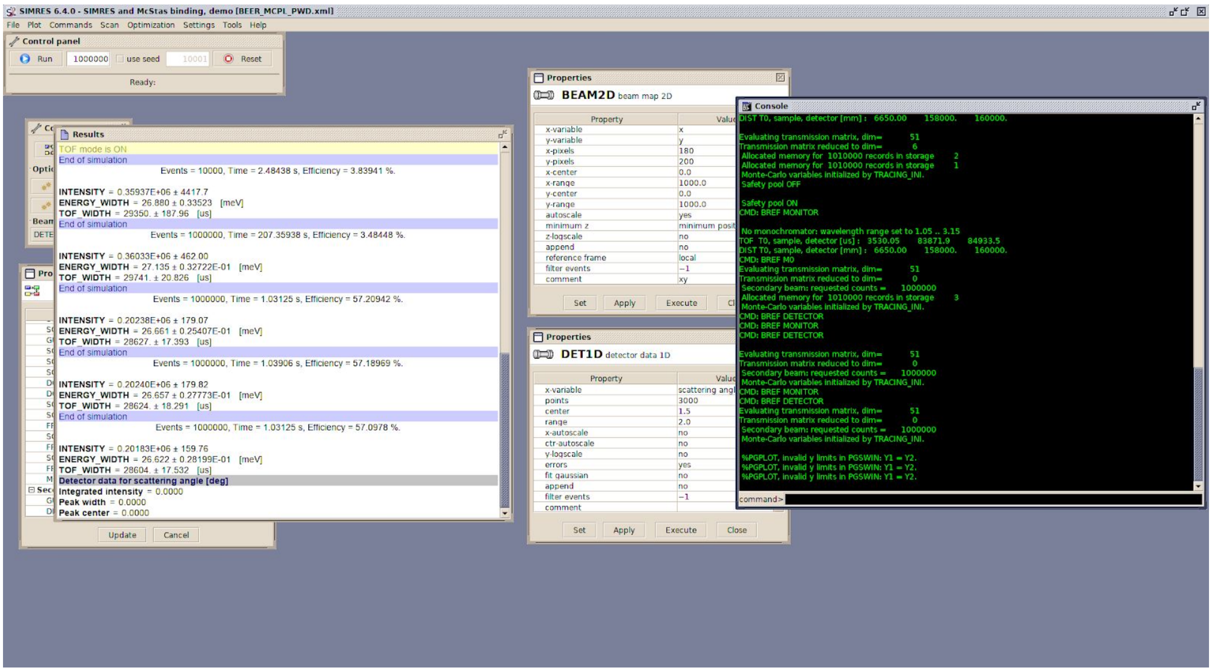


Figure 6: The main window when running SIMRES.

Running the simulation as described in section 6 in the SIMRES user manual[5], results in a powder diffraction signal as:

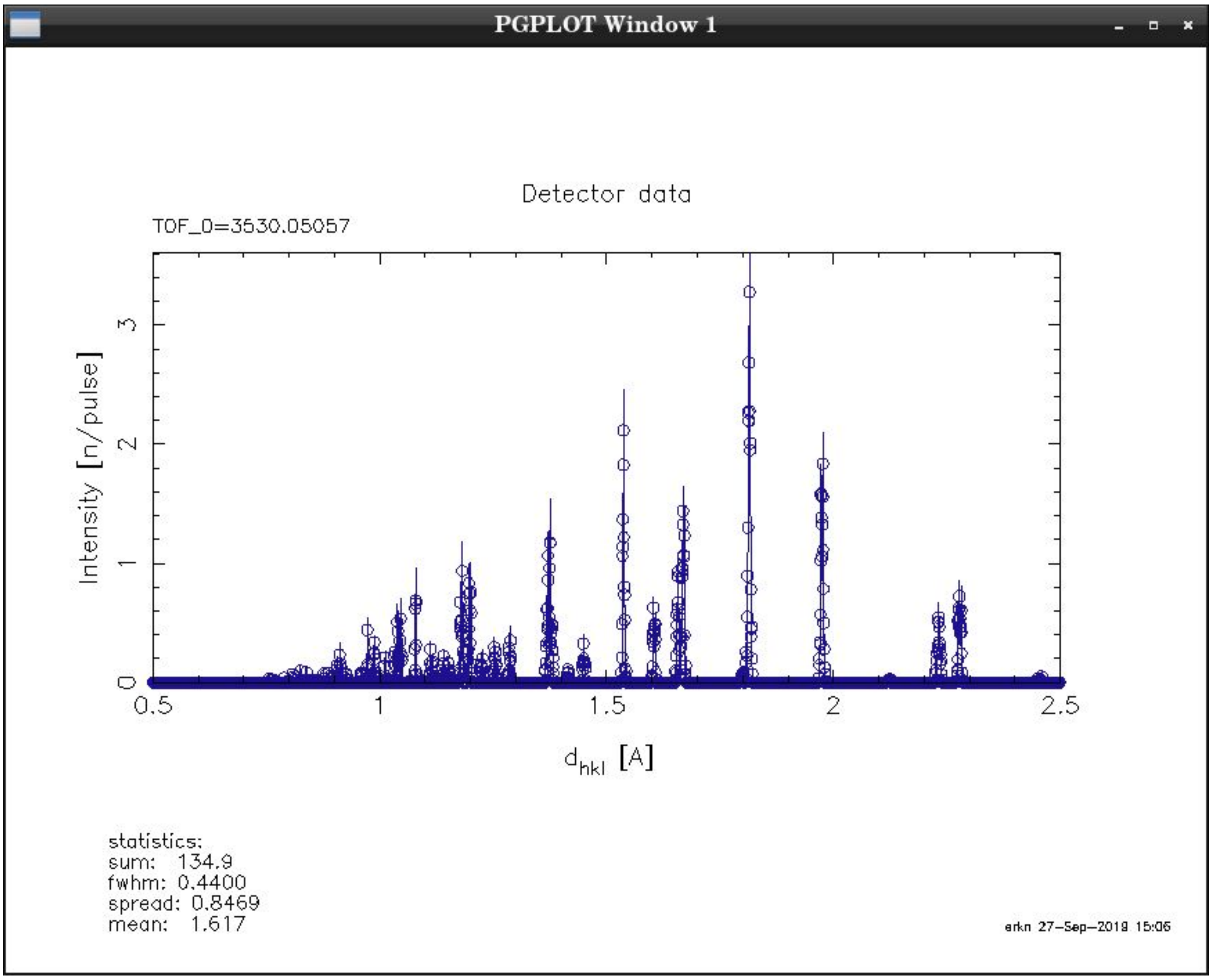


Figure 7: Neutron scattering signal from a duplex steel powder sample, simulated by the SIMRES-McStas-SIMRES pipeline developed in WP8.

Supposing the sample is replaced by a different powder, we simply need to replace the reference to the ".laz" file in the script running SIMRES with an appropriate similar .laz file containing nuetron scattering structure factors for the new sample material. For instance, if we replace the deafult sample with LiF we arrive at the following pattern.

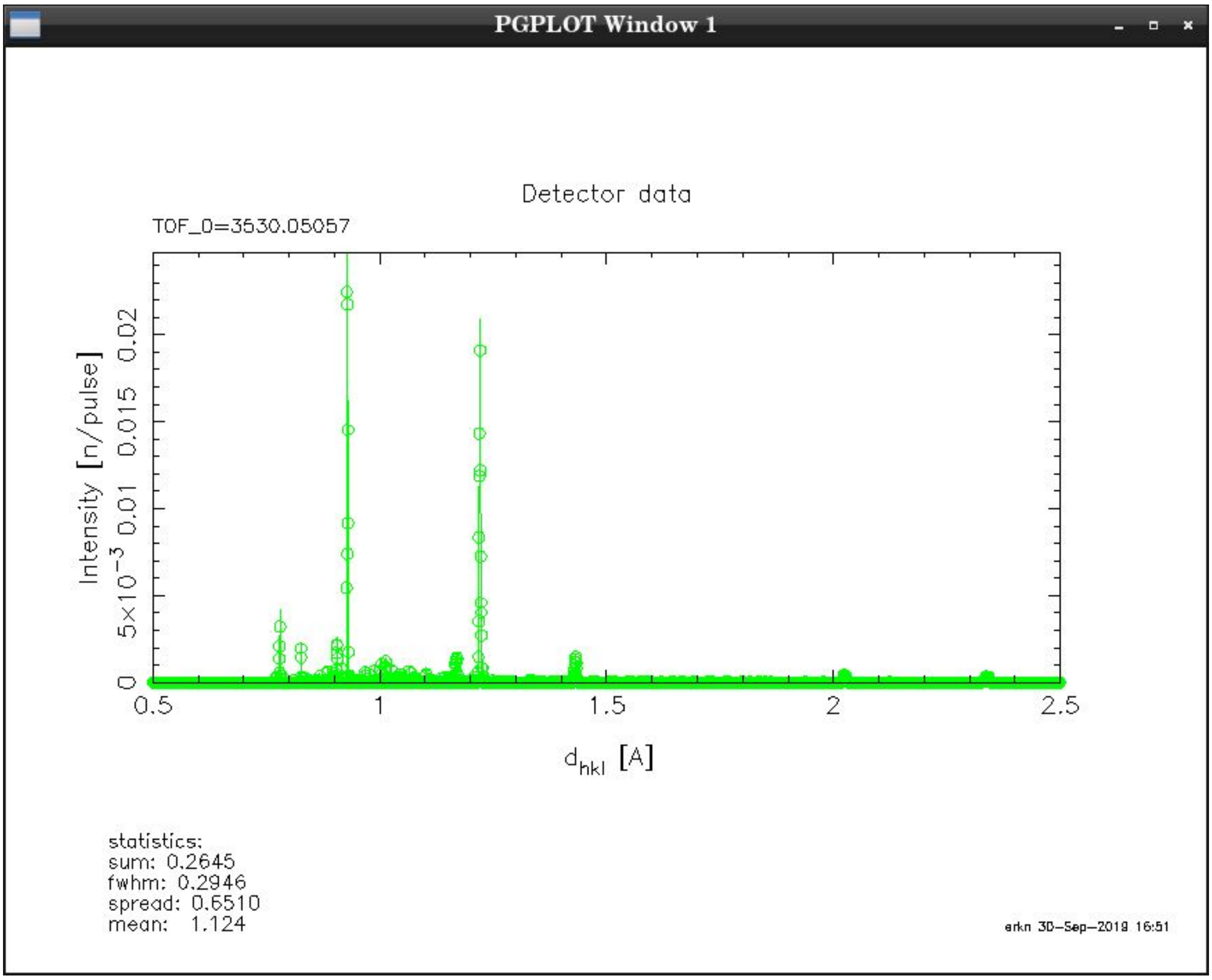


Figure 8: Neutron scattering signal from a Lithium Flouridel powder sample, simulated by the SIMRES-McStas-SIMRES pipeline developed in WP8.

The switch is easily performed by (in the automated run script distributed with SIMRES) replacing the line “sample.mcstas=duplex.laz” with “sample.mcstas=LiF.laz”.

To conclude, we note that these simulation required < 1 min complete runtime on a standard laptop computer. Not bad, considering that this may be seen as a simulation of complete instrument.

6) Scatter logger with MCPL

This example shows how to use the Scatter logger interface to McStas to extract information about neutron intensity lost in the walls of a neutron guide. In this case the definition of *lost* is intensity that is *not reflected* at the guide wall surface. This is important to keep in mind. McStas in general treats reflectivity phenomenologically as something that happens on the mirror surface plan - i.e. there is no distinction of which surface layers reflect what (and at what depth) in a suppermirror setting [6].

As a very simple first example of such use - we here plot the escape vectors for the first 2000 neutron events for a standard m=1, 10 m straight guide which is illuminated by a 5 Å neutron source with 1% bandwidth. For clarity we have scaled the velocity vectors’ length by 1/1000.

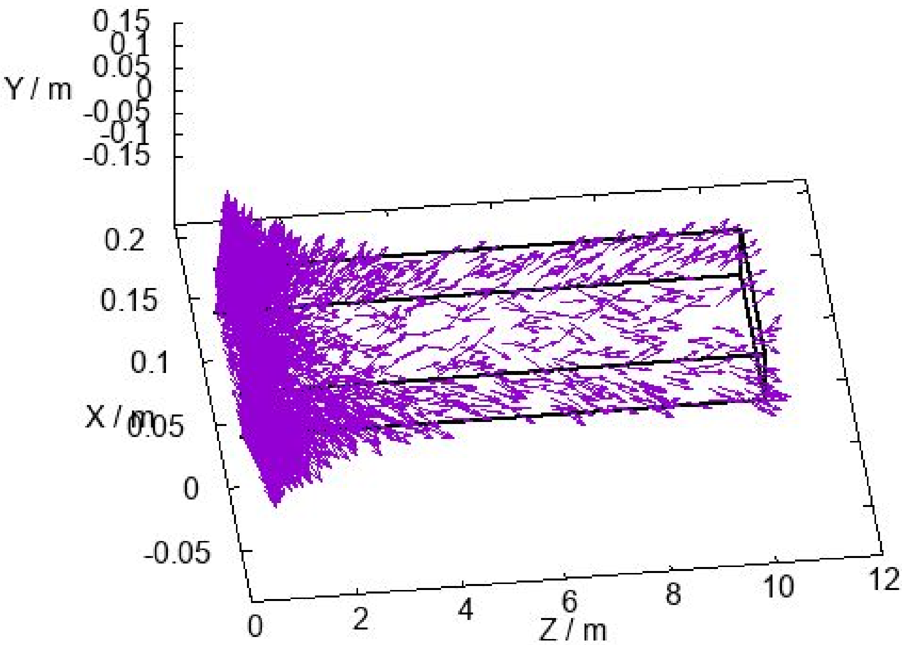


Figure 9: Velocity vectors of neutron events that escape a straight 10 m guide, at the points where the guided rays are reflected in the guide supermirrors.

Some care needs to be taken when interpreting this kind of plot as it does not directly correspond to the lost intensity, merely the statistical events which may be processed further to reveal what intensity is lost where. The simulation calculates the point along the guide where a neutron ray is reflected and with what intensity lost. These data points are logged and later revisited to generate a set of neutron rays which is saved to an MCPL-file. Such events can then further be processed using dedicated software to provide a handle on for instance shielding characteristics.Recent results developed by R. Kolevatov [7] show that such data can be transformed into gamma ray generation estimates in realistic guide settings.

In outlook, it is conceivable to generate geometrical object directly from the data in an MCPL-file that describe surfaces in MCNP and fluka to ease the transition between neutron scattering simulation codes such as McStas and VitESS and the more general codes like MCNP and fluka.

References

[1] Kittelmann, T., Klinkby, E. B., Bergbäck Knudsen, E., Willendrup, P. K., Cai, X. X., & Kanaki, K. (2017). Monte Carlo Particle Lists: MCPL. Computer Physics Communications, 218, 17-42. https://doi.org/10.1016/j.cpc.2017.04.012

[2] https://confluence.esss.lu.se/display/MCSTAS/Using+MCPL+as+source+term+in+McStas

[3]https://www.helmholtz-berlin.de/forschung/oe/em/transport-phenomena/neutronmethods/vitess/index_en.html
[4] https://confluence.esss.lu.se/pages/viewpage.action?pageId=238390110

[5] http://neutron.ujf.cas.cz/restrax/#

[6] Kolevatov, R., Neutron absorption in supermirror coatings, Journal of Neutron Research, 2012

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

Acknowledgements

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- Erik Iverson and Igor Remec from the ORNL neutronics group have found several applications of MCPL in their work, and helped disseminate its use also in the US.
- Klaus Lieutenant (formerly HZB, now FZ Jülich) has implemented support for MCPL in the Vitess code.
- 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.