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Abstract

The possibility to combine capabilities of two ray-tracing programs, McStas and RESTRAX, in one simulation were exploited within the task 8.12. Utilities allowing to redirect ray-tracing process to/from McStas simulation have been developed in SIMRES (the ray tracing program from the RESTRAX project). The method builds on the Monte Carlo Particle Lists format library (MCPL), which enables binding of the programs without extra costs for porting codes and maintenance of interfaces. The development chains and working environments of both the programs can therefore remain completely independent. This report documents the method and shows four use examples, where this technique brings substantial benefits to users, including large improvement of simulation speed and the possibility to employ a wider choice of component models by both programs. Beamline configurations which could not be simulated so far by either of the programs due to the lack of suitable components or simulation speed become thus feasible.

1. Introduction

Development of several neutron ray-tracing software packages started independently in 1990's, motivated by (i) availability of sufficient CPU power provided by commonly available personal computers and (ii) growing demand for simulation support in instrumentation upgrade programs taking place at large scattering neutron centers. In Europe, three such packages have been developed till present: McStas, Vitess and SIMRES (the ray-tracing program from the RESTRAX package). McStas became clearly the most used one and de facto a standard tool for neutron ray-tracing simulations. At the same time, it has been recognized that development of the other simulation packages is not a mere duplicity of efforts. It provides an important added value in several ways:

- 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.

The purpose of the task 8.12 was to better exploit synergy effects arising from the possibility to combine McStas and SIMRES in a single simulation. The expected benefit consists in much higher simulation speed provided by SIMRES especially in simulations of the primary beam with tight collimation and small gauge volumes. At the same time, using McStas to simulate the secondary beam allows to employ the very large library of sample and monitor models, which are not available in SIMRES, as well as high configurability allowed by the McStas meta-language framefork. The work carried out within this task included development of necessary features in the SIMRES code and providing users with a documented example, which demonstrates the method and serves as a template usable by the neutron community in their own projects. The program code and documentation will be distributed as a part of the next SIMRES release.

2. METHOD

The main instrumental allowing for the combination of neutron ray-tracing codes in one simulation is the Monte Carlo Particle List (MCPL) library [1]. As it has been shown in another report (D8.8, *Port of selected scattering kernels from McStas to SIMRES*), it enables to use McStas [2] scattering kernels in SIMRES [3] without the need of actual copying of the McStas code or its translation into the SIMRES core language (Fortran). Work duplicity and extra maintenance effort are thus avoided, while the whole portfolio of McStas sample components can be employed in SIMRES. The basic scheme of such a simulation is shown in the figure 1 below.

In fact, this procedure can be used not only for modelling scattering from sample components unavailable in SIMRES. The McStas part of the instrument description can represent an arbitrary beam line. As a part of the work package WP8, we have implemented necessary code in SIMRES for import and export of MCPL files, as well as control functions allowing to run McStas simulations directly from the user environment of SIMRES as a single command. In the next section, the implementation of this method in SIMRES is described in more details.

The first practical application of such a combined simulation was the modelling of the engineering diffractometer BEER, which is to be built at ESS in Lund. In this report, four use cases for this instrument are given as examples demonstrating usefulness of the combined simulations:

1) Standard *medium resolution strain mapping* experiment with a small gauge volume of 1x1x3 mm3 in duplex steel.

2) High resolution strain mapping experiment employing the novel beam *modulation method* proposed for BEER.

3) Measurement of a small *single crystal* (α-SiO2) using a white beam on BEER.

4) *Simultaneous diffraction and SANS measurement o*n a rod sample in axial strain geometry typical for thermo-mechanical loading experiments. This is one of special operation modes planned for BEER once it is equipped with a SANS detector within the ESS completion program.

In the cases 1, the simulation model was also written and executed completely in McStas. The results serve for validation and evaluation of simulation speed gain achieved by combining McStas and SIMRES codes.

3. SOFTWARE DESCRIPTION

Description of SIMRES from the users' perspective is available in the program manual. This report focuses only on the new features developed within the SINE2020 project.

In the standard mode, each simulation in SIMRES is split in between three sections: (i) primary beamline, (ii) sample and (iii) secondary beamline as schematically shown in Figure 1. Neutron ray-tracing within the primary beam can be optionally executed in reverse order, starting just before the sample and propagating towards the source. This enables usually much higher event transmission probability due to a more efficient choice of sampling volume, particularly when simulating experiments with small samples or small gauge volumes defined by a tight beam collimation. The

primary beam neutrons are stored in memory and used in subsequent cycle for tracing through the sample and secondary beamline.

The newly developed code in SIMRES includes:

1. Export and import of neutrons to/from the primary beam storage (and in fact any other monitor defined on the model) in the MCPL format.
2. Execution of a McStas simulation in a separate thread. Configuration and compilation of the McStas instrument model is fully independent on SIMRES. Only the executable is required. The only obligatory parameters are the "input" and "output" MCPL file names, and the number of MCPL rewinds required for MCPL input. The McStas model can use any additional parameters, which are accessible to SIMRES by parsing the simulation output executed with the "-help" option. It is therefore possible to pass parameters of the SIMRES model to McStas. Of course, any monitor export defined in the McStas part is available at the end of McStas simulation as usually and can be visualized by the McStas front end, in addition to the output files and graphics provided by SIMRES.
3. Implementation of a timer thread which controls the top level of the simulation flow, including transitions between the SIMRES and McStas simulations and exchange of the MCPL files.

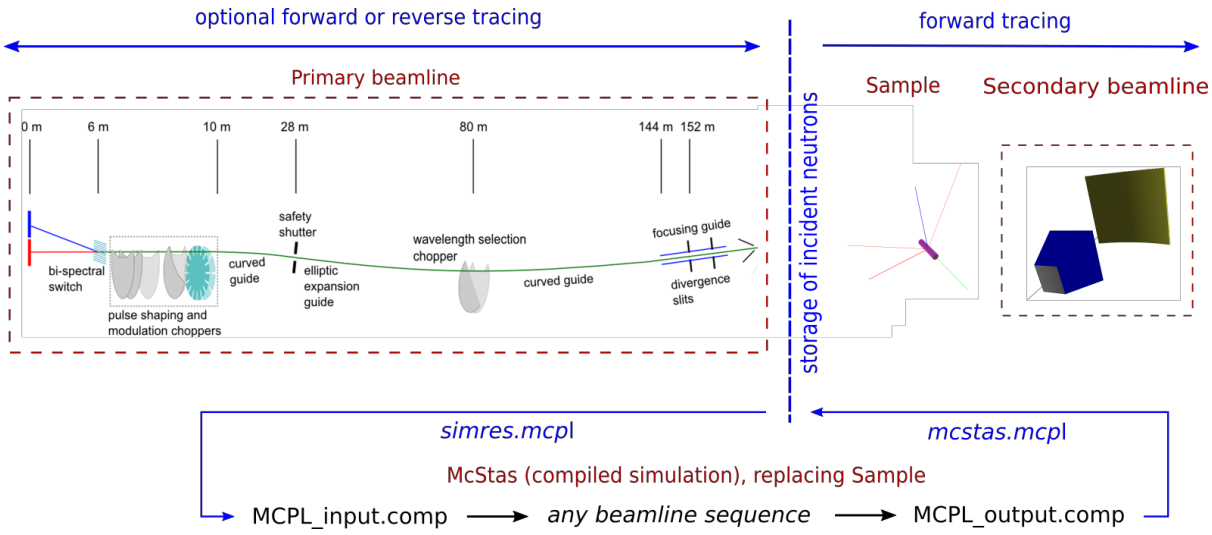

Figure 1. A schematics showing the flow of neutrons in a simulation combining SIMRES and McStas. The sample component of SIMRES is replaced by a compiled McStas simulation executable. It uses primary beam neutrons from SIMRES monitor and returns back the result by using the MCPL input/output components. The 3rd step (secondary beam simulation by SIMRES) is optional, simulations can be finished already by the McStas part.

4. EXAMPLES

4.1. Medium resolution strain mapping

The engineering diffractometer BEER (ESS) operated in medium resolution pulse shaping mode has been simulated by (i) McStas only and (ii) by using the combination of SIMRES and McStas ray-tracing. The basic configuration parameters were:

- **Source**: bi-spectral, W2 beamport of ESS
- **Resolution choppers**: a pair of choppers separated by 400 mm gap and rotating at 280 Hz in optically blind mode.
- **Wavelength bandwidth**: from 1 Å to 3 Å.
- **Primary collimation**: vertically focusing neutron guide, primary slit 1x3 mm^2 placed at 50 mm before the sample axis.
- **Sample**: rod (diameter=10 mm, length = 50 mm) made of duplex steel, oriented in axial strain geometry (axis along the mean scattering vector); modelled by the component PowderN.com.
- **Secondary collimation**: Radial collimator with gauge FWHM = 1 mm (ENGIN-X setup).
- **Detector**: cylindrical, resolution 2x5 mm, span 30 x 30 deg, take-off angle 90°; modelled by the component `NPI_tof_dhkl_detector.comp`.

The SIMRES configuration included the primary beamline down to the primary slit followed by a primary beam monitor. The reverse tracing mode of SIMRES was used to improve the simulation speed by more than an order of magnitude. Neutrons were exported from the monitor to an MCPL file and then loaded by the subsequently started McStas process, which exported the result in another MCPL file. At the end of McStas simulation, SIMRES loaded the McStas MCPL output into the same monitor and ray-tracing continued in SIMRES to the detector.

An equivalent BEER model has also been fully written in McStas. Both SIMRES and McStas models (including 35 components on the primary beam) defined the same component sequence with parameters generated from the same data source by a Python script. However, implementation of underlying physical models by both the programs is different, with various levels of approximation, and hence exact match of the results cannot be expected. Figure 2 shows the resulting diffractograms produced by the SIMRES detector during the combined simulation (red line) and by the McStas detector in the complete McStas BEER model (black points). Both simulations were executed to a similar accuracy for the flux at the sample and produced similar results, but required very different computing times (single Pentium i7 CPU on a standard laptop), as illustrated in Table 1.

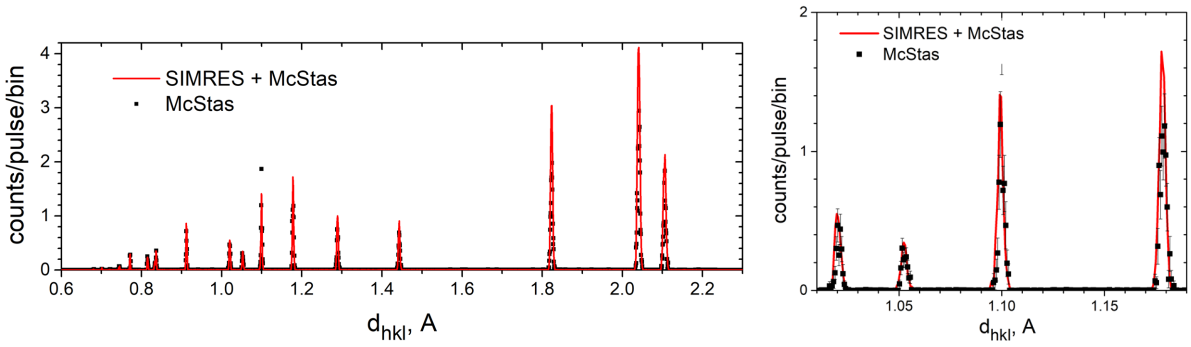

Figure 2. Diffractograms simulated by the combined SIMRES+McStas ray-tracing (red line) and by McStas only (black points).The detail on the right permits to assess differences, which are within the statistical errors.

Table 1. Comparison of computing times and statistical errors for the primary beam intensity.

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

4.2. BEER in modulation mode

The combination of SIMRES and McStas tracing described above has also been applied to test event based data reduction procedure for strain measurements in beam modulation mode of BEER. In this mode, the primary beam is modulated by a fast chopper with multiple windows, placed close to the source. As a result, a chain of several diffraction lines is measured by the detector for each diffracting plane. Whereas SIMRES enables fast simulation of the primary beam even with the small gauge volume required for strain mapping, McStas enables to easily implement new or derived component models. The detector component `NPI_tof_dhkl_detector.comp` has been developed for data reduction of the modulated data. It permits to reconstruct single high-resolution diffraction lines from the modulated pattern, which have higher peak intensity compared to the usual pulse shaping mode with similar resolution. In this example, the primary beam has been simulated by SIMRES in reverse tracing direction, while the sample (`PowderN.comp`) followed by the radial collimator and detector was simulated in McStas. The modulation chopper MCB rotating at 280 Hz, with 8 x 4° slits was used to modulate the beam. The gauge volume of 1x1x2mm^3 was defined by a primary slit and secondary radial collimator similarly to the previous example. The sample was again a duplex steel rod of 7 mm diameter oriented with the axis parallel to the mean diffraction vector (45° orientation). In Figure 3, the wavelength-time maps of neutrons at the sample (SIMERS output) and detector (McStas output) are shown. The diffractograms produced by the McStas detector are then plotted in Figure 4.

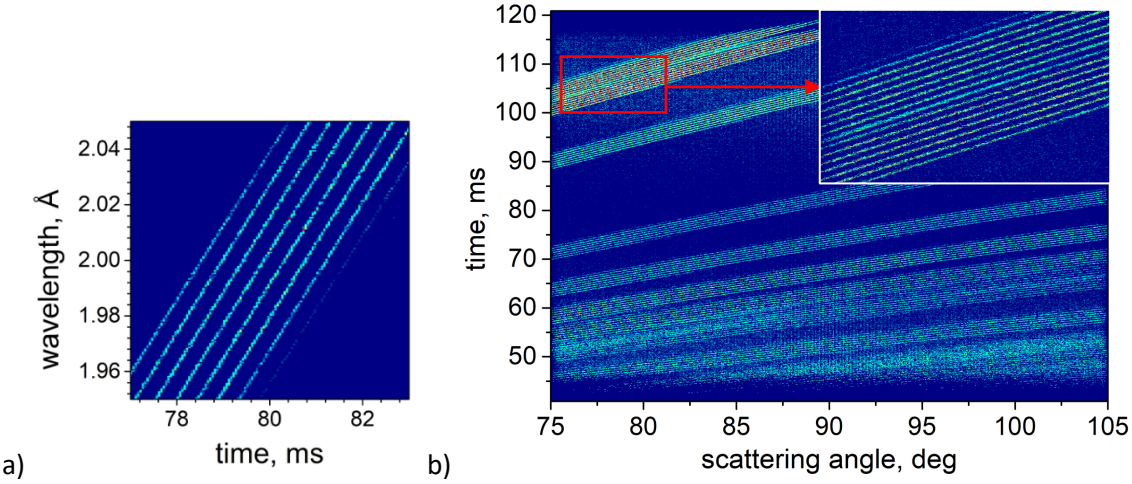

Figure 3. (a) Modulated beam structure at the primary slit – SIMRES MCPL output passed to McStas. (b) ToF – 2θ map of events registered by the detector component (`NPI_tof_theta_monitor.comp`) in McStas; multiplexed diffraction lines from the duplex steel sample (`PowderN.comp`).

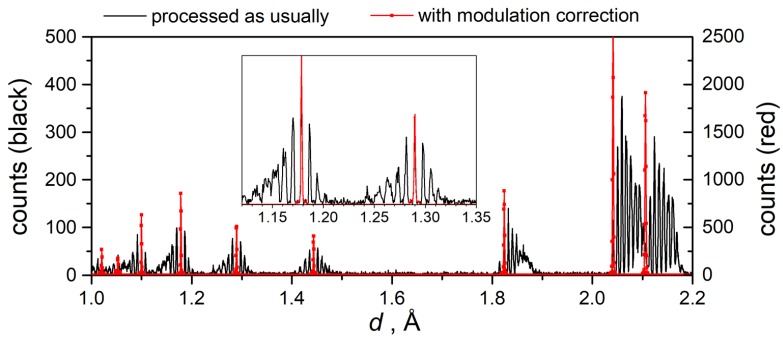

Figure 4. Diffractogram produced by the McStas component `NPI_tof_dhkl_detector` with the modulation analysis switched off (black, left scale) and on (red, right scale).

4.3. Single crystal diffraction

To test the variety of scattering models in McStas, the BEER instrument was simulated with a single crystal sample (`Single_crystal.comp`) in white beam mode (Laue diffraction). This configuration used following settings:

- **Choppers**: switched off (white beam).
- **Wavelength bandwidth**: from 0.5 Å to 2.7 Å.
- **Primary collimation**: divergence slit 15x15 mm (6 m before the sample), primary slit 4x4 mm^2 placed at 50 mm before the sample axis.
- **Sample**: α-SiO2 cube 3x3x3mm^3, mosaicity 30' (data file `SiO2_quartza.lau`)

- **Detectors**: cylindrical (`PSDcyl_monitor`) and 4PI (`PSD_monitor_4PI`) monitors, and 1x1m^2 ^{3}He detector at 90° (`PSD_Detector`).

As before, the primary beam was simulated by SIMRES, ray-tracing through the sample was performed by McStas. Scattered beam monitors were defined in both McStas and SIMRES. Note that the wide cylindrical detector is not part of the BEER project and this simulation serves merely as a demonstration of bringing new scattering models to SIMRES via MCPL event exchange. The simulated scattering pattern as detected by SIMRES detector is shown in Figure 5.

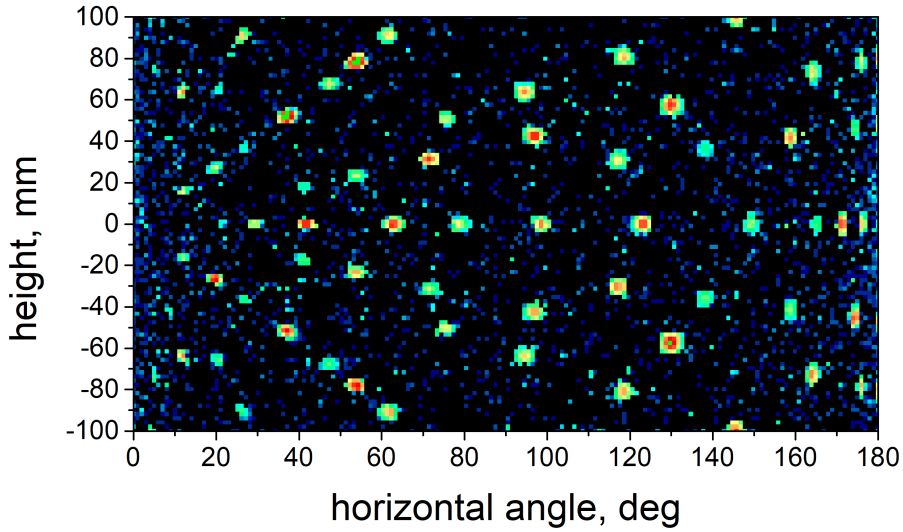

Figure 5. Single crystal diffraction pattern (α-SiO2) recorded by the SIMRES detector. The primary beam was simulated by SIMRES. Simulation of the sample was redirected to McStas. The secondary beam was traced by both McStas and SIMRES.

4.4. Simultaneous diffraction and SANS measurement

Unlike the previous example, simultaneous measurement of diffraction and small-angle scattering belongs to the scope of the BEER project, assuming installation of a SANS detector as a part of the ESS completion program. The chopper system of BEER permits to operate the instrument in the so called alternating wavelength frame mode, when the sample is exposed alternatively to thermal neutrons in one source period, followed by cold neutrons in the next period. The bandwidth in both ranges is limited to about 1.75 Å, while the mean wavelengths of the thermal and cold beams are separated by 3.5 Å.

Although there is no component in McStas or SIMRES which combines diffraction and SANS scattering models, it was rather easy to extend the existing component `PowderN` so that it handles SANS in addition to diffraction and incoherent scattering. The simplest case of monodisperse spheres was used for demonstration. Following instrument setup was considered:

- **Resolution choppers**: a pair of choppers separated by 925 mm gap and rotating at 280 Hz in optically blind mode.

- **Wavelength bandwidth**: about 1.1 Å to 2.9 Å in one period for diffraction, 4.6 Å to 6.4 Å in the other period for SANS.
- **Primary collimation**: divergence slit 15x15 mm (6 m before the sample), primary slit 5x10 mm^2 placed at 50 mm before the sample axis.
- **Sample**: rod (diameter=10 mm, length = 50 mm) made of duplex steel, oriented in axial strain geometry (axis along the mean scattering vector). Microstructure consisting of 1 vol. % of monodisperse spherical particles with radius 10 nm and scattering contrast of $1x10^{-6}$ $Å^{-2}$ was assumed.
- **Secondary collimation**: Radial collimator in the diffracted beam ($2\theta = 90^o$, gauge width 4 mm)
- **Diffraction detector**: cylindrical, resolution 2x5 mm, span 30 x 30 deg, take-off angle 90°; modelled by the component `NPI_tof_dhkl_detector.comp`.
- **SANS detector**: 1 x 1 m^2 3He detector at 6 m from the sample (`PSD_detector.comp`).

Results of this simulation are summarized in Figures 6 to 8.

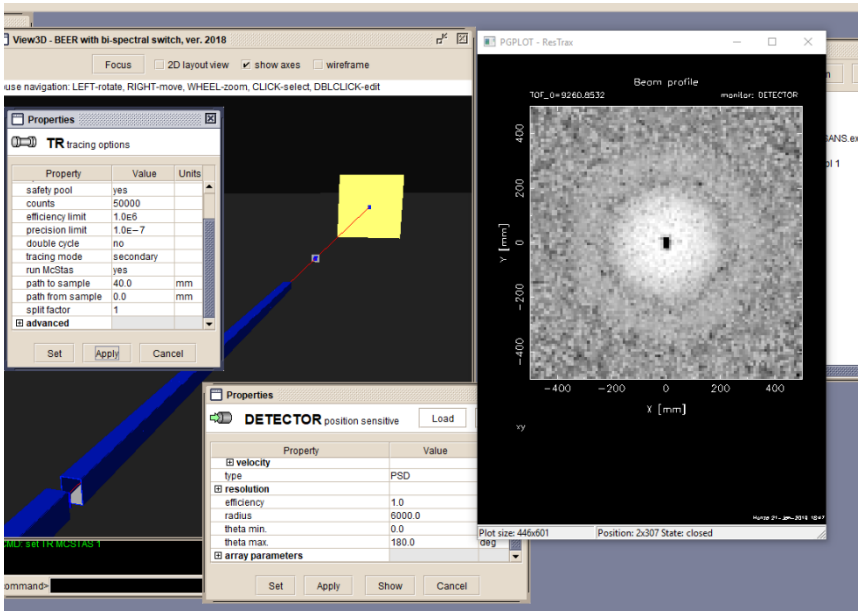

Figure 6. Screenshot of the SANS pattern shown in the SIMRES user environment. Primary and secondary beams were simulated by SIMRES. Simulation of the sample was redirected to McStas.

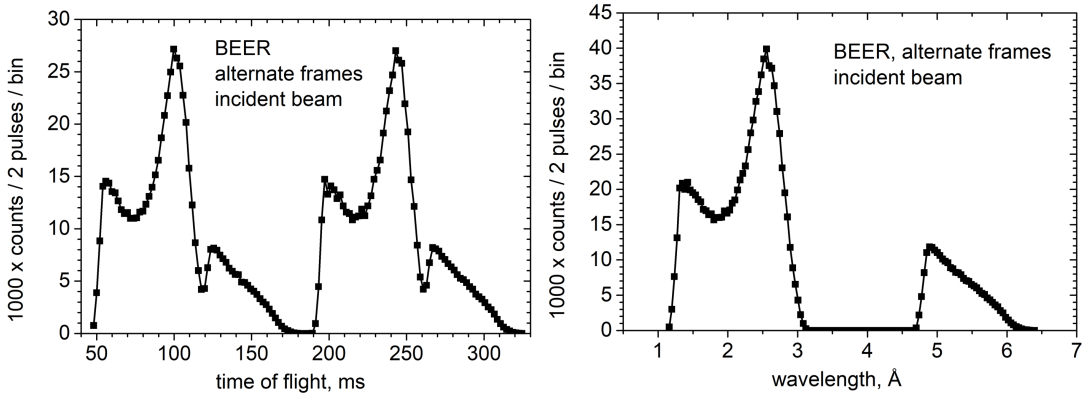

Figure 7. Time structure (left) and spectrum (right) of the primary beam simulated by SIMRES for BEER in the alternating frame mode. It was used as MCPL input to the subsequent McStas simulation of the sample and secondary beamline (see Figure 8).

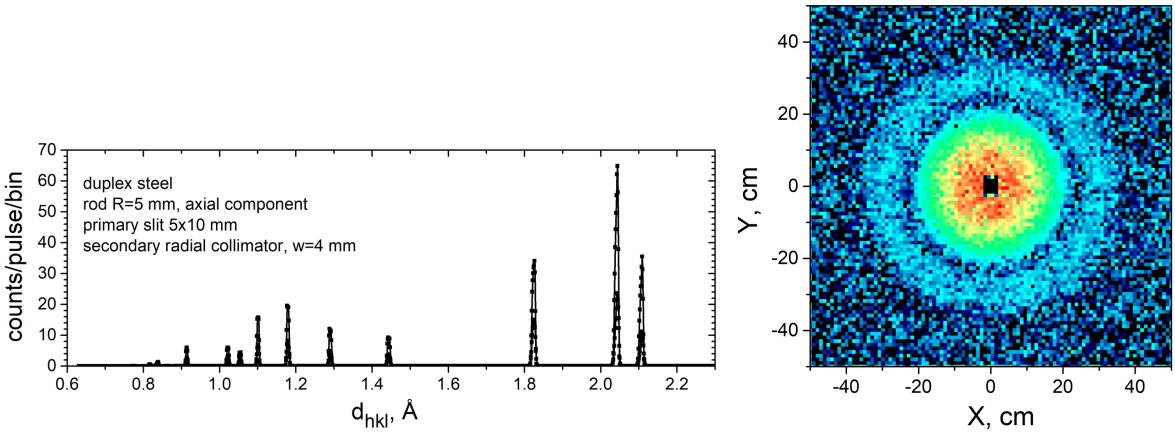

Figure 8. Diffractogram and SANS pattern "measured' simultaneously on the same sample - output of the McStas simulation of the secondary beam.

5. Discussion and conclusions

Combination of SIMRES and McStas codes in one simulation brings obvious benefits to users. Those demonstrated in this report include

- higher simulation speed by more than an order of magnitude,
- wider library of components which can be used to configure the instrument model,
- the possibility to use already configured and tested instrument models together with the components available only in the other program, without extra effort needed for code porting and maintenance.

Obviously not all possibilities have been fully exploited so far and more use cases are anticipated in future. For example, the middle part of the simulation process run by McStas does not have to include any sample at all. Instead, McStas can ran any, possibly complex component sequence, making use of all unique McStas features not available in SIMRES, such as GROUP, SPLIT etc.

Of course, there are limitations that can hardly be overcome. For example, the ray tracing algorithm of SIMRES does not permit to employ souce models developed in McStas. The primary part has always to start by the SIMRES source. However, this does not prevent users from defining another source in the McStas part, simply ignoring the SIMRES input. Possiblity to use the MPI interface for parallel computing is not obvious, since this feature is not available in SIMRES. However, SIMRES simply runs the compiled McStas simulation and all it needs is a message when the simulation ends and the MCPL output is available for import. Therefore there should be no principal obstacle for McStas to employ paralel computing on its part of the ray-tracing job.

The presented examples were produced with the McStas version 2.5, which includes some newly added contributed components. Hence these examples would not run with the older McStas versions. The option for redirection of part of the ray-tracing process to McStas has been implemented and tested in the pre-release version of SIMRES (ver. 6.3.6). A stable release with an updated manual and demo examples is expected during spring 2019.

6. Acknowledgements

The author would like to express thanks to the McStas development team for their support in developing McStas components and including the components developed within this project in the new McStas release. This work would not be possible without Thomas Kittelmann (ESS) and his efforts in developing the MCPL library as an open source software available to the neutron community.

7. References

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