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1. Abstract

Simulations of target-moderator-reflector system at spallation sources are conventionally carried out using MCNP/X whereas simulations of neutron transport and instrument performance are carried out by neutron ray tracing codes such as McStas. The coupling between the two simulations suites typically consists of providing analytical fits from MCNP/X neutron spectra to McStas. This method is generally successful, but as will be discussed in the this paper, there are limitations and a more direct coupling between MCNP/X and McStas could allow for more accurate simulations of e.g. complex moderator geometries, interference between beamlines as well as shielding requirements along the neutron guides. In this paper different possible interfaces between McStas and MCNP/X are discussed and first preliminary performance results are shown.

2. Introduction

In the target-moderator-reflector system of a spallation source, neutrons are slowed down from being fast at the formation in the spallation target to thermal or cold neutrons in the beam extraction guides. Simulation of this neutron moderation as well as the neutron scattering instruments plays a central role in the design of the European Spallation Source (ESS), where the aim is to optimise neutron fluxes for the scattering experiments.

To model the thermalization of neutrons in spallation target and moderators, the MCNP/X code is a standard of its field [1]. Since mainly being developed for high energy applications, however, the MCNP/X code does lack in description of coherent scattering applicable to the cold/thermal range, not accounting for e.g. reflectivity and Bragg scattering, or inelastic scattering arising from phonons.

The transport of cold/thermal neutron through guides and optics and the scattering instruments on the other hand are well described using neutron ray-tracing codes such as McStas [2, 3], where Risø DTU has been the main development centre. To bridge the gap between MCNP/X and McStas, the approach has generally been to use analytical formulae fitted to MCNP/X event spectra, using these as input for the McStas simulation. This approach has strong limitations as it in general does not allow the re-entry of cold neutrons into the thermal regime.

In order to resolve this issue, a more direct coupling between MCNP/X and McStas is required.

Below, various possibilities for such MCNP/X McStas coupling are described. Based on experience gained during implementation and tests of the interfaces, the feasibility and usefulness of the individual approaches are evaluated.

At the time of writing, the validation work is ongoing, and is performed within the framework of the ESS target-moderator-beam-extraction geometry. The software developments, however, are general and longer term, foreseen to be useful for other applications.

3. Concepts for automated interfacing between MCNP/X and McStas

3.1. Tally option

This approach is based on fitting MCNP/X distributions, allowing to model neutron states on a statistical basis. In short, detailed MCNP/X simulation of e.g. the ESS target, reflector and moderator system is performed, and the resulting neutron fluxes and spectra at the moderator surface are approximated by simple distributions (fitted by simple analytical formulae). McStas then 'draws' random neutron states from these distributions. A challenge faced when using this approach is to correctly describe the correlations between the parameters constituting a neutron state. For example non-trivial correlations between the neutron starting coordinates on the moderator surface and the momentum could exist. Quantifying correlations is thus an important part of validating the *Tally* method. In section 4 this discussion is quantified.

The advantage of the *Tally* method, as seen from a user perspective is, that the cumbersome MCNP/X simulation step is decoupled from McStas and this makes the method fast and thus very useful for e.g. instrument designers, who might not have access to the neutronics code. The drawback is that the precision of the simulation may be questionable; it is one of the things that the remainder of this project aims at investigating.

A McStas ESS component which follows this approach exists, but it is based on an outdated target-moderator geometry and energy spectrum. In section 4 the development of an revised version is discussed.

3.2. Ptrac option

This approach utilises an intermediate step of event files, so that MCNP/X at a given user-defined surface, outputs to a file the state of individual neutrons (position, momentum, time and Monte Carlo weight). The McStas component: *Virtual_MCNP_input* allowing McStas to interpret *Ptrac* files was developed prior to the present work [4]. It was confirmed that the McStas neutron ray code is able to correctly interpret the data as produced by an MCNP/X simulation. Apart from the sizable intermediate files, a drawback by this approach is that the MCNP/X code is unable to re-import data in the *Ptrac* format. i.e. this approach can only be a one way interface. Moreover the method is limited by the fact that MCNP/X only allows particles crossing *one* surface to be written to file, and that the *Ptrac* option is unavailable under MPI‡. For these reasons, relying on intermediate *Ptrac* files is inadequate as a general solution to the problem faced. Nevertheless, it is a useful tool for specific problems as well as for validation against other approaches listed below.

3.3. SSW/SSR *option*

The *SSW/SSR* is a MCNP/X feature that allows to stop a simulation at a given surface, and restart it later. It was never intended to work as a switch allowing external programs to be linked with a MCNP/X simulation. For this reason the intermediate files exist in an undocumented MCNP/X version dependent binary format only. However, we have succeeded to interpret the binary files allowing us to read and write *SSW/SSR* file with external code.

We have developed a McStas interpreter so that McStas can run based on a *SSW/SSR* file input, and produce a *SSW/SSR* output once the simulation is complete. The main advantage of the *SSW/SSR* option as compared to the *Ptrac* option is that MCNP/X can run based on the *SSW/SSR* files. In this way one could first do a MCNP/X simulation of the thermal neutron moderation. Once the neutrons enter the beam extraction region the neutron states are outputted through the *SSW/SSR* interface, and based on this a McStas simulation is carried out, e.g. involving mirrors and coherent scattering (which is not possible in MCNP). The scattered neutrons and/or the non-scattered can then be handed back to MCNP/X using the same interface. The corresponding McStas components to read and write from/to the SSW/SSR format are called: *Virtual_MCNP_ss_input* and *Virtual_MCNP_ss_output*, and are expected to be included as official McStas components, before the next major McStas release. In section 4 below, the *SSW/SSR* functionality is tested against the *Tally* approach (section 3.1).

‡ MPI is an abbreviation for: Message Passing Interface, which is a method of parallelising computer processing. For additional information, see e.g.: http://www.mcs.anl.gov/research/projects/mpi/

3.4. Compile option

Closely resembling the above approach, an even more direct coupling of the MCNP/X and McStas codes was successfully attempted. Rather that writing out intermediate files using *SSW/SSR* interface, the McStas and MCNP/X codes were simply compiled together so that once a neutron, arrived at a 'McStas surface', a McStas simulation was launched from within MCNP/X. The present status is at the proof-of-concept level, where we have an existing MCNP/X build that calls a McStas routine with a given neutron state as input. After completion the updated neutron state is returned to MCNP/X which proceeds the simulation. For an illustration see figure 1. The advantage of this approach is the truly unified nature of the two codes, but there are drawbacks: Firstly, the above relies on rather comprehensive changes to the MCNP/X code. Changes that would need to be redone, if one would want to upgrade to later versions of MCNP/X. Secondly, given the enormous differences in typical simulation times of the MCNP/X and McStas code respectively (many orders of magnitude), there is an advantage in being able to separate them. If not, those designing/simulating e.g. neutrons experiments at the end of the beam-line, would have to cope with a very long simulation times, which is many cases could have been avoided if the McStas simulation was somehow bootstrapped using e.g. *SSW/SSR* interface (or *Ptrac*). Thirdly, there is a licensing issue at hand when merging the codes: McStas is licensed under GNU GPL v.2., whereas MCNP/X requires individual personal certification something which many users are not able to obtain. It is planned to develop a preliminary version of the *Compile option*, so that it can be tested against the other interfaces. Only then is it possible to fully judge whether or not the advantages of the compile option balance the disadvantages§.

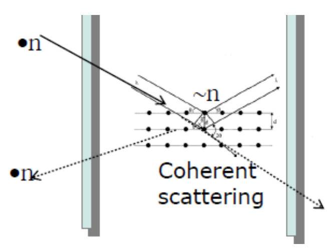

Figure 1. The McStas surface interfaces MCNP/X and McStas simulations.

3.5. Super-mirror option

As the above, this approach is based on modifying the MCNP/X source code. In this case, however, the idea is not to launch a McStas simulation from within MCNP, but rather to update MCNP/X shortcomings, with functionality inspired from McStas. The first and most important shortcoming when using MCNP/X for low energy neutron

§ A special internal DTU and ESS project license for this usage was applied.

scattering is the lack of coherent scattering. Coherent scattering, or in particular, super-mirrors (reflects some wavelengths, and allows others to penetrate) is well described in McStas. As for the *SSW/SSR* option , maintenance across MCNP/X releases is problematic for the super-mirror approach and also other McStas functionality than super-mirrors may need to be implemented, potentially causing heavy code development.

Existing implementation of super-mirrors in MCNP/X was done by collaborators from PSI and Oak Ridge National Laboratory [5, 6] and was ported to the most recent MCNP/X release (2.7.0). This allows for a direct comparison to the other described interfaces. As of yet, no such comparison was carried out.

4. Validation - first steps

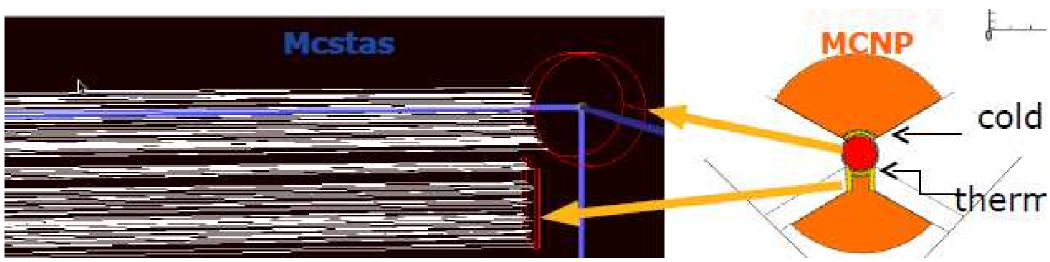

Figure 2. SSW exported at moderator surface, and neutron states transported to McStas (individual white traces).

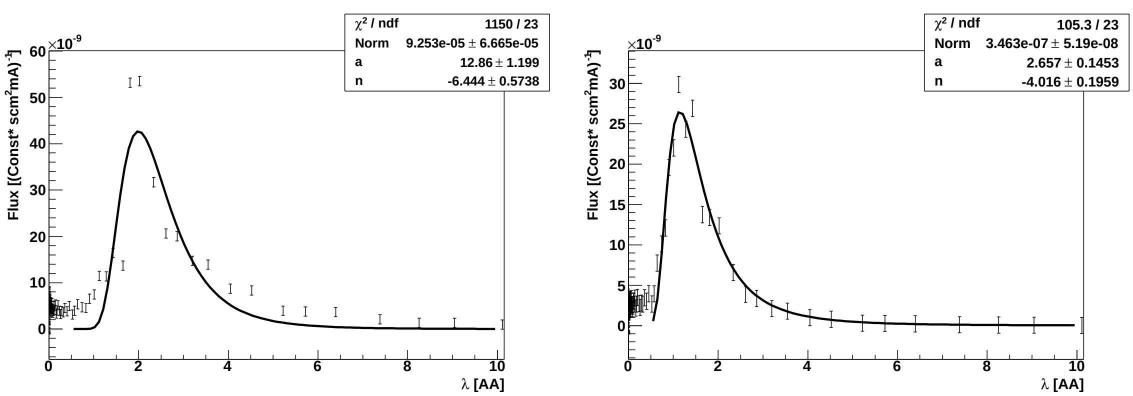

Figure 3. Fits to cold/thermal spectra of ESS-Bilbao preliminary ESS target-moderator geometry.

Despite the shortcomings of the *Tally* approach, the immense gain in computational speed with respect other coupling choices, ensures that there will be a need from instrument designers etc to use it. For this reason, it is important to evaluate its performance - in particular to study to which extent the approximations made by omitting possible correlations introduce systematic errors on the final distributions.

To make such study in the framework of the ESS, first the McStas component describing the ESS source was updated. According to present (preliminary) ideas within the target group, the moderation at ESS is likely to employ a bi-spectral principle, where some or all beam-lines have access to both cold (from H_2 moderator) and thermal neutrons (from H_2O moderator). Based on the geometry of the preliminary bi-spectral moderator from ESS-Bilbao, a new McStas component was prepared - for an illustration see figure 2. Also, based on the the preliminary MCNP/X geometry a full scale simulation was performed and the neutron flux was tallied, giving rise to cold and thermal spectra as shown in figure 3.

A revised McStas component, containing the updated spectra and geometry, *ESS_Moderator_Revised* is expected to be released shortly.

5. Prospects

We foresee that the combination of MCNP/X and McStas will become a new standard for detailed simulation of cold/thermal neutron moderators. Besides being directly applicable to the simulation of the target-moderator-reflector system of the spallation source, it will enable McStas-based descriptions of e.g. reflecting material and crystals to be included in the design and optimisation of advanced moderators, such as recently proposed Si-crystal vanes [7] or nano-diamond coatings [8], to a level beyond what is possible with the MCNP/X codes alone. Also we foresee that the combination of MCNP/X and McStas will enable more accurate calculation of photon production along neutron guides, and thus ultimately yield better shielding calculations. Finally, existing spallation sources have experience problems with crosstalk between neutron guides. Given that the beam-lines at ESS are expected to be closer than at existing facilities, it is important already before the construction phase to start studying these effects, and we expect to do this using the coupled MCNP/X McStas interface.

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