Full Simulation of Detector Performance of Neutron Instrumentation at ESS

PhD Thesis booklet

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Introduction

Understanding the nature of materials is fundamental for many scientific fields such as engineering, physics, chemistry, geology, biology and medicine. Scientists probe the structure and behaviour of materials using different methods like microscopy, X-ray scattering and neutron scattering. Different techniques usually give complementary information about the observed sample of material due to the different interaction between the probing particles (e.g. photons, electrons, neutrons) and the building blocks of the sample.

Neutrons have the unique advantage of being able to penetrate bulky materials due to their weak interaction with atoms through the short-ranged nuclear force, and can provide information of the atomic scales. On the other hand, this weak interaction is also a major drawback of the neutron scattering techniques, as it necessitates the use of powerful neutron sources with high fluxes which are not as easily accessible as for other techniques such as X-ray scattering. For this reason, scientific experiments involving neutron scattering techniques are concentrated in research facilities using strong neutron sources, that are mainly research reactors or spallation sources.

In order to push the boundaries of science, it is inevitable to upgrade scientific instruments and to build new facilities which exceed the capabilities of their predecessors. Both upgrading instrument at existing facilities and building new ones at new facilities require significant development in many fields of neutron scattering. This is especially true for the European Spallation Source (ESS) [Peggs, 2013], a new research facility being built in Lund, Sweden, that is designed to operate using the most powerful spallation neutron source in the world. Building ESS is one of the largest science and technology infrastructure projects today, and when finished, it will provide unprecedentedly high neutron fluxes for instruments of various neutron scattering techniques [Andersen, 2020].

Harnessing this powerful neutron source carries a high potential risk for detector rates that can saturate the detectors and therefore degrade the performance of the instruments. In order to avoid the detectors becoming the bottleneck of the instrument's performance, simulation studies can be carried out as part of the design process to serve basis for detector requirements.

Monte Carlo simulation [Lux, 1991] plays a key role in the development and characterization of instruments as a reliable, cheap and versatile tool [Kanaki, 2018], as CPU cycles are cheaper than prototyping cascade for complicated scientific instrumentation. Feedback from simulations taken into account in the development of the instrument design can reduce the number of physical prototypes needed, and also enable the quantification of otherwise unmeasurable properties. Development of complete and detailed instrument simulation models enables simulations from source to detectors, offering the opportunity to discover and decouple otherwise undetectable cumulative effects.

The simulation of a complex system such as a neutron scattering instrument is not straightforward and is subject of certain limitations. At the moment, there is no single software that enables detailed and efficient simulation of all aspects like production of neutrons, their transport for long distances through neutron guides, transport in crystalline materials, and detection via production of secondary particles. There are, however a handful of simulation tools such as McStas [Lefmann, 1999] and Geant4 [Agostinelli, 2003] with different strengths and weaknesses. Recent developments enabled interchange of particle data between some of these tools using dedicated MCPL files [Kittelmann, 2017], making it possible to use a chain of simulations to carry out the full simulation of a neutron scattering instrument using the adequate software at each part of the system.

Objectives

In this PhD work multiple Monte Carlo simulation tools such as McStas and Geant4 are used together to implement full simulation models of two ESS instruments, namely the small-angle neutron scattering (SANS) instrument, LoKI [Jackson, 2015], and the indirect geometry cold neutron spectrometer, BIFROST [Ronnow, 2014]. The main purpose of these models is to define the anticipated detector rates for both instruments in various scenarios including those which are expected to result in the highest rates, and thus can help to formulate detector requirements.

Elaborating and implementing the simulation model of the LoKI instrument served dual purpose. The first part of the work aimed at acquiring a good understanding of the rates LoKI is going to achieve by looking at how the neutrons scattered on the sample are distributed in space and time. A realistic worst-case scenario is reproduced, based on which the detector requirements for rate capability can be extracted. The main focus of this evaluation concerns the neutron scattering taking place within the forward solid angle after the sample, as this happens to be the primary area of interest for the SANS technique. This translates to a typical 1 m^2 detector area considered for the rate estimates of the scattering characterisation system. The second part of the work aimed at using a part of the full simulation model to perform a comprehensive characterisation of the novel Boron-Coated Straws (BCS) [Lacy, 2013] neutron detector technology in order to evaluate its performance and confirm its applicability for neutron scattering applications and for the LoKI instrument in particular. Detection efficiency is one of the key performance parameters of a detector, that is known to be low for a single BCS detector tube, therefore it is natural idea to increase the efficiency by using multiple layers of them. On the other hand, this leads to an increased amount of material in the system that raises the problem of absorption in the structural materials and their activation by neutrons. Another side effect of the added detector material budget is the increase in the scattering of neutrons inside the detector system. In contrast to absorption, scattering can degrade the detector performance by producing intrinsic background, which in turn can impact the signal-to-background ratio. The scope of the performance study included all these aspects of a potential BCS detector system.

The work concerning the BIFROST instrument aimed at extending the pre-existing model of the instrument to carry out full simulation of the instrument from to the neutron source to the detectors, and to develop a methodology to acquire time-averaged and peak incident detector rates for this instrument. Determination of anticipated detector rates for an instrument is a key part of defining requirements for the detectors to be used. It can prevent the detector rate capability from becoming the bottleneck of experiments or a source of performance degradation. This is particularly the case for BIFROST where the scattering characterisation system is designed to detect weak inelastic signals from small samples, but the exceptionally high intensity on the sample carries the danger of extreme rates in case of coherent elastic (Bragg) peaks. For this reason, simulations are performed to determine the highest time-averaged and peak incident rates for the detector tubes. The effects of some instrument and sample parameters on the incident detector rates are not necessarily straightforward, therefore parameter scans are performed including sample and analyser mosaicity, sample size, pulse-shaping chopper opening time, and accelerator source power. Beside considering the worst-case conditions in terms of the incident detector rates, it is also important to evaluate conditions that are closer to normal operation, therefore simulations are done for conditions representative for normal operation, aiming at defining time-averaged and peak incident rates for the detector tubes.

New scientific results

The new scientific results of the thesis can be summarised in the following points:

1. I developed a generic Geant4 Monte Carlo simulation model of the Boron-Coated Straws, a solid ^{10}B-enriched boron-carbide converter based, Ar/CO_2-filled neutron detector. I used this model to estimate the incident and detection rates that are anticipated for detectors operated in small-angle neutron scattering instruments planned for the European Spallation Source. I found that for instrument configurations representing realistic operational conditions, the instantaneous detection rate will significantly exceed the rate capability of the detectors having conventional parameters, and therefore they would limit the scientific performance at higher source power. The model has since been adopted as the full simulation model for simulating instrument performance of LoKI instrument at the European Spallation Source. [P0 and P1]

2. With the Geant4 model of a Boron-Coated Straws detector system from thesis point 1 I carried out a simulation study of absorption, activation and efficiency in order to evaluate the detector performance. I found that in the wavelength range of 0.6–11 Å 13–33% of the incident neutrons are absorbed in the detectors without enough energy deposited in the counting gas to trigger detection event. This level of absorption is acceptable for neutron scattering application. However, at smaller wavelengths the fraction of neutrons transmitted through the detector is high (60–27% for 0.6–1.8 Å) and therefore absorbant shielding behind the detector is a must for applications below 5 Å. I demonstrated that the radiation from activated materials will not influence the signal-to-background ratio, or cause limitation due to high doses for maintenance in case of envisaged application at the European Spallation Source. I showed that the detection efficiency of the detector is low, however with application of overlapping layers of detectors, 50–66% detection efficiency is achievable in the 1.8–11 Å wavelength range. [P1 and P2]

3. With the Geant4 model of a Boron-Coated Straws detector system from thesis point 1 I studied the impact of scattering inside the detectors on the signal-to-background ratio for quantities relevant for different neutron scattering techniques. I found that the fractional scattering (as generally defined as the ratio of the background intensity, and the combined intensity of signal and background) increased with the amount of the material budged, it became the highest at low wavelengths, and significant below the Bragg cut-off. According to the results, the scattering can be considered to remain on acceptable levels for applications such as small-angle neutron scattering, however, may be considerable for applications which are highly sensitive to it such as spectroscopy. I found the application of a polyethylene "afterburner" block placed behind the detector system to noticeably increase the number of neutrons contributing to the signal, however significantly increase the background, therefore the only considerable application field could be homeland security, where position resolution is not a concern. [P2]

4. I elaborated and implemented the first simulation model with complete geometrical coverage of the scattering characterisation system of the BIFROST instrument designed for the European Spallation Source. This is the first application of the special NCrystal pyrolytic graphite material, developed for modelling analysers for neutron scattering applications. I connected this Geant4 model with the existing McStas model of the BIFROST instrument using the MCPL tool and carried out the full simulation of the instrument from source to detector position, which is very novel for neutron scattering. I demonstrated the usefulness of the model by simulating the incident detector rates in case of a common vanadium calibration sample, and matched the acquired energy resolutions of the analyser system to the intended values of the instrument. [P3]

5. I elaborated and implemented a McStas model of the scattering characterisation system of the BIFROST instrument, and used it with the same configurations as the Geant4 model of the system in order to compare the two software packages, and define the highest possible incident detector rates. I demonstrated that Geant4 is more suitable for modelling such a complex geometry, and that the results of McStas and Geant4 are in perfect agreement with the only exception being the transmission where in one case I found a difference of 10%. I found that for instrument configurations and sample parameters representing worst-case conditions the instantaneous rates can be in the range of 1–1.7 GHz for a single detector tube with time-averaged rates of 40–70 MHz. These numbers are well beyond the rate capability of the detector tubes of state of the art, therefore the saturation of the detectors is expected that may last for longer than 6 ms for electronically coupled triplets. [P3]

6. With the joint McStas and Geant4 model of the BIFROST instrument from thesis point 4 I studied the impact of parameters such as sample and analyser mosaicity, sample size, pulse-shaping chopper opening time, and accelerator source power on the incident detector rates for elastic peaks. I demonstrated the impact of the listed parameters, and concluded that in case of a representative operational scenario the incident detector rates are orders of magnitude lower than in the worst-case scenario, however, the values are still beyond the rate capability of the detector tubes. This implies that the detector features of recovery time and high rate tolerance have to be carefully evaluated by measurements to prove that the presumed scientific performance will be provided. [P3]

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Utilisation of the results

Regarding BIFROST, the rate challenge was anticipated even at the proposal of the instrument, however the magnitude of the peak rates exceeded the expectations. The acquired rate values were used at advisory meetings at the European Spallation Source, and the studies helped the instrument team to better understand the challenge of the detector rates. The simulations offered valuable input in finalising the detector requirements before the instrument tendered the procurement of the scattering characterization system. As a result, the detectors are expected to withstand Bragg peak bursts of 3 ms duration, with peak fluxes up to 10^8 n/s/cm^2, and with time-averaged flux below 10^7 n/s/cm^2 [Whitelegg, 2020]. Careful evaluation of the performance of the detectors is planned, but the foreseen potential solutions to the detector rate challenge include the limitation of sample size and type for the instrument.

The implemented simulation tools, and acquired results for the LoKI instrument and the BCS detectors are also in use. The results of the detector rate study were used in the decision making and review processes at the European Spallation Source, e.g at the "Phase 2" review of LoKI [Kanaki, 2017], and the generic model of the BCS detectors, presented in this thesis has been expanded into the full simulation model of the LoKI detector system by the LoKI instrument team and the ESS Detector Group [Houston, 2019].

The full simulation model of the LoKI detector system is connected to the Mantid software, where reduction and analysis of simulated data is done. With this connection, the full simulations of the LoKI instrument from the neutron source to the data analysis software will be used to facilitate corrections and calibration routines prior to the start of the operation of the instrument.

The complex study of the BCS detector tubes is not exclusively in the interest of the ESS, as this is the first time that such study of the scattering effects of the structural materials of the detector is done, and the producing company intends to reduce secondary scattering inside the detector [Lacy, 2019].

Thesis point related publications

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