



Deliverable Number: D8.4

Deliverable Title: Experimental Tests

Delivery date: Month 24

Leading beneficiary: DTU

Dissemination level: Public

Status: version 2.0

Authors: Erik Bergbäck Knudsen, DTU Physics

Esben Bryndt Klinkby, DTU Nutech

Emmanouela Rantsiou, PSI

Project number: 654000

Project acronym: SINE2020

Project title: World-class Science and Innovation with Neutrons in Europe 2020

Starting date: 1<sup>st</sup> of October 2015

Duration: 48 months

Call identifier: H2020-INFRADEV-2014-2015

Funding scheme: Combination of CP & CSA – Integrating Activities

## Abstract

Two benchmark experiments were performed during back-to-back beamtimes at BOA (PSI) in August/2017.

The first set of measurements consisted of two parts: 1. Split the beam in in 3 pts. and block one to create background in the other paths. 2. Examine the beam emerging from the back of a supermirror surface. Both sets of measurements were compared with simulated experiments in augmented versions of MCNP and McStas, as well as MCNP and McStas connected. The software additions and connections enable a qualitatively good agreement between simulation and experiment.

For the second set we performed a polarized neutron experiment at BOA (PSI) in August/2017. This was a calibration measurement intended to provide a validation benchmark for the effect of partially polarized beams impinging on a polarization dependent supermirror(ref). This often-ignored situation has needed careful validation for several years. The early analysis of the data indicates that the data is useful and thus the experiment was a success.

## Introduction

Both experiments were designed to form benchmarking and validation data-sets to be used in conjunction with aspects of neutron scattering instrument simulation, yet the experiments were to separate campaigns. While it was originally conceived that the second experiment would be performed at ChipIR @ISIS, we decided to do this also at BOA@PSI. This was due to beamtime availability at ISIS, for more efficient use of personnel, and for flexibility of experimental set-up.

We will in the following report separately on Experiments 1 and 2, which form deliverable 8.4.A and 8.4.B.

## Experiment 1 (Deliverable 8.4.A)

The express aim of the experiments was to create simple yet realistic benchmarks to validate simulation codes, and combinations of simulation codes with. In particular, we have targeted two types of benchmarks:

1. Background emanating from scattering of objects in the beam path.
2. Background arising from objects, not directly in the beam path, such as behind a mirror etc.

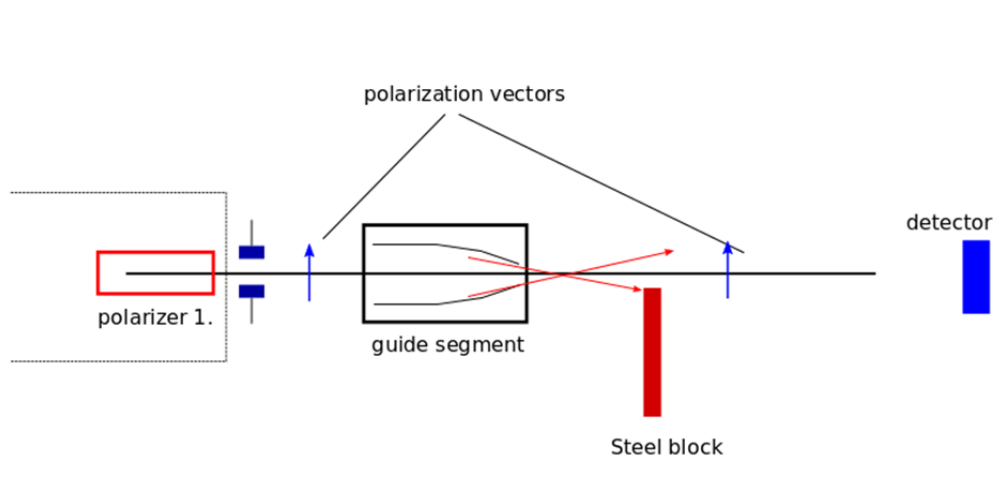


Figure 1 Sketch of Experiment 1.1.

Some computer codes work well with objects in any order (MCNP, Geant4), whereas other are more strictly sequential (McStas, VitESS). In general, the latter is less computationally expensive, but requires far-reaching assumptions about the beam path.

### Experiment 1.1.

The experiment was designed to create three beam paths with separate characteristics. The beam is allowed to enter an elliptical neutron guide. The guide is set such that parts of the beam will be reflected, and one part will simply be transmitted through to the detector, as sketched in figure 1.

From a simulation point of view the transmitted part holds little novel interest, but can serve as a calibration. The reflected beam paths offer more information. In the experiment, one of the reflected paths was “blocked” by a 3x2 cm steel block.

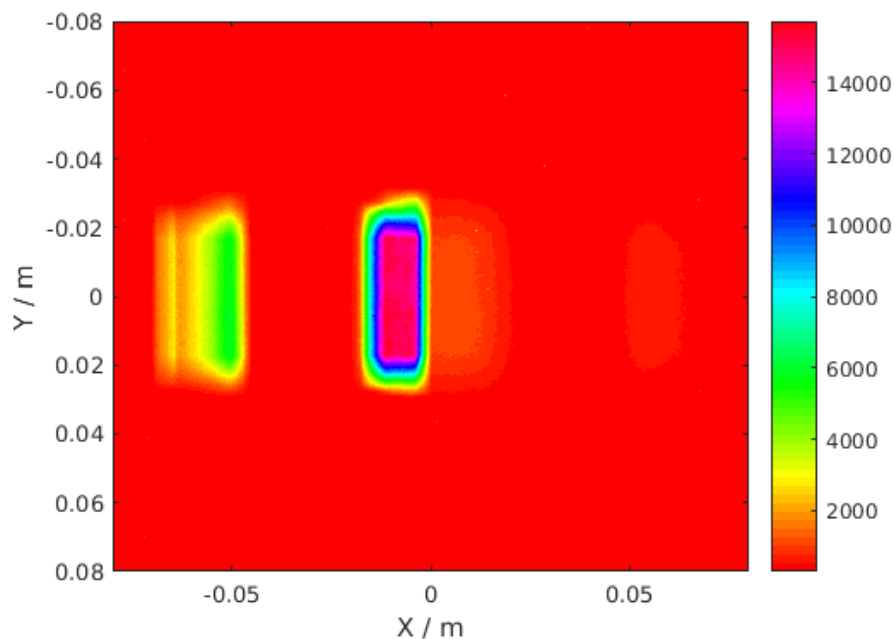


Figure 2 Raw experimental detector image. The steel block is set to block appr. half of the direct beam. Detector in the "near" position, catching all 3 beam paths.

Figure 2 shows examples of data from the experiment at PSI. Its simulated counterparts are shown

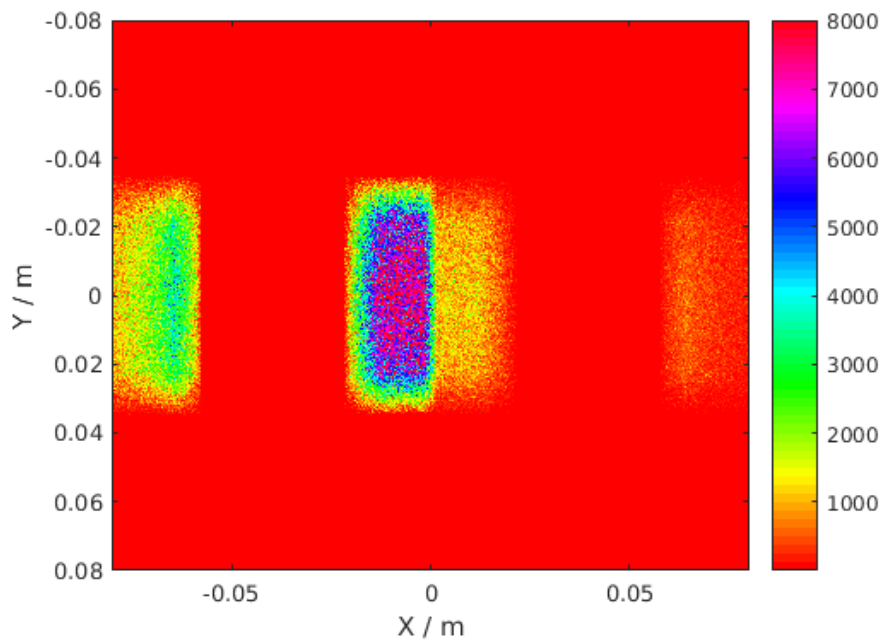


Figure 3 Detector image simulated by McStas. The steel block is set to block appr. half of the direct beam. Detector in the "near" position, catching all 3 beam paths.

in figures 3 (McStas) and 4 (MCNP). We find good agreement in qualitative terms between simulation and experiment. There are a number of geometrical issues to tweak – for instance the side-peaks in the McStas simulations are further from the central peak than for the experiment. This situation is expected as the instrumental geometry is never ideal. More importantly, the single-domain simulation models will allow us switch software domain at several points along the beam path, using the interfacing tools developed within the work package.

We note that, by design, that the steel block does not completely block the beam. In addition, the steel block creates background which is present on the detector images. We find that qualitatively the simulations agree. More work is required to match absolute intensities. E.g. one thing missing

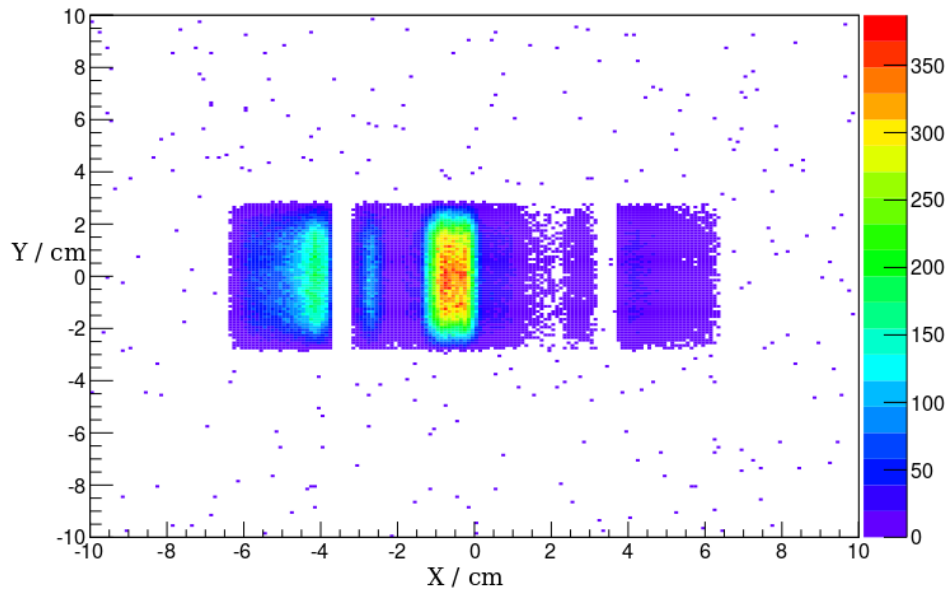


Figure 4 MCNP simulated detector image

from the simulations is the support structure of the neutron guide.

### Experiment 1.2.

This is a variant of the previous experiment where the focusing neutron guide has been replaced by a flat supermirror set at an angle such that it may reflect the beam. The aim of the experiment is to test software features developed for McStas and MCNP that deal with reflecting surfaces and includes the non-reflected part of the beam.

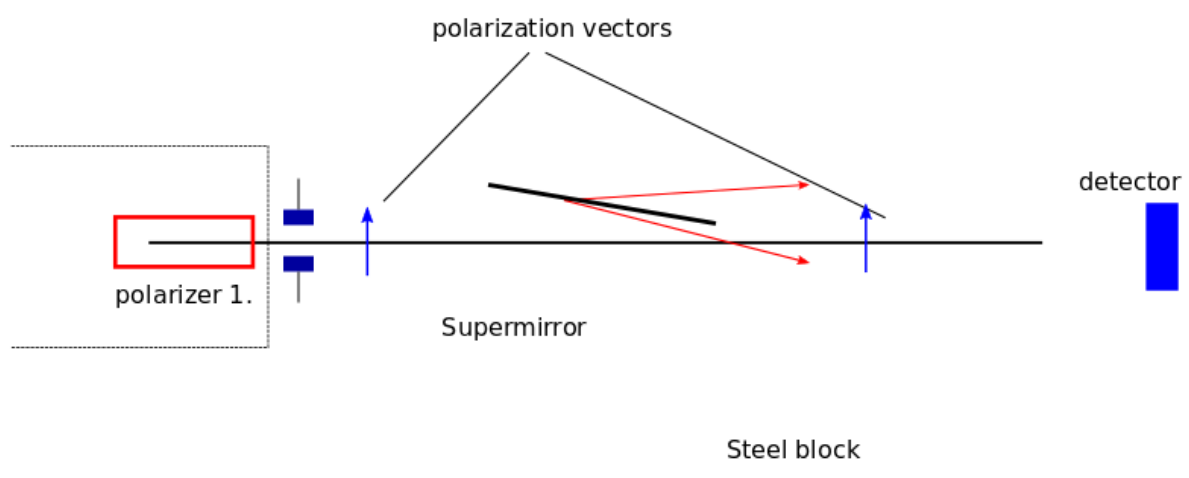


Figure 5 Sketch of Experiment 1.2

The aim of the experiment was to provide a benchmark for code that targets neutrons passing through a supermirror reflector. A benchmarked procedure is expected to handle more complex

situations such as neutron-gamma conversion inside shielding material. In terms of code gamma conversion can be targeted by e.g. MCNP and Geant4. Thus, there is a need for a benchmark experiment of this type.

The elliptical neutron guide in experiment 1 was not used since it has a Gd-coating on the back of the reflector substrates. This, in combination with the 10Li scintillator detector meant that any neutrons passing through would be so fast they could not be detected. Hence the decision to go for a flat mirror and redesign the experiment.

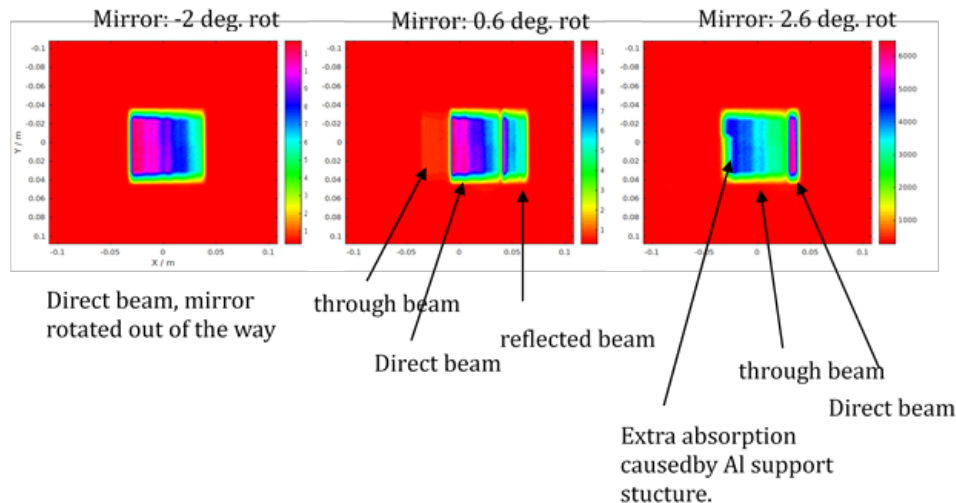


Figure 6 Raw detector images.

In figure 4 we show results obtained via an MCNP-model of the 2nd set up. To facilitate this some new code development had to be made, since MCNP does not (as distributed by RSICC) include models for reflecting guide surfaces. The software to do so originates from SNS (US), whereas PSI has contributed by patching it to run efficiently on MPI-enabled platforms. Further patches were made by the DTU team to run on the ESS HPC cluster installation.

We show raw detector images from experiment 2 in figure 5. The images are part of a series where the mirror was rotated from not interfering with the direct beam to “completely” deflect it. It is clear, that we can (using the full models of BOA) model the situation in MCNP. As is the case for experiment 1 and McStas, much work remains to match absolute intensities. This is expected as we can a-priori only use nominal values for instrument parameters. For a close match between experiment and simulation some measures would need fitting and other closer analysis.

## Conclusion and Outlook

In conclusion we consider this experiment to constitute Experimental test A of Deliverable 8.4 of the SINE2020 program.

The data obtained in the experiment will form the basis of further investigations, where we intend to mix the software domains in several ways

1. Use an MCNP-source to drive a McStas-model of BOA
2. Model the glass reflector (experiment 2) in McStas but store transmitted intensity.
3. Add generated gammas to the detector signal (in addition to the simple through-beam).
4. Add a realistic detector model, including quantum efficiency etc.

5. Model the support structure for the neutron guide piece.'

All in all, this requires switching from MCNP-McStas-MCNP-McStas-Geant4 (or a similar sequence). This is facilitated by the newly developed MCPL-library.

### Experiment 2 (Deliverable 8.4.B)

Supermirror devices are common in polarized neutron scattering experiments, yet the available tools for simulating these kinds of experiments are often lagging behind their unpolarized counterpart techniques. Further, there is in some cases a significant lack of benchmarks that new developments can target to provide accurate software tools.

One particular aspect wrt. McStas is the computation of a partially polarized beam passing through a supermirror polarizer/analyzer. It has long been known that the code works well for fully polarized beams, whereas the code partially polarized beams has long remained unproven. This experiment seeks to remedy that situation and put one of the most common tool for neutron scattering simulations on an even stronger footing. BOA is an ideal choice for beamline for several reasons:

1. The geometry set-up is very flexible.
2. The beam is already polarized (to a high degree) by an in-tube supermirror bender polarizer.
3. The beamline is already prepared for guiding a polarized beam. i.e. it has the option of setting up a vertical guide-field along the beam.

### Method

Using a set up as sketched in figure 1, we let an almost fully spin-up polarized beam pass through a spin-flipper. The beam is now almost fully spin-down polarized. This beam is transported by a guide field to a slit after which it goes through a bender analyzer, which reflects the spin-up state, to a detector. Thus, when the flipper is on, the intensity recorded at the is  $\sim 0$ , when the flipper is off it is at a maximum.

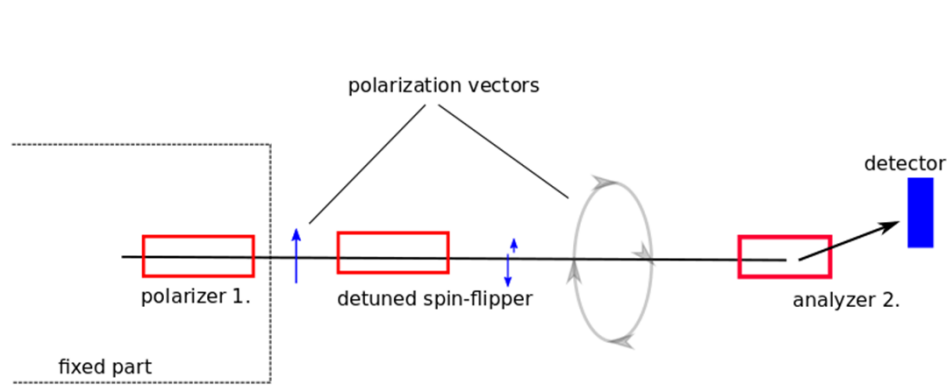


Figure 7 Sketch of the partial polarization experiment.

If we run the spin-flipper at non-ideal conditions, such as turning down the voltage for the RF-coil,

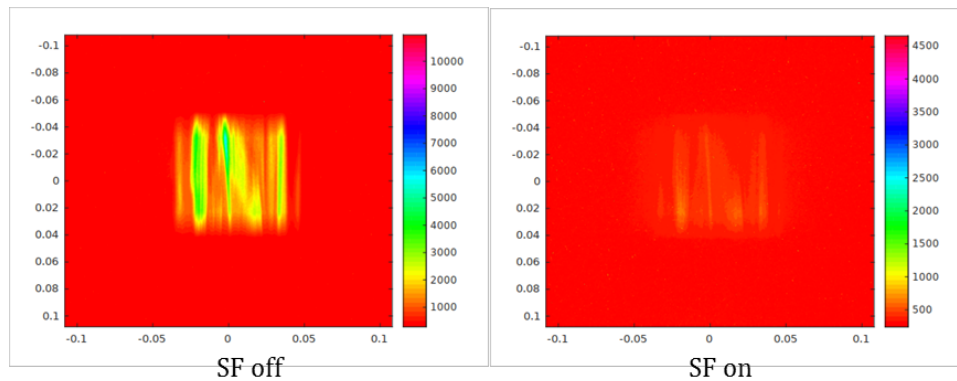


Figure 8 Detector images. Left: spin flipper off. Right spin-flipper on. There are clear signs of structure coming from the analyzer blades.

the result is an incomplete flip. The upshot of this is a beam with controllable depolarization which hits the analyzer.

We used a well characterized analyzer built as a prototype of the analyzer that PSI built for HySPEC at SNS (ref). The detector used was the standard BOA 10Li area detector. Although in principle the experiment could be performed using a single counter, we used a 2D area detector – that way we gain an option to calibrate the blade structure of the analyzer.

## Results

We show examples of data from the experiment in figure 2. Here we show the two extremes, i.e. spin-flipper off and on. We clearly see a non-ideal structure from the analyzer blades. For the present we study the integrated counts on the detector as a function of spin-flipper voltage and hence as a function of spin-polarization degree (figure 3). As expected the polarization is a non-linear function of voltage.

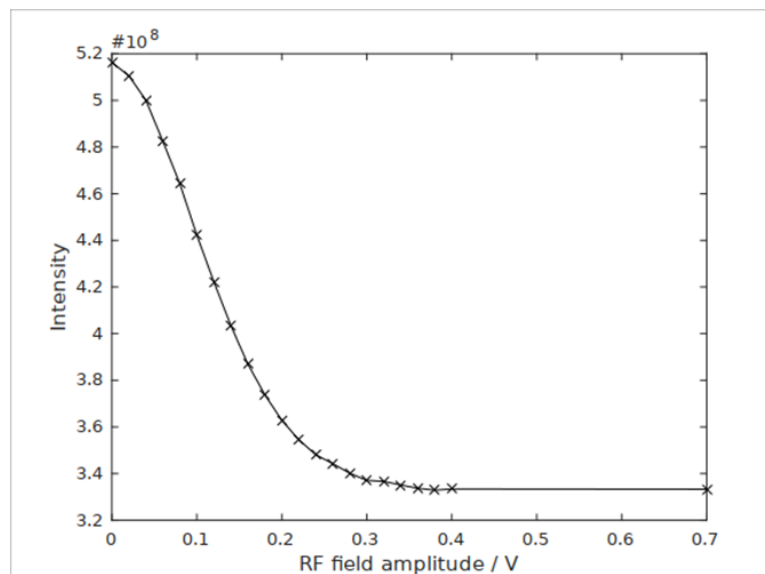


Figure 9 Intensity as a function of spin-flipper driving voltage. Below 0.4 V the flipper does not work properly creating a partially polarized beam.



At a voltage of 0.4 V the polarization of the beam can no longer track the magnetic field adiabatically, and so the net polarization of the beam decreases, until at 0 V the spin-flipper is completely off.

## Conclusion and Outlook

In conclusion we consider this experiment to constitute Experimental test B of Deliverable 8.4 of the SINE2020 program.

The data obtained in the experiment will serve as validation of several McStas supermirror components. We expect to be publish a detailed study of these results and further simulations in late 2018. Ideally this could also include comparative simulation studies using e.g. ViTESS, and or other software packages.

## *Acknowledgements*

This work was supported by the Horizon 2020 project 654000, PSI(CH) through its grant of beamtime for the experiment.

Furthermore, the authors wish to acknowledge the work of Franz Gallmayr (SNS) and Ryan Bergmann (PSI) who programmed the reflector card to MCNP, and Emmanouela Rantsiou (PSI) for invaluable help during the experiment beamtime.