New features in McStas for polarised neutron beams

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Abstract

We present work on simulation of polarised neutron beams within the framework of the McStas, Monte Carlo ray-tracing software package. Simulation work has been epecially amimed at describing the Spin-Echo SANS-instrument located at TU-Delft.

New kernel procedures are introduced to McStas as well as new simulation components that are specific to the Delft instrument. New Components include a model of the magnetized foil spin-flipper magnets which form the functional basis for the instrument - we compare our model to published work.

Features for propagation of polarised beams of the new kernel include a choice of precession routines and the option to nest magnetic environments, realized through a stack-concept.

Polarization Kernel

Spin-polarized neutron beams are modelled using the well known concept of a mean polarization vector, $\mathbf{P} = < s_x, s_y, s_z >$, which is very suited for Monte Carlo simulation techniques, as the mean Polarization becomes a simple weighted mean of contributions from the independent virtual neutrons.

For instance, when such a beam travels through a magnetic field, whose amplitude and direction does not change too rapidly we may simply apply the standard Larmor precession formula to the polarization vector.

Tests of polarization behaviour in different magnetic fields have been carried out. Conclusion: These tests match up perfectly with similar ones reported in the litterature.[5]

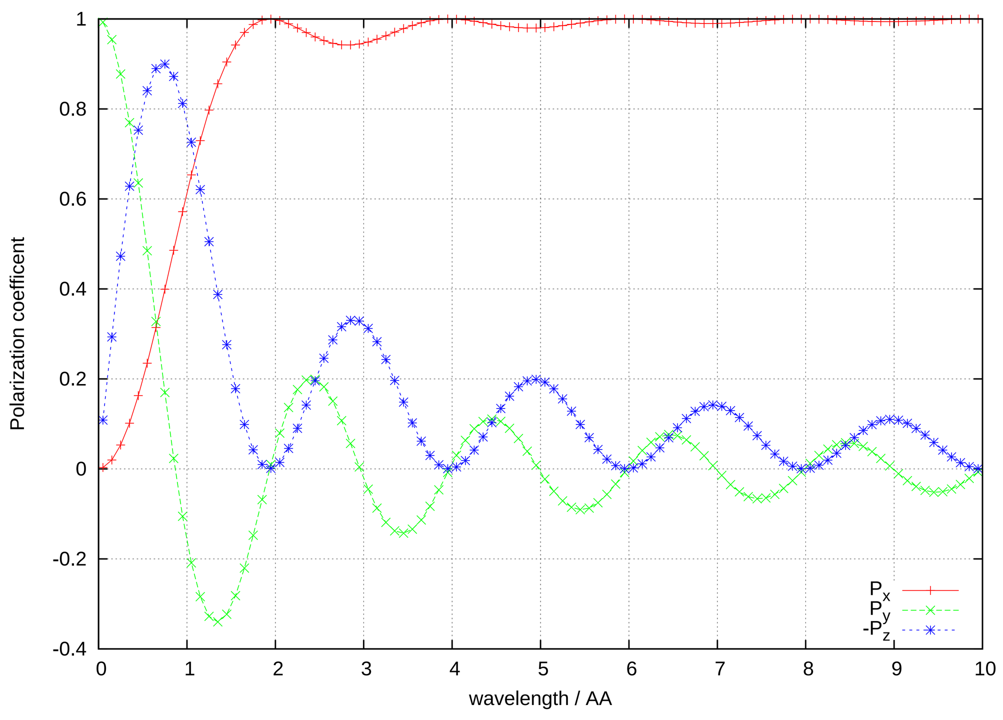

Figure 1: Polarization vs. wavelength for a geometrically rotating magnetic field.

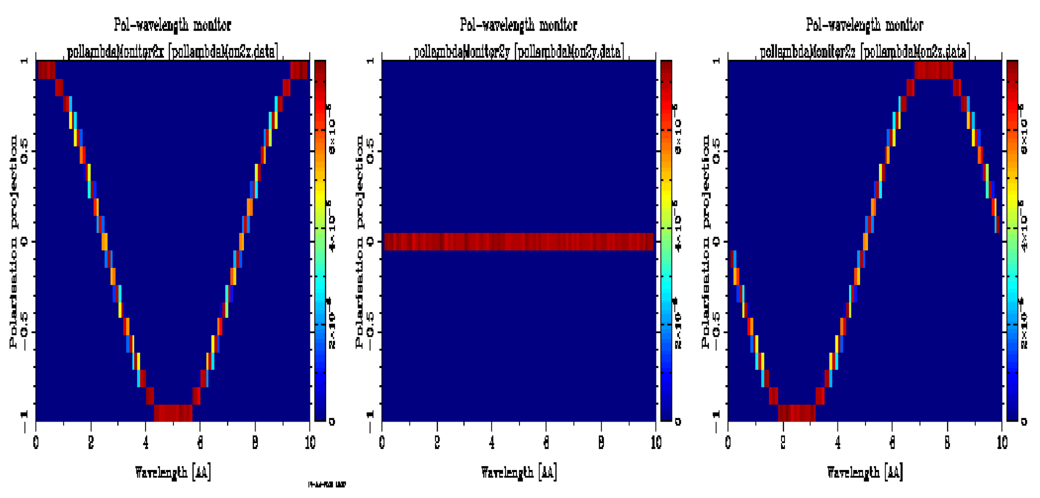

Figure 2: Resulting polarizations from neutrons that have been through a polarizing filter and a magnetic field set to flip the spin at one wavelength (5 AA)

Magnet Stack

Magnetic fields are set up in a stacked manner, so that field may be additive or not. As an exmaple we let a broad bandwidth neutron beam, polarized along $(-1, 0, 0)$ travel through a $1m$ long magnetic field of $+0.01T$ along the y-axis, resulting in the following polarization components.

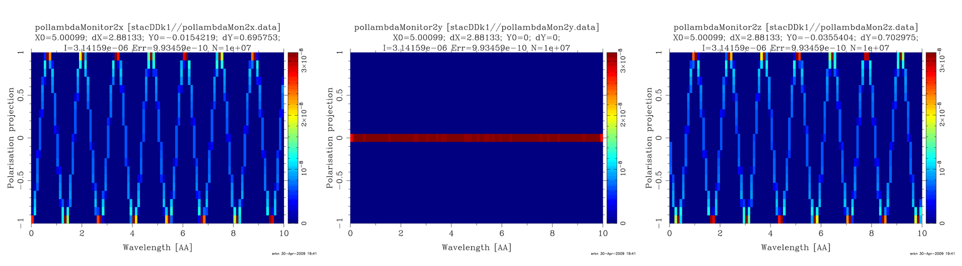

Figure 3: Resulting polarization after precessing in a $+0.01T$ field for $1m$

Now, to create an spin echo we insert a field of oppsite direction and appropriate strength in the last quarter of the field region, which results in an echo.

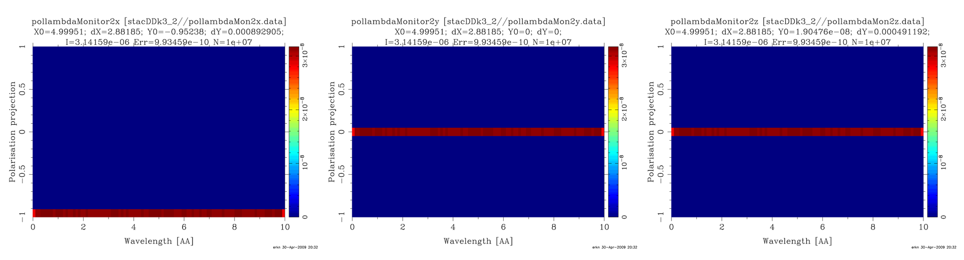

Figure 4: Resulting polarization after precessing in a $+0.01T$ field for $0.75m$ and a $(+0.01 + -0.04)T$ field for $0.25m$

SE-SANS Principle

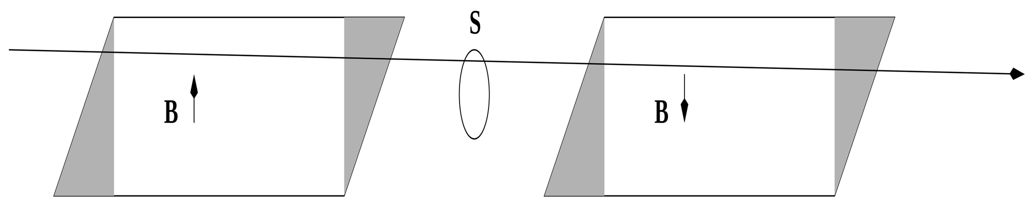

Figure 5: Drawing of the "classical" SESANS setup with inclined magnetic regions. The gray areas are the ones that actually contribute (to 1st order) to the Spin-Echo signal

The regular Spin-Echo SANS setup consists of two opposite field regions in which the neutron beam polarization precesses. Due to the opposite sign, the precession angle of the first region will be "echoed" by the second region, unless a scattering event in between (at position S) diverts the neutron beam. If the beam is scattered the path length difference through the magnetic regions induces a difference in precession angles which may be detected and analyzed. Further, the inclination of the magnetic field regions causes a 1st order difference in the precession angles, thus greatly enhancing sensitivity — and makes the principle practical.[4]

Following [4] the precession angle difference may be calculated (assuming a collimated beam) as

$$\phi_1 = c\lambda BD \quad (1)$$

$$\phi_2 = \frac{c\lambda BD\,(1 + \Delta\lambda/\lambda)}{\cos\theta\cos\phi - \sin\theta\tan\theta_0} \quad (2)$$

where θ_0 is the inclination angle of the field regions with respect to the plane perpendicular to the beam, θ and ϕ denote scattering angles from the beam direction, B the magnetic field strength and D the length of the magnetic regions along the beam. To 1st order eq. 2 expands to

$$\phi_2 \approx c\lambda BD\,(1 + \Delta\lambda/\lambda)\,(1 + \theta\tan\theta_0) \quad (3)$$

Eqs. 1 and 3 yield:

$$\delta\phi = \phi_1 - \phi_2 \approx -c\lambda BD\,(\theta\tan\theta_0 + \Delta\lambda/\lambda) \quad (4)$$

I.e. if the inclination angle is large, the difference in precession angle is significant, whereas it vanishes (to 1st order) for $\theta_0 = 0$. Further we observe that the field regions in between the inclined ends do not contribute to $\delta\phi$ except through the distance D. This has lead to the novel design of a SESANS machine at Delft.

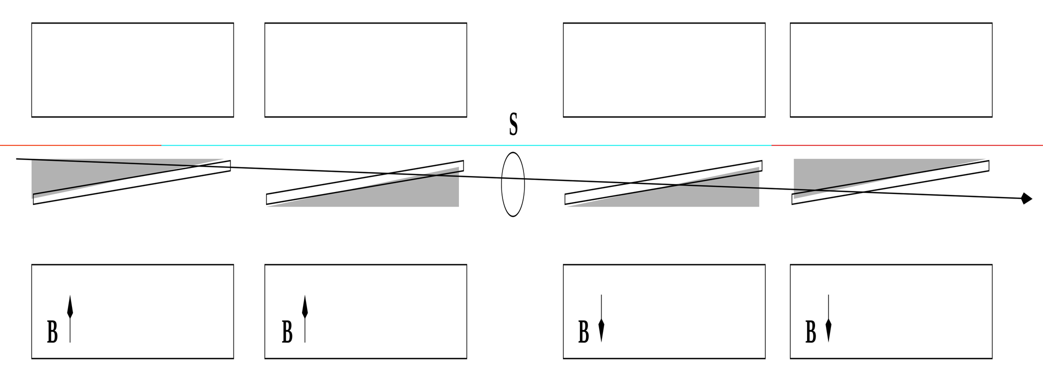

Figure 6: Schematic drawing of the magnetic regions in a spin-flip foil SESANS. Again the gray areas are the ones contributing to the Spin-Echo signal.

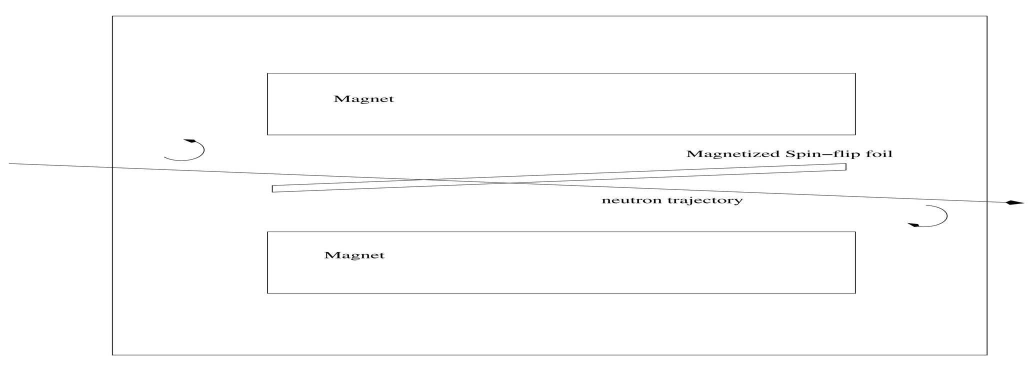

Figure 7: Schematic drawing of a single magnet with magnetized foil.

Instead of the regular SESANS setup with oblique field regions the same effect may be targeted by a setup with pairs of magnets with magnetized foils, acting as spin-flippers in the gap. One advantage of this setup, is that the difficult issue of creating and rpecisely controlling the oblique field regions is avoided. Precise positioning of the foils is vital, but may fairly easily be achieved by utilizing the spin-echo signal of the instrument, and tune the foils until the echo condition is fulfilled. The gray regions act as the inclined magnetic field regions of the regular setup, only with a factor of 2.

Instrument model

We've constructed a mcstas model of the instrument setup at Delft.

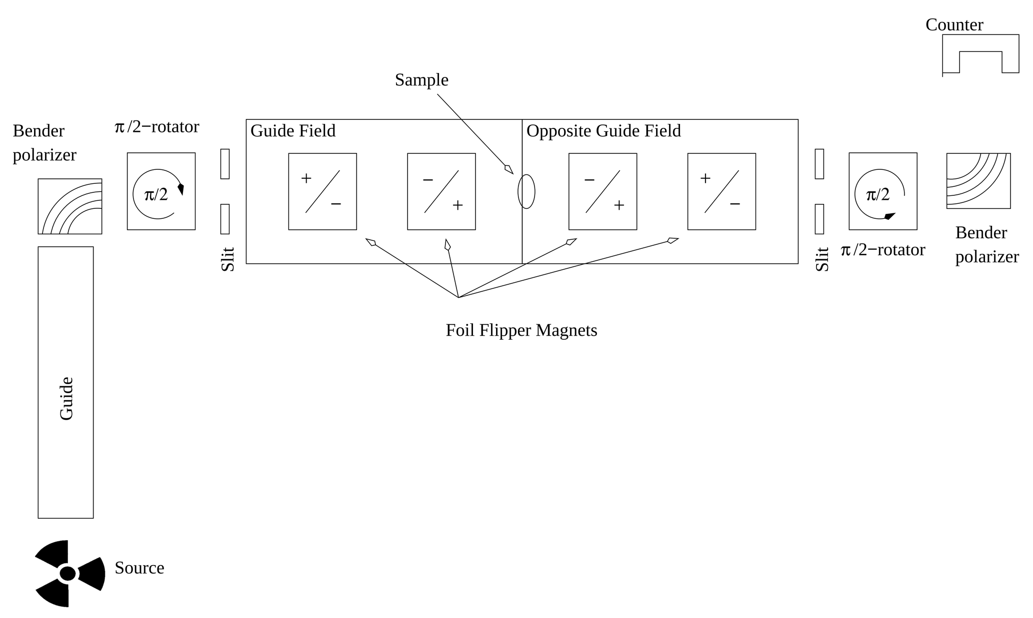

Figure 8: Schematic drawing of the SESANS instrument at Reactor Instituut Delft.

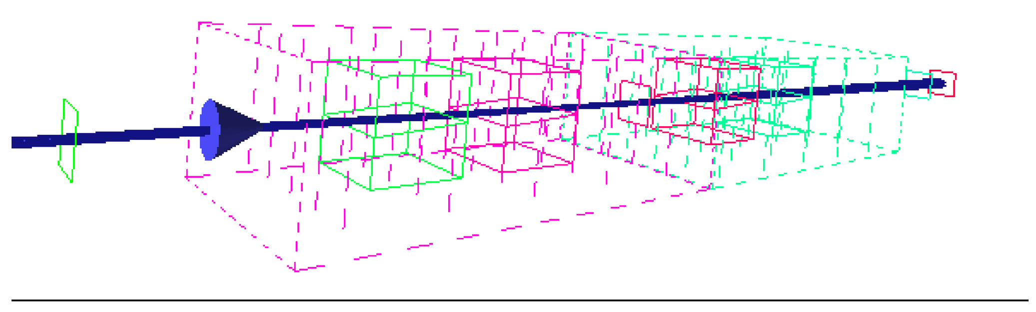

Figure 9: McStas simulation displaying neutron trajectories travelling through a Foil-flipper SESANS setup

An instrument simulation has been constructed to simulate the SESANS instrument in the McStas[6] framework. Although in its early stages, we may follow the neutron trajectories through the instrument (Figure 10).

Limitations in the current model:

- The bender-polarizer is currently a perfect, non-physical component yields a polarization of $\equiv 1$ along the X-axis.
- The Flipper foils are considered infinitesimally thin perfect planes, flipping the spin exactly π.

References

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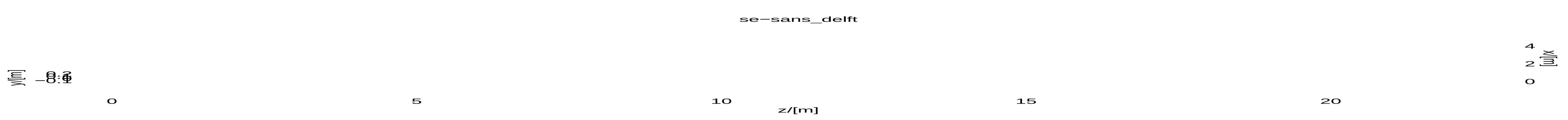

Figure 10: Component plot of the McStas-model of the se-sans instrument