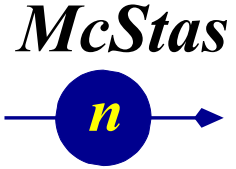
McStas-model of the Delft SE-SANS

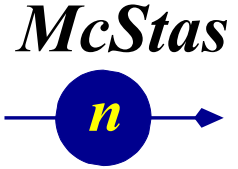
E. Knudsen[1], P Willendrup[1], L. Udby[2], K. Lefmann[2], W. Bouwman[3]

[1]Risø DTU, Denmark
[2]University of Copenhagen, Niels Bohr Institute, Denmark
[3]TU Delft, The Netherlands

PNCMI 2010



Outline



Ray tracing

Monte Carlo Simulation of Triple Axis Spectrometers

- Now used for simulation of any kind of neutron scattering instrument
- Used at all major facilites across the globe

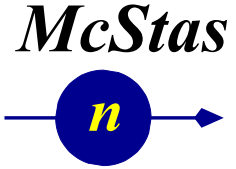
McStas

McStas particulars

- Neutron described as a “ray” with state parameters: position,velocity,time,polarisation vector,weight

$$(x, y, z, vx, vy, vz, t, sx, sy, sz, p)$$

- Components are instrument entities (such as monchromators, guides etc.)
- Instrument file: positions Components relative to each other



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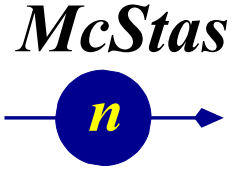

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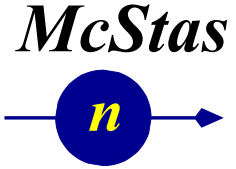

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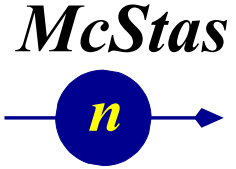

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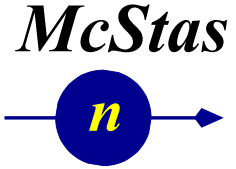

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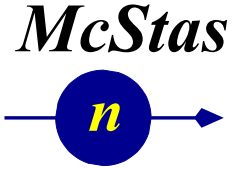

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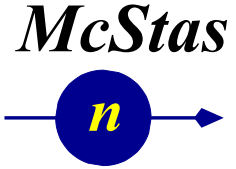

Example Entries I in Instrument file

A circular source (radius 10 cm) aimed at a guide opening 1 m downstream, with main wavelength `Lambda` ± `DL`

```
COMPONENT source = Source_simple(
  radius = 0.01, dist = 1.0,
  focus_xw = 21.5e-3, focus_yh = 80e-3,
  lambda0 = Lambda,dlambda = DL)
AT (0, 0, 0) RELATIVE Origin
```

Example Entries II in Instrument file

Entry into a region with nonzero magnetic field $\mathbf{B} = (0, B_y, 0)$.
Field starts 2 mm after the component `something`

```
COMPONENT guide_field=Pol_simpleBfield(
  xwidth=0.5,yheight=0.3,
  Bx=0, By=By, Bz=0,
  fieldFunction=const_magnetic_field)
AT (0,0,0.002) RELATIVE something
```

... and ends 2.025 m thereafter

```
COMPONENT guide_field_stop=Pol_simpleBfield_stop(
magnet_comp_stop=guide_field)
AT(0,0,2.025) RELATIVE guide_field
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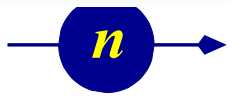

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Virtual Experiments

The aim of the project: Enable **V**irtual **E**xperiments of SE-SANS.

VE What? Lefmann et al JNR **16**(3-4), 97-111 (2008)

- The neutrons rays must have absolute intensity units and should be traced through the whole instrument, from source to detector.
- The description of the instrument should be as close as possible to the reality. This is in particular the case for the sample.
- The virtual instrument is controlled like the real instrument, and the resulting data are analyzed like real data.

VE Why?

- Instrument optimization
- Data analysis
- Teaching

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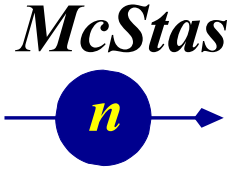


The SE-SANS Technique sketched

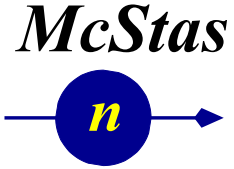
Scattering at small angles gives a difference in flight path through the precession regions on each side of the sample yielding a net precession which causes the beam to depolarise.

SE-SANS measures the transmission of polarisation $P(Z)$ which is directly related to the projection of the autocorrelation function of the sample density distribution along the neutron path.

Spin echo length ("the lengthscale at which sample features are probed"):

$$Z = \frac{c\lambda^2 L < \cot(\theta_0) >_\alpha}{2\pi} B$$

I.e. Z can be scanned by scanning B, λ or L.
In a virtual experiment anything can be scanned.



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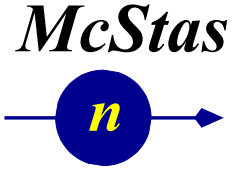
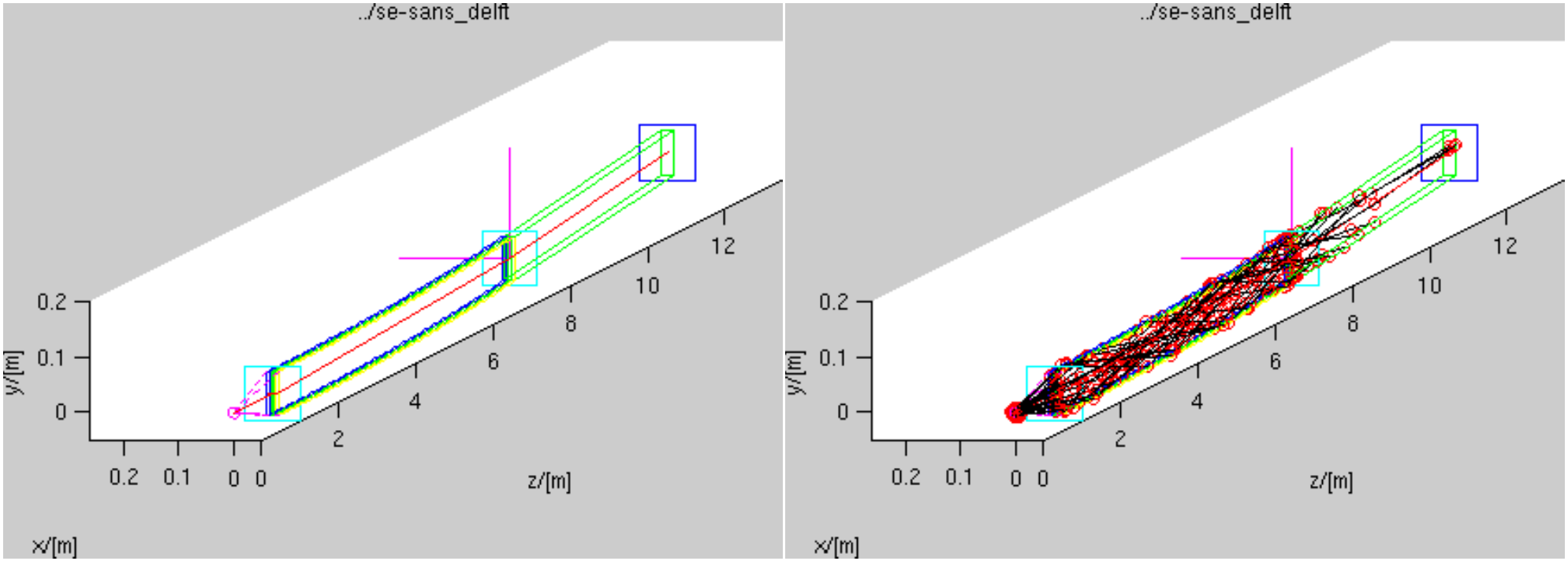


Guide system

The guide system at Delft



Bent triple channel $m = 2$ guide followed by straight $m = 2$ 1-channel. Modelled on the exact dimensions of the Delft reactor guide system

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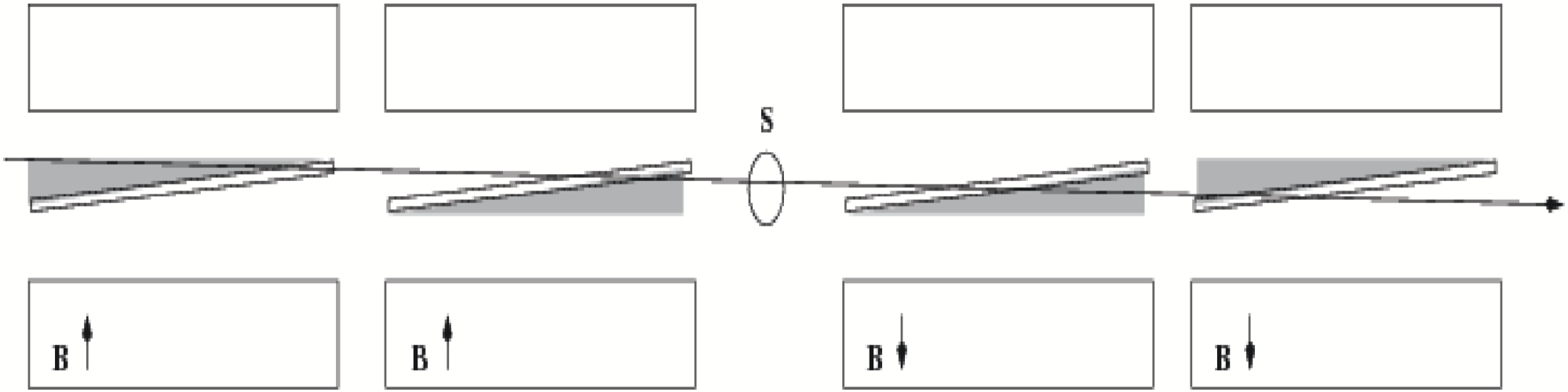
Variant of SE-SANS modelled

Focus on the “magnetized foil flipper” version of SE-SANS.



4 magnets $\rightarrow$ 2 sets of “regular” oblique SE-SANS precession sections $\rightarrow$ factor of 2 in spin echo length:

$$Z = \frac{c\lambda^2 L < \cot(\theta_0) >_\alpha B}{\pi}$$

Rekveldt et al Rev. Sci. Instr. **76**, 033901 (2005)

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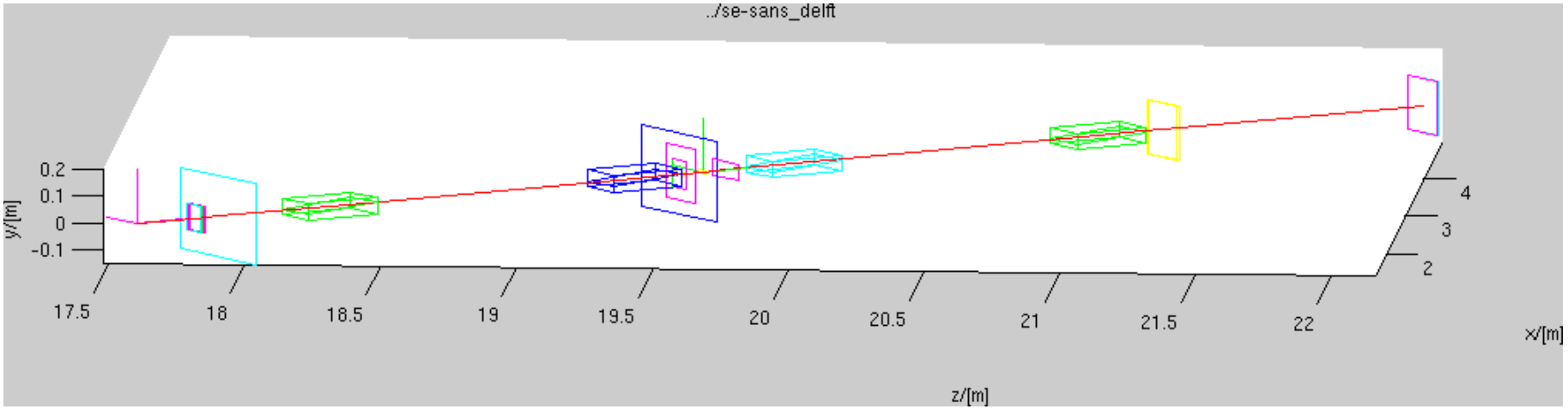
Precession Region

The precession region contains the 4 magnets with magnetized foils. Shown in green, blue, cyan and green.



Varius squares in the beam path (red) represent monitors.

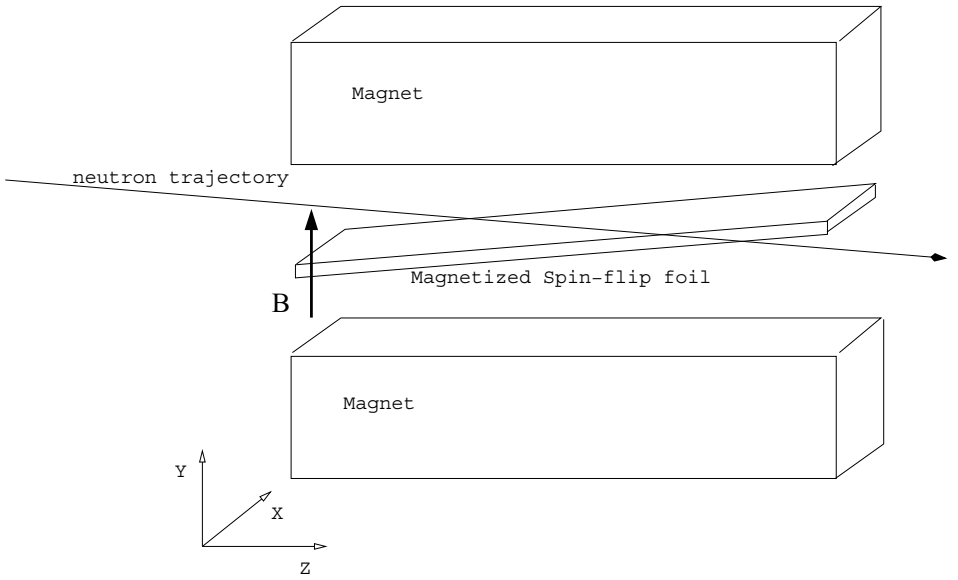
Foil Flipper Magnets

Model is parameterized by:

- Pole shoe geometry.
- Spin-flip foil inclination.
- Magnetic field (correction) function inside.

Ideal: spin-flip in xz-plane.

The error may be corrected by a small $Bz \neq 0$ component.



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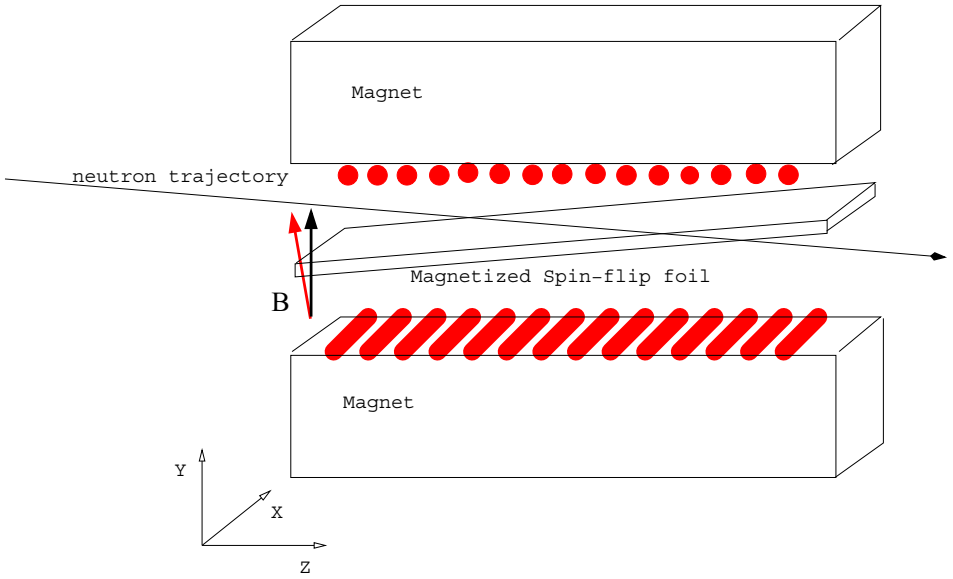

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Polariser/Analyser

Idealized versions.

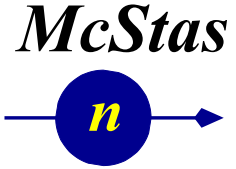
- Polariser (assuming unpolarised beam):

$$I_{in} = I_0,\ \mathbf{P}_{in} = (0,0,0) \quad \Rightarrow \quad I_{out} = \frac{I_{in}}{2}, \mathbf{P}_{out} = (0,1,0)$$

- Analyser:

$$I_{in} = I_0,\ \mathbf{P}_{in} = \mathbf{P} \quad \Rightarrow \quad I_{out} = I_0 \frac{1 + \mathbf{P} \cdot (0,1,0)}{2}, \mathbf{P}_{out} = (0,1,0)$$

. . . for polariser/analyser set to transmit $\mathbf{P} = (0,1,0)$

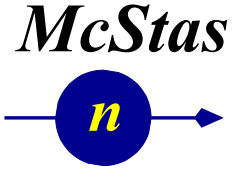


Sample Models

1. Forced Scatterer
2. Vanadium incoherent scatterer
3. Hard dilute spheres

Forced Scatterer

- When scattering, divert neutron by specified 2θ
- Cross section defined by single probability
- Depolarization depends simply on cross section and L



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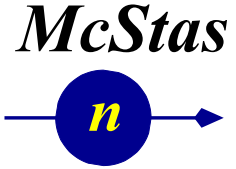
Vanadium incoherent scatterer

- Solely incoherent elastic scattering.
- Probes broad Q-range instrumental response.



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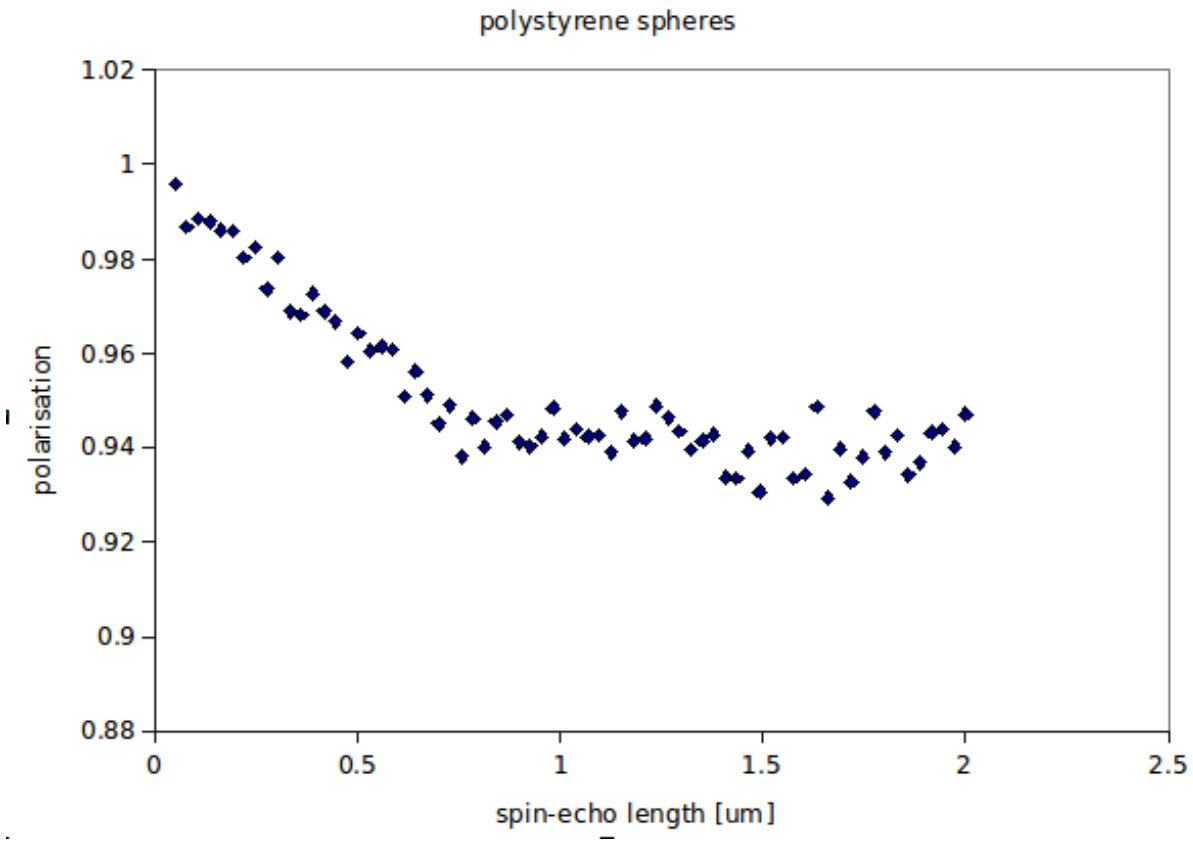
Hard dilute spheres

- Realistic type of sample.
- Testcase is polystyrene in H_2O/D_2O mixture. 55μm diameter spheres.

Results

An example of a real SE-SANS scan at Delft:



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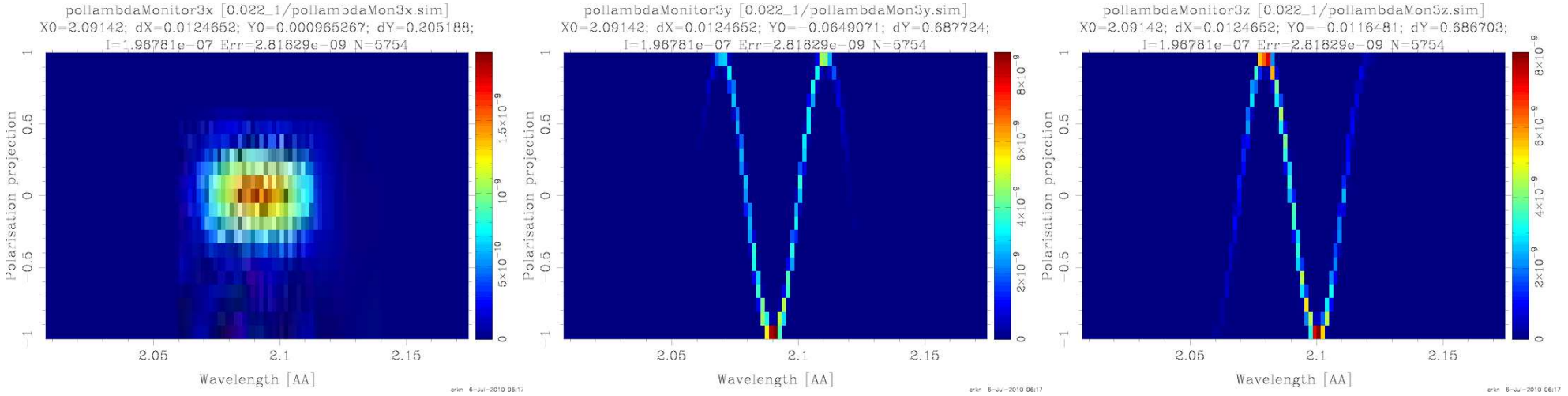
Simulated Results

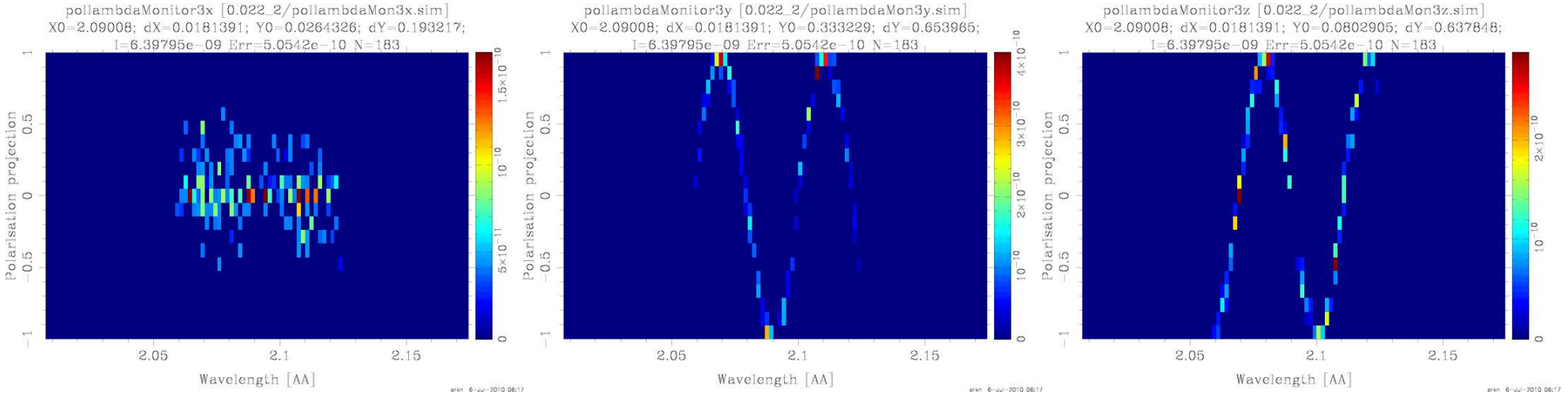
Example results of polarisation vs. wavelength.
sample 1: Forced scatterer



Further analysis will provide direct comparisons to real data.

Simulated Results

Example results of polarisation vs. wavelength.
sample 2: Vanadium incoherent scatterer



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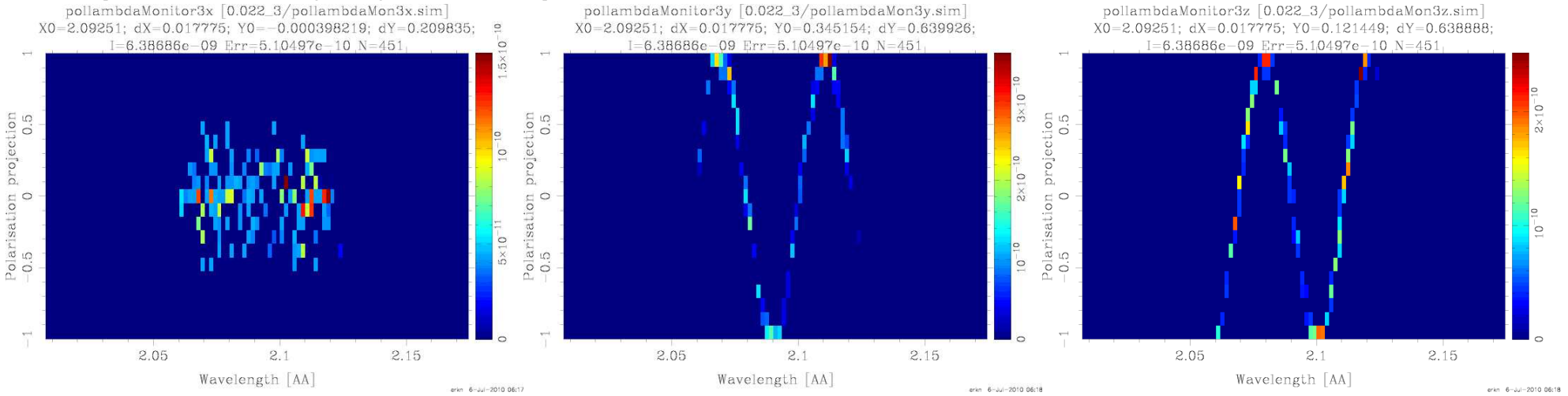
Example results of polarisation vs. wavelength.
sample 3: Polystyrene spheres



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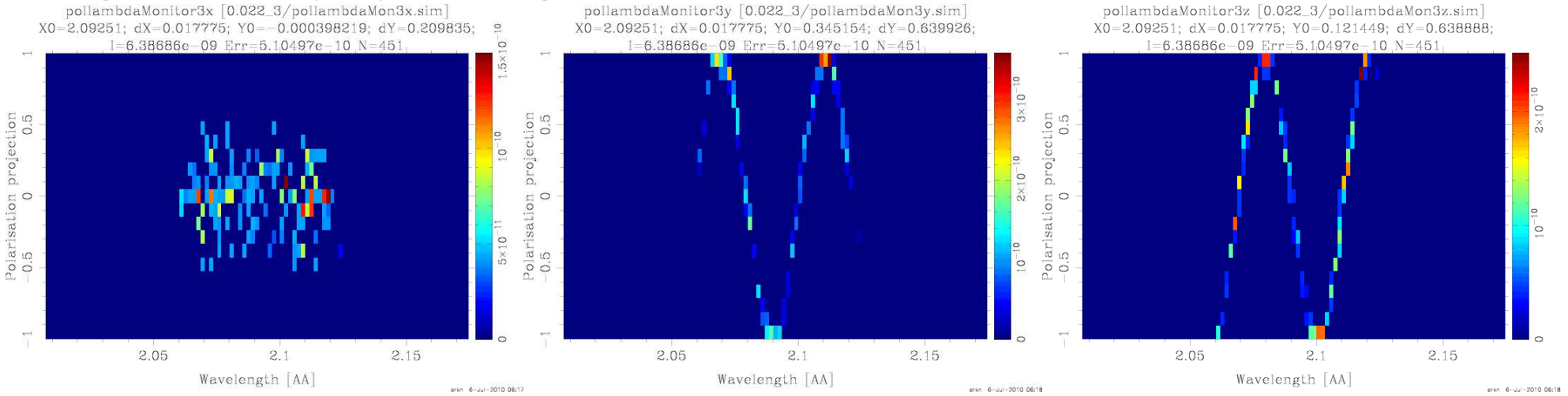

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We are on the way towards Virtual SE-SANS Experiments *but* much needs to be done

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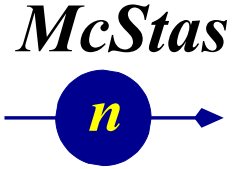
  stray fields, imperfections, read from F.E.M.
- Better source model (spectrum)
- Realistic polariser/analyser



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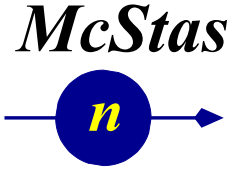

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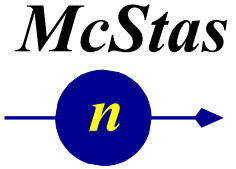

Thank you for your attention!