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McStas

Simulating Polarized Neutron Scattering Experiments and Equipment with McStas

Erik Bergbäck Knudsen, DTU Physics

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Mcstas “particle” model

Neutron ray/package:

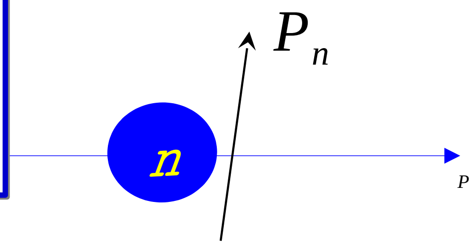
Weight: (p) # neutrons left in the package

Position: (x, y, z)

Velocity: (v_x, v_y, v_z)

Polarization: (s_x, s_y, s_z)

Time: (t)



$$\boldsymbol{P}_n=\frac{1}{p_n}\sum_i^p \boldsymbol{P}_{i,n};\quad n=raynumber$$

$$\boldsymbol{P}=\frac{1}{N}\sum_{n=0}^{N} \boldsymbol{P}_n$$

$$\boldsymbol{P}_{i,n}=2\left(\langle \hat{s}_{x,i}\rangle \hat{i}_{x,i}+\langle \hat{s}_{y,i}\rangle \hat{i}_{y,i}+\langle \hat{s}_{z,i}\rangle \hat{i}_{z,i}\right)$$

From G. Williams: *“Polarized neutrons”, Oxford Science Publ.*, 1988

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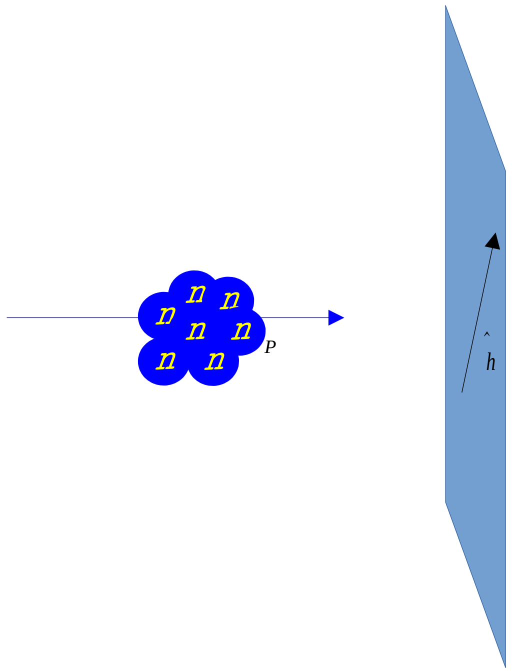
McStas detectors/monitors

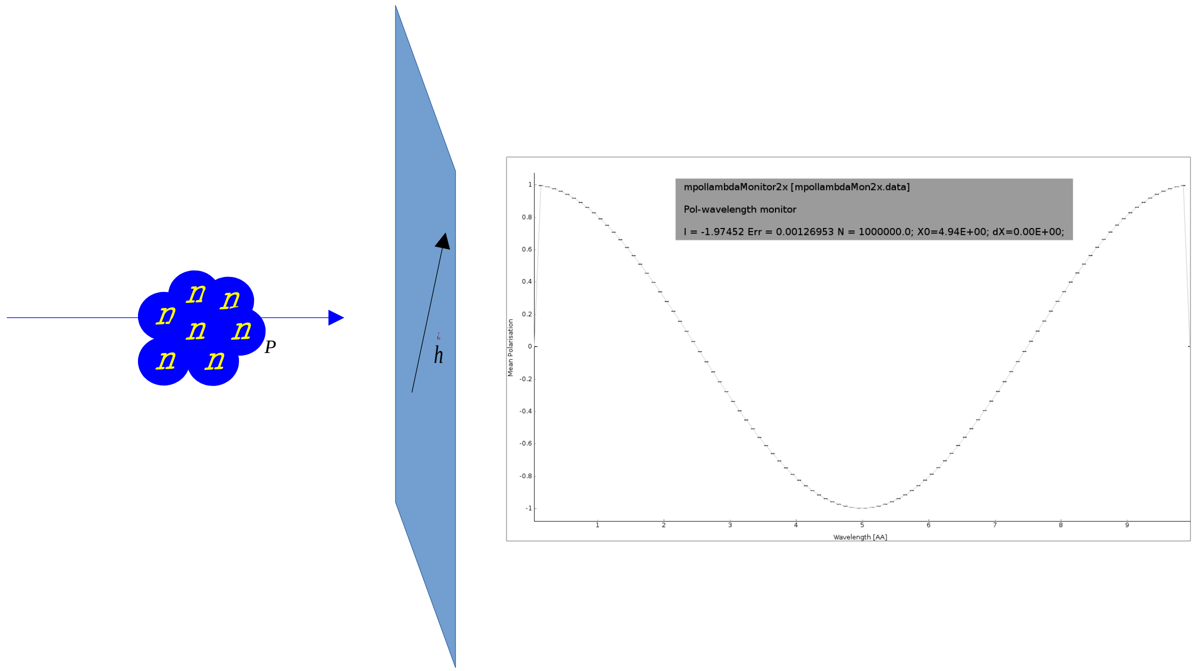
Monitoring: How and What do we monitor?



$$P_{\hat{h}} = \frac{\sum_{n=0}^{N} p_n P_n \cdot \hat{h}}{\sum_{n}^{N} p_n}$$

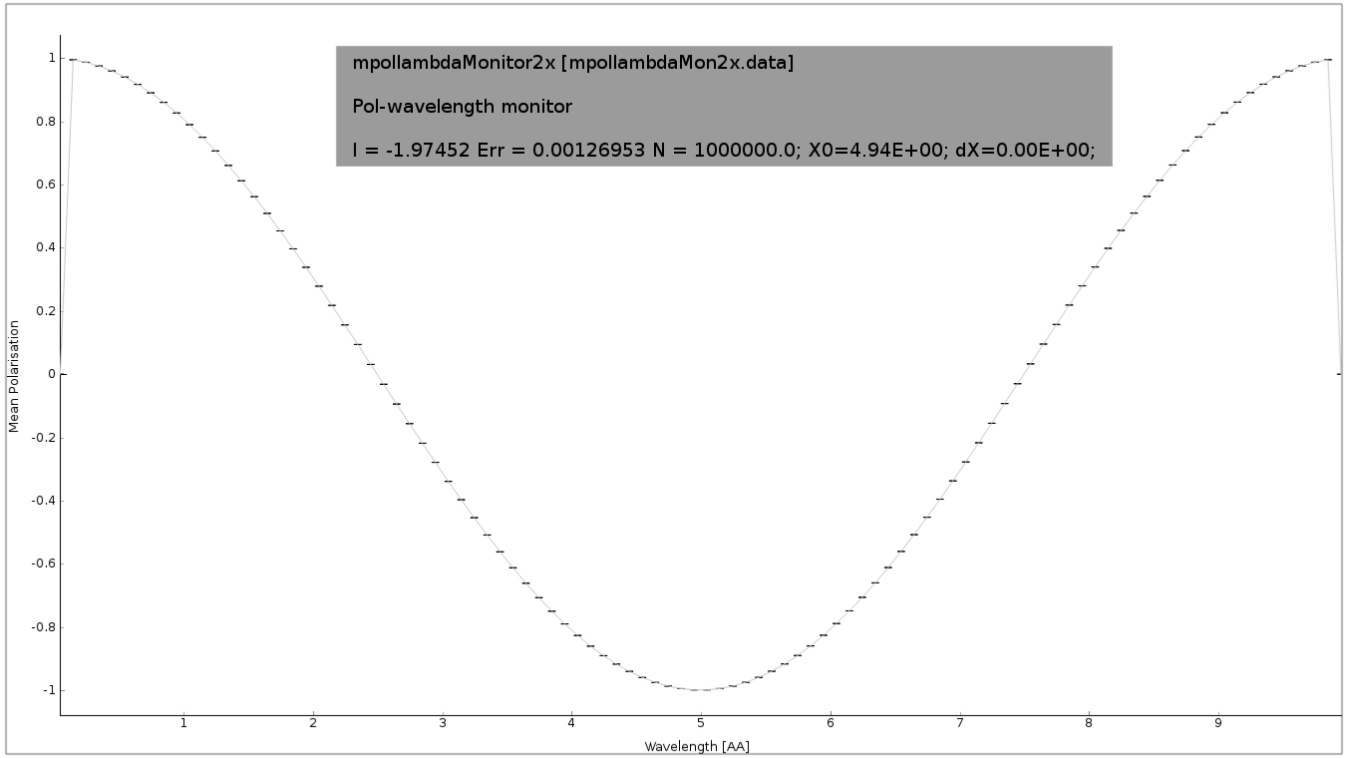
McStas detectors/monitors

Monitoring: How and What do we monitor?



McStas detectors/monitors

Monitoring: How and What do we monitor?



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Polarization monitors

- Available monitors:
- `Pol_monitor.comp`: 0D
- `PolLambda_monitor.comp`: 2D
- `MeanPolLambda_monitor.comp`: 1D

McStas precession algorithm

- Magnetic fields in McStas
- The challenge:
  - Fast beam/ray transport: $\#rays > 10^6$
  - Unknown magnetic field and field strength
  - >1 Magnet → nested fields.

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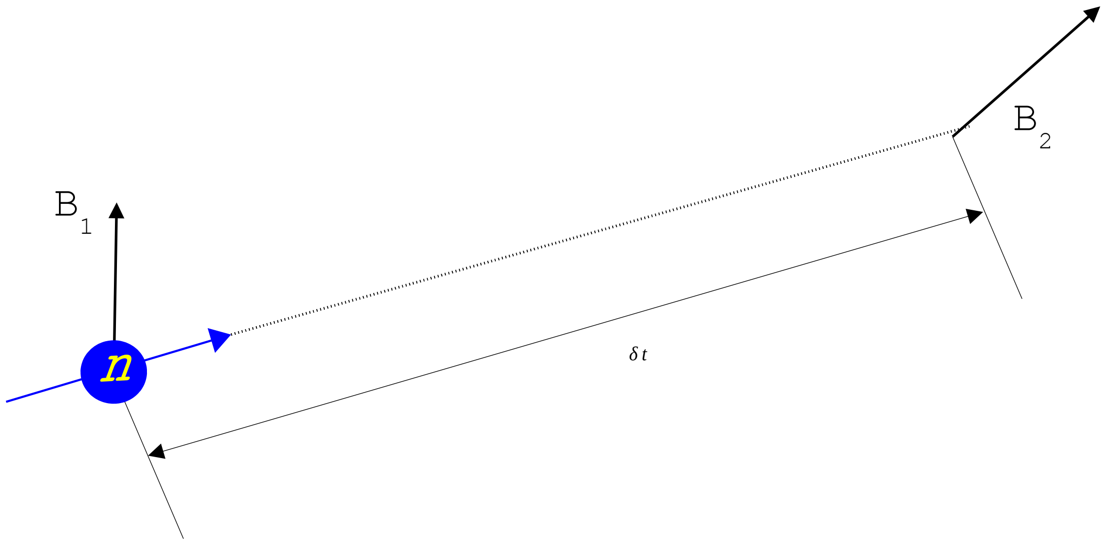
McStas precession algorithm

while $n_t < t_{target}$ **do**
- store neutron;
- sample magnetic field: $\mathbf{B}_1 = \mathbf{B}(n_x, n_y, n_z, n_t)$;
- propagate neutron: $\delta t(< \Delta t)$;
- sample magnetic field: $\mathbf{B}_2 = \mathbf{B}(n_x, n_y, n_z, n_t)$;
- **while** $|\mathbf{B}_1 - \mathbf{B}_2| > \delta B_{threshold}$ **do**
  - restore neutron;
  - $\delta t := \delta t/2$;
  - propagate neutron: $\delta t(< \Delta t)$;
  - sample magnetic field: $\mathbf{B}_1 = \mathbf{B}(n_x, n_y, n_z, n_t)$;
- precess polarization: $\mathbf{P_n}$ by ω around $\frac{\mathbf{B}_1 + \mathbf{B}_2}{2}$;

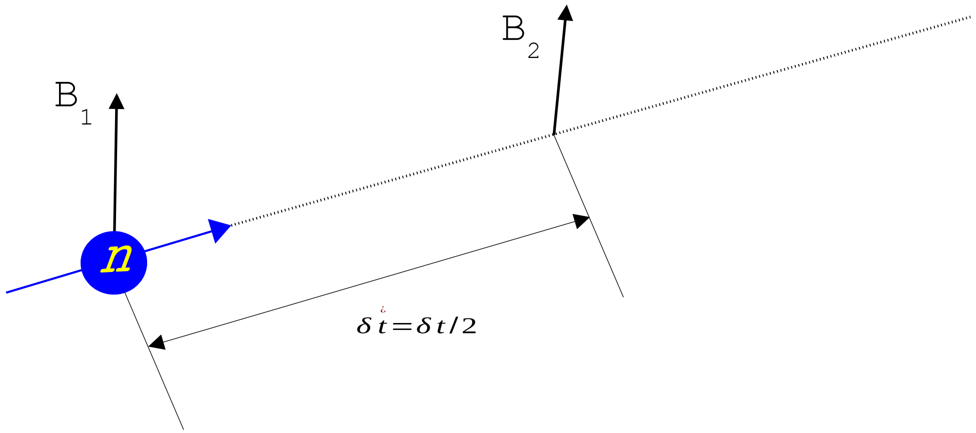
Algorithm 1: SimpleNumMagnetPrecession: Simplistic algorithm for tracking polarization of a Monte-Carlo neutron in a magnetic field. The neutron's state is stored as a position (n_x, n_y, n_z), a velocity $\mathbf{v}$, time n_t, and polarization vector $\mathbf{P_n}$.

From: Knudsen et.al., *J. Neutron Research*, 2014

McStas precession algorithm



McStas precession algorithm



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McStas precession algorithm

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McStas precession algorithm

while $n_t < t_{target}$ **do**
- store neutron;
- sample magnetic field: $\mathbf{B}_1 = \mathbf{B}(n_x, n_y, n_z, n_t)$;
- propagate neutron: $\delta t(\boxed{< \Delta t})$;
- sample magnetic field: $\mathbf{B}_2 = \mathbf{B}(n_x, n_y, n_z, n_t)$;
- **while** $|\mathbf{B}_1 - \mathbf{B}_2| > \boxed{\delta B_{threshold}}$ **do**
  - restore neutron;
  - $\boxed{\delta t := \delta t/2;}$
  - propagate neutron: $\delta t(< \Delta t)$;
  - sample magnetic field: $\mathbf{B}_1 = \mathbf{B}(n_x, n_y, n_z, n_t)$;
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From: Knudsen et.al., *J. Neutron Research*, 2014

McStas precession algorithm

while $n_t < t_{target}$ **do**

store neutron;

sample magnetic f eld

```
void mc_pol_set_timestep(double dt);
```

propagate neutron: δ

sample magnet

while $|\mathbf{B}_1 - \mathbf{B}$

```
void mc_pol_set_angular_accuracy(double domega);
```

restore neutron;

$\boxed{\delta t := \delta t/2;}$

propagate neutron: $\delta t (< \Delta t)$;

sample magnetic f eld: $\mathbf{B}_1 = \mathbf{B}(n_x, n_y, n_z, n_t)$;

precess polarization: $\mathbf{P_n}$ by ω around $\frac{\mathbf{B}_1 + \mathbf{B}_2}{2}$;

Algorithm 1: SimpleNumMagnetPrecession: Simplistic algorithm for tracking polarization of a Monte-Carlo neutron in a magnetic f eld. The neutron's state is stored as a position (n_x, n_y, n_z), a velocity $\mathbf{v}$, time n_t, and polarization vector $\mathbf{P_n}$.

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McStas polarization components

Magnetic fields:
- Pol_FieldBox.comp
- Pol_constBfield.comp
- Pol_Bfield.comp
- Pol_Bfield_stop.comp
- Pol_triafield.comp

Optics:
- Monochromator_pol.comp
- Pol_bender.comp
- Pol_guide_vmirror.comp
- Pol_mirror.comp
- Pol_pi_2_rotator.comp
- Transmission_polarisatorABSnT.comp
- Pol_bender_tapering.comp

Monitors:
- Pol_monitor.comp
- MeanPolLambda_monitor.comp
- PolLambda_monitor.comp

Idealized components:
- PolAnalyser_ideal.comp
- Set_pol.comp

Contrib:
- Foil_flipper_magnet.comp

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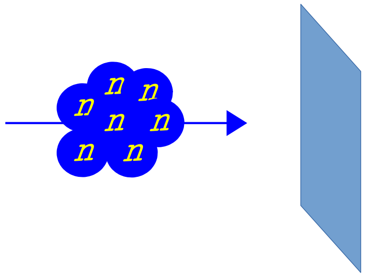
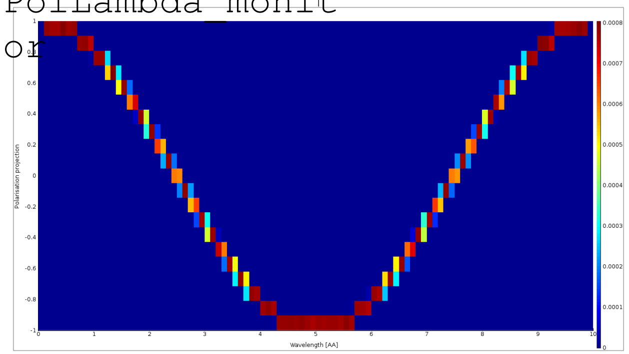
McStas polarization monitors

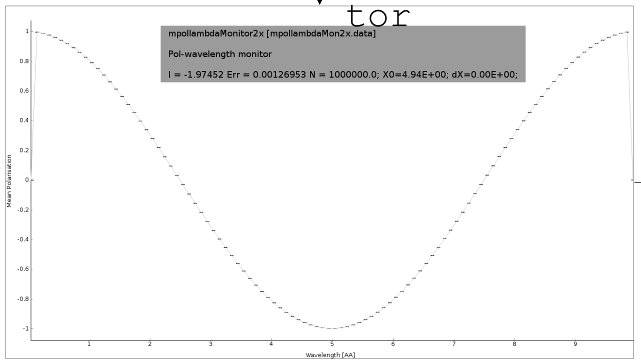
Monitors



PolLambda_monitor



MeanPolLambda_monitor

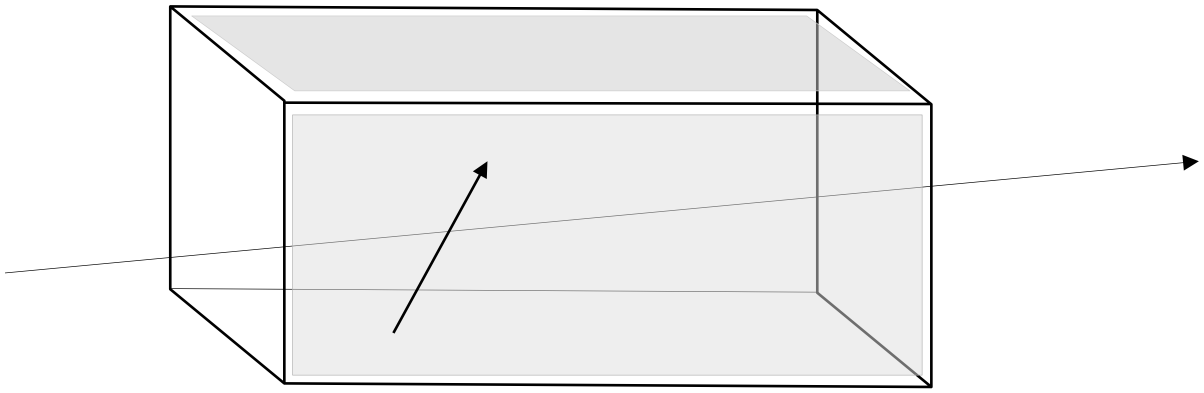


Pol_monitor

$$P \| (m_x, m_y, m_z) = 0.87$$

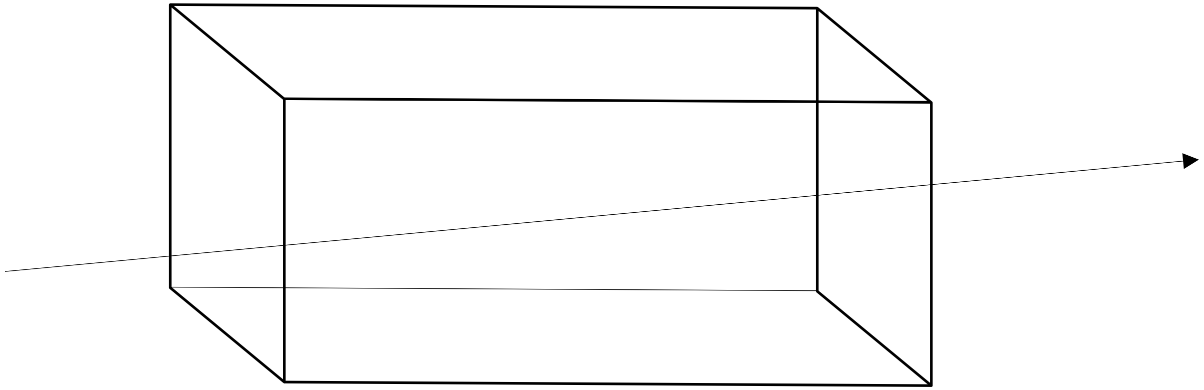
McStas magnetic fields

- `Pol_constBfield.comp`
- Single constant Magnetic field in a "box".
- - user may specify a wavelength to flip.
  - blocking walls



McStas magnetic fields

- `Pol_FieldBox.comp`
- Single Magnetic field in a “box”
- - optional user supplied field c-function



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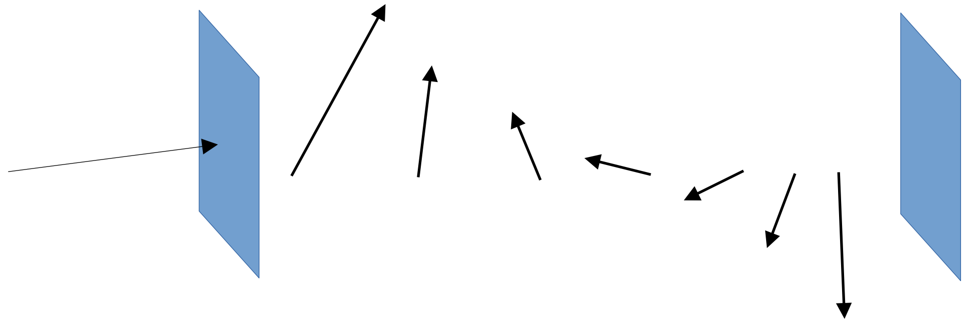
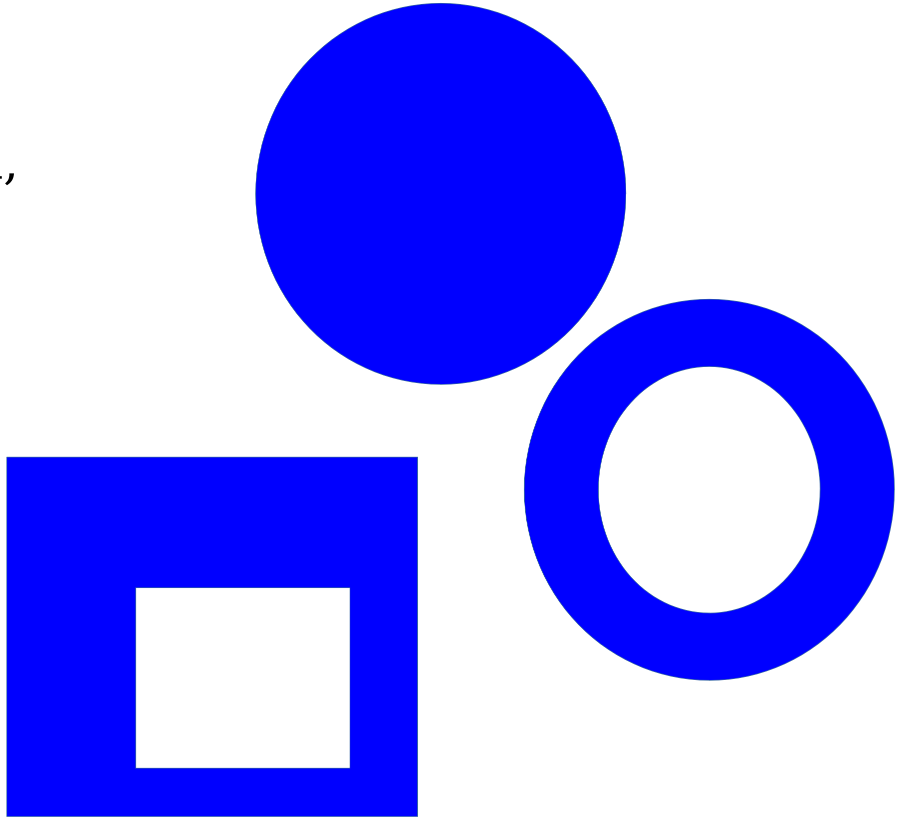
McStas magnetic fields

- `Pol_Bfield.comp`
- `Pol_Bfield_stop.comp`
  - - Entry/Exit contruction allows for nested magnetic field descriptions.
    - Any magnetic fields through user supplied c-function
    - Tabled magnetic fields



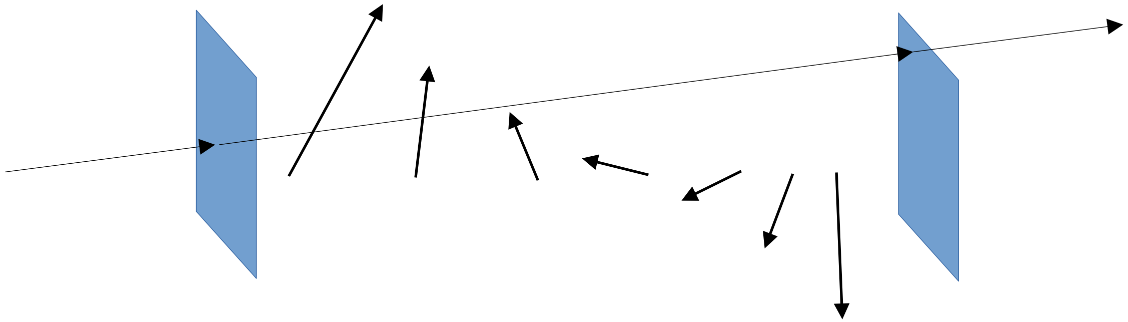
Windows can be many shapes

B-Fields: constant, functional, tabled,
… in more general shapes



McStas Polarization Capabilities IV

- `Pol_simpleBfield.comp`
- `Pol_simpleBfield_stop.comp`
  - - Entry/Exit contruction allows for nested magnetic field descriptions.
    - Any magnetic fields through user supplied c-function
    - Tabled magnetic fields



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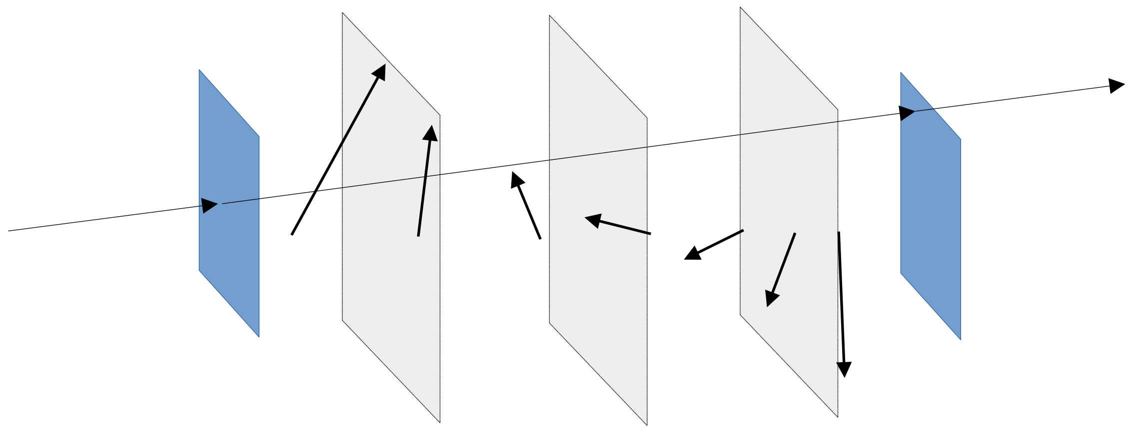
Pol_monitors along the way...



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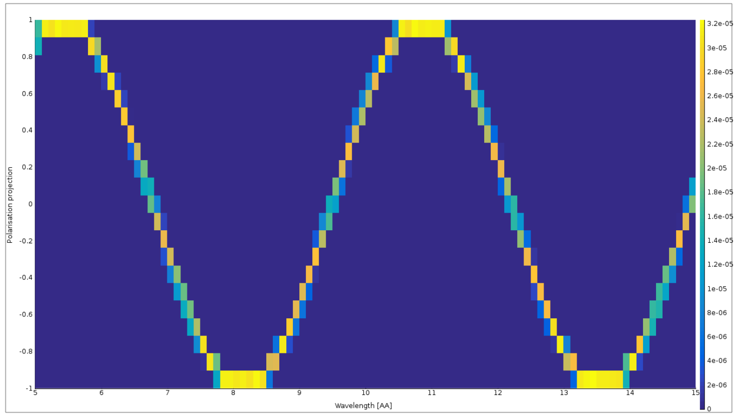

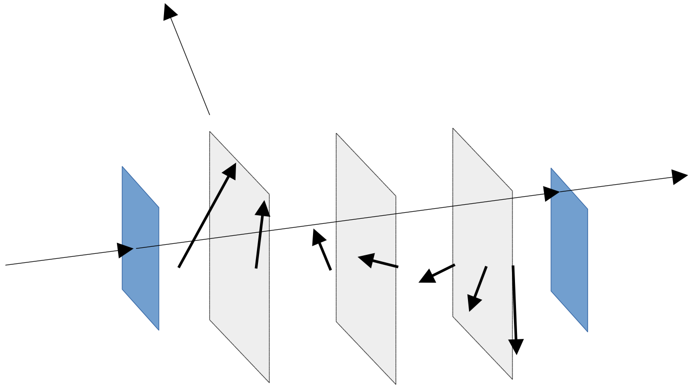

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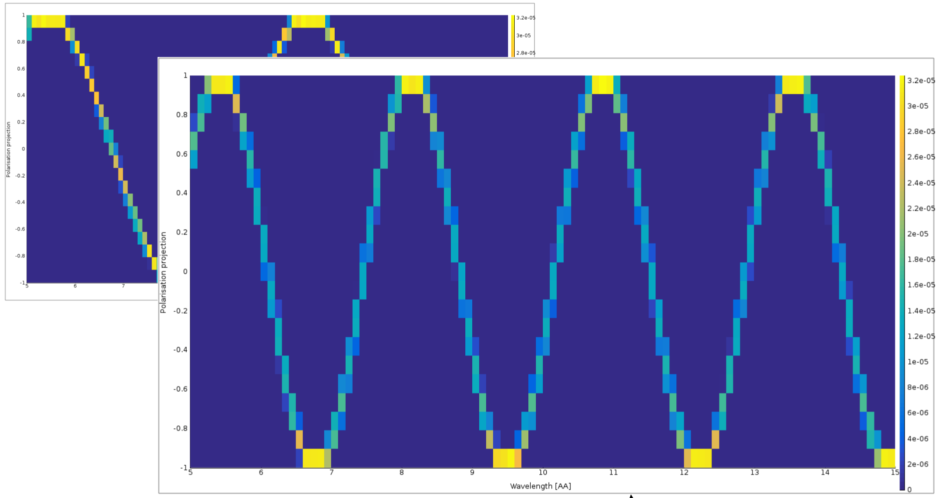
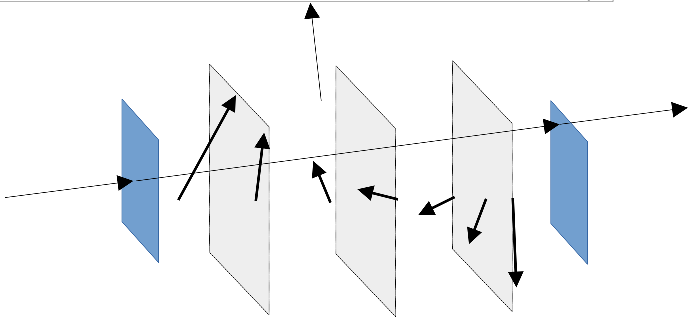
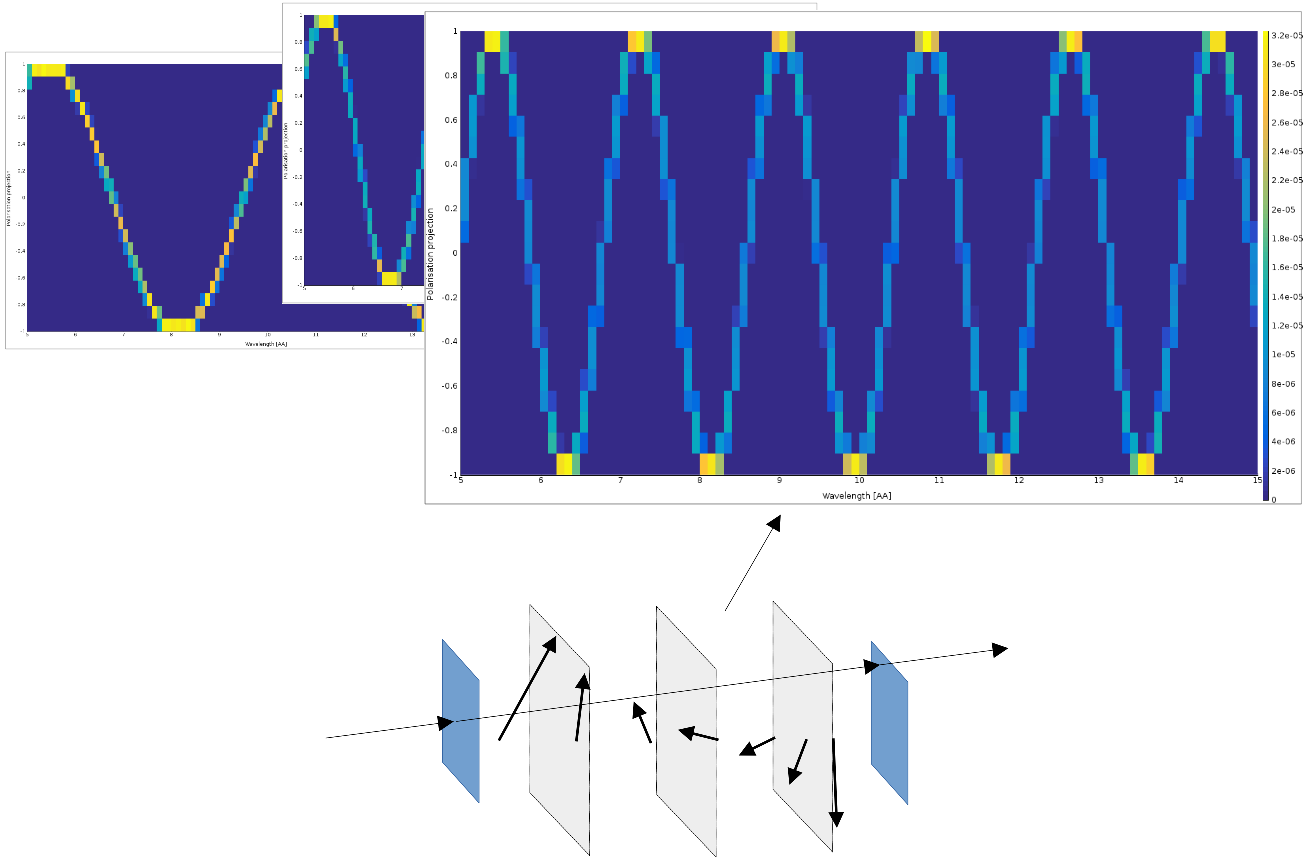
Pol_monitors along the way...

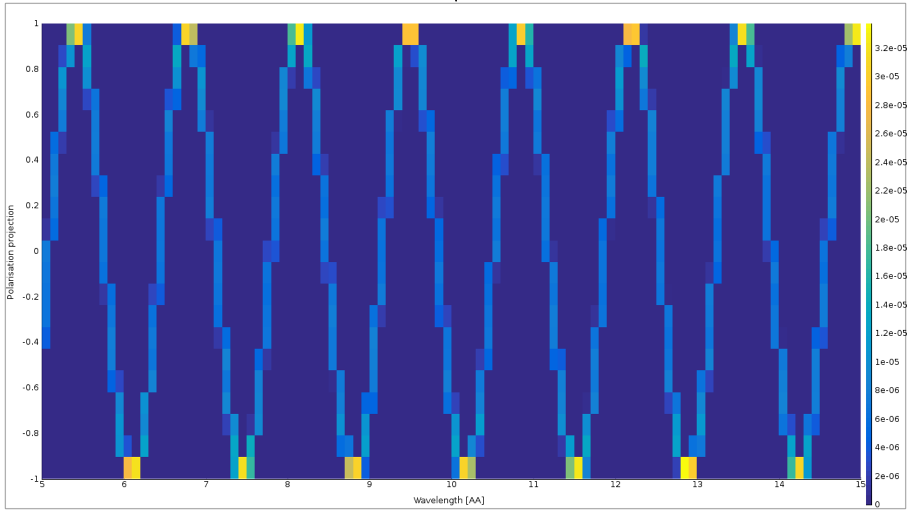


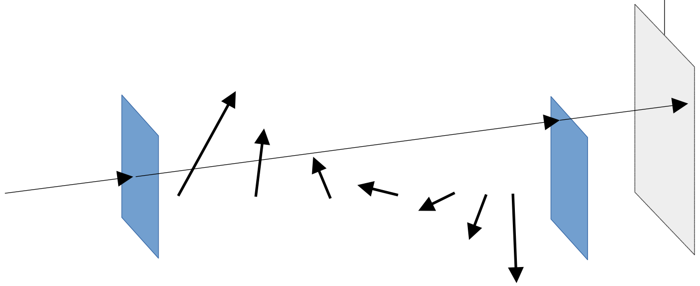


Pol_monitors along the way...



Nested fields





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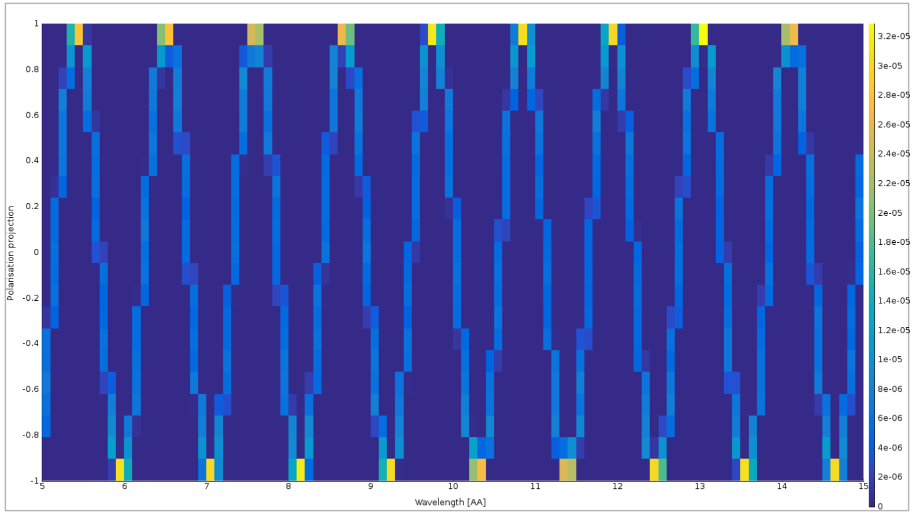
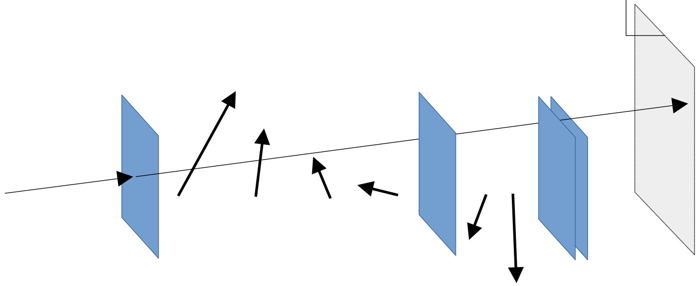
Nested fields





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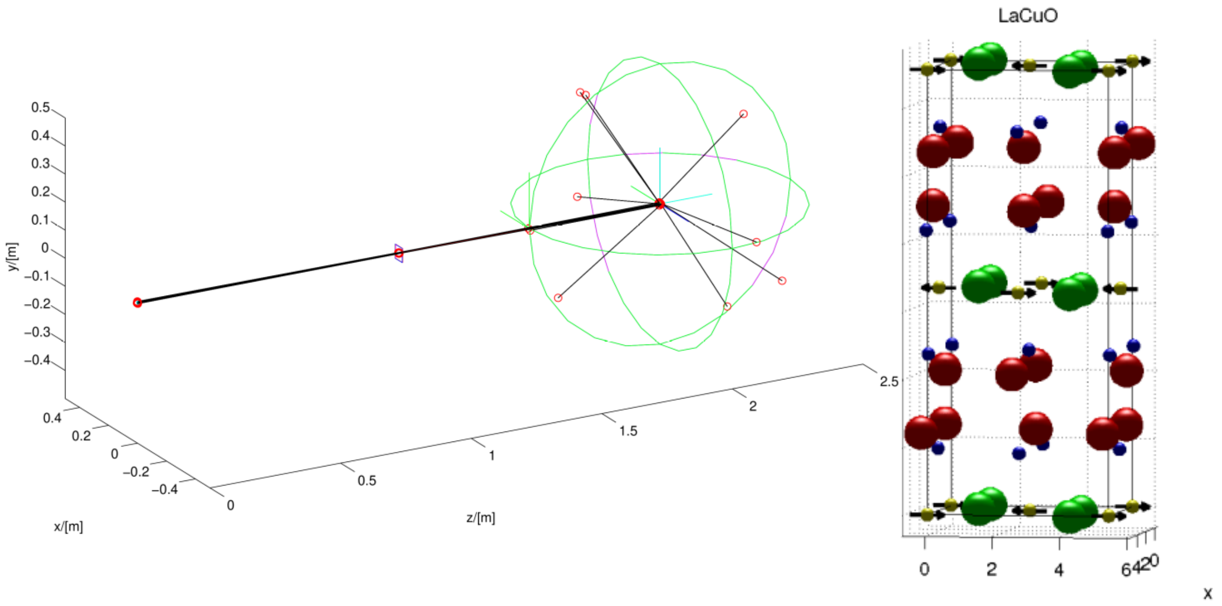
McStas component on the way

Magnetic single crystal



index	iontype	x	y	z	b_{coh}[fm]	g_S	S_x	S_y	S_z	g_L	L_x	L_y	L_z
1	Cu2+	0.5	0.5	0	7.718	2	0	-0.5	0	0	0	0	0
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮

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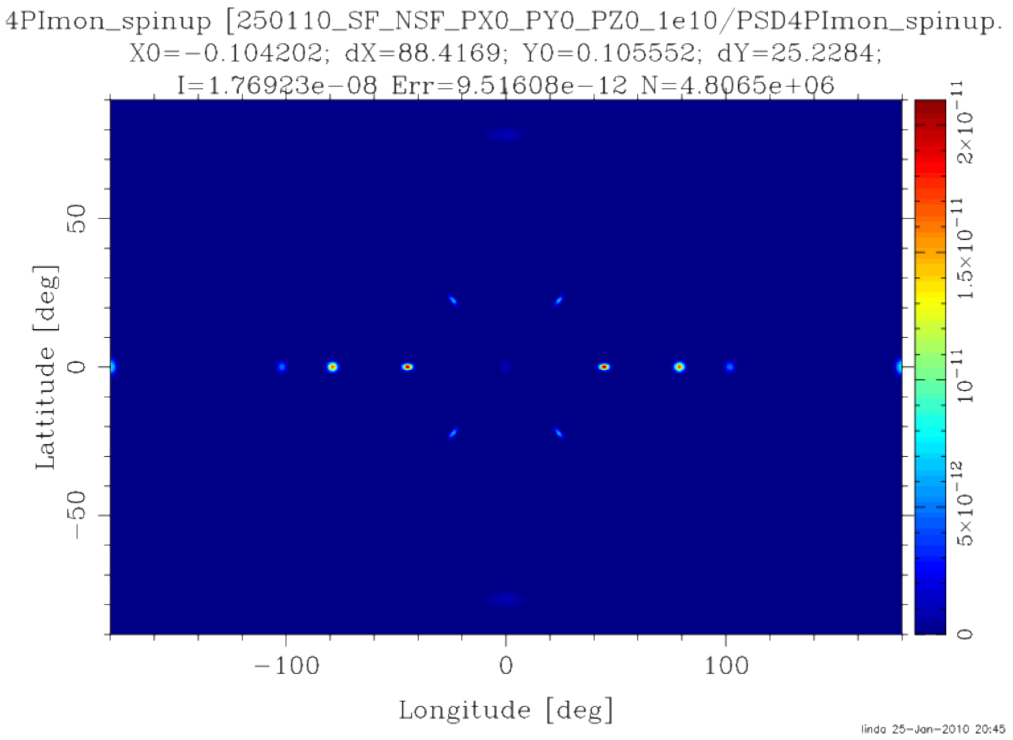
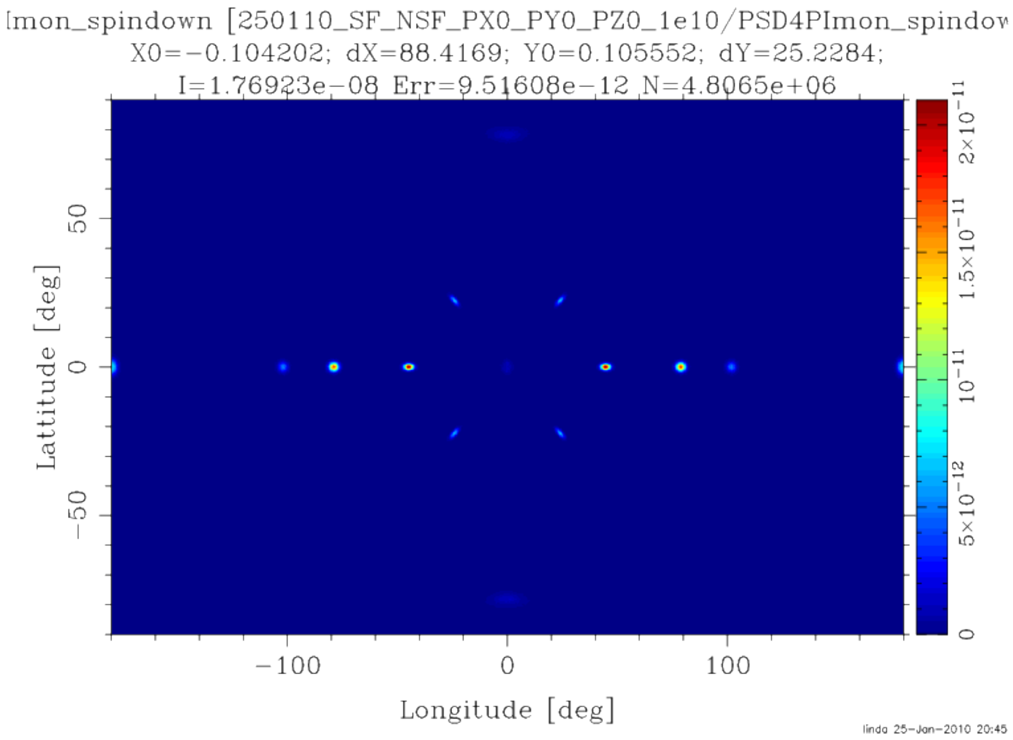
McStas component on the way

Magnetic single crystal – Unpolarized beam





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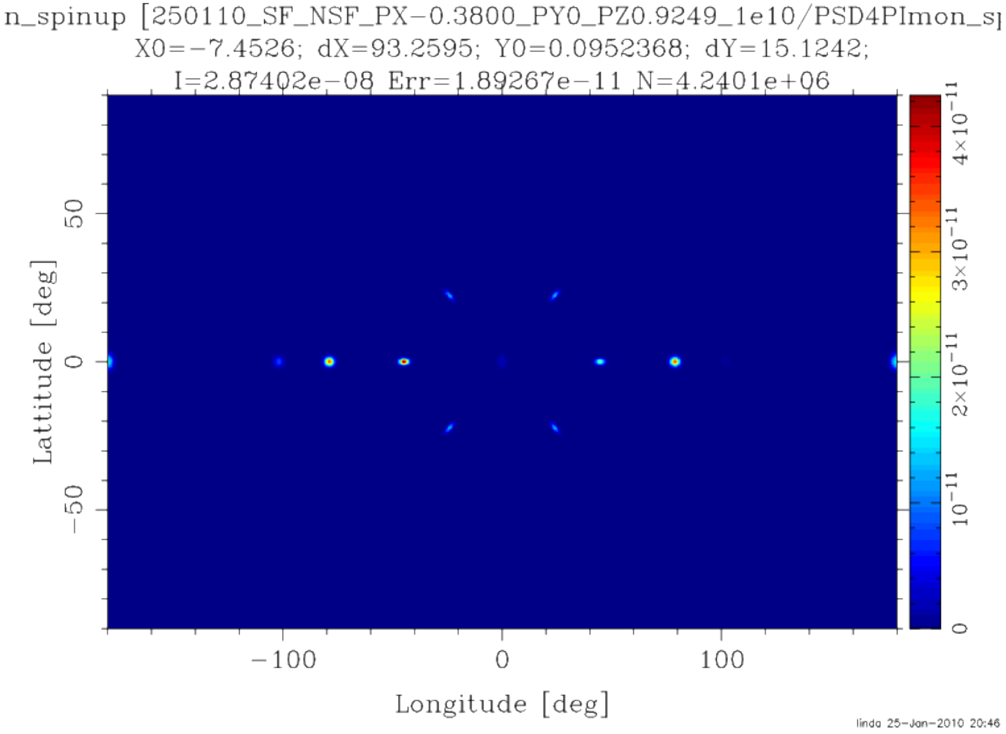
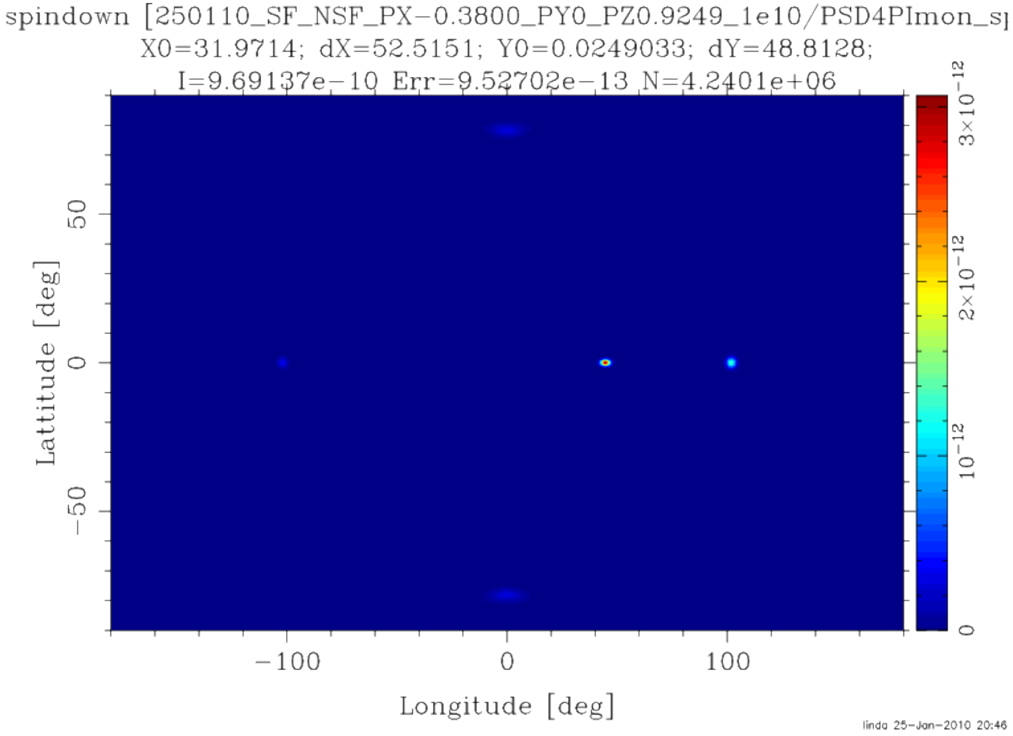
Magnetic single crystal – Polarized beam





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McStas components on the way

Magnetic single crystal

The magnetic scattering cross-section for a sample with localised spin+orbital angular moment $g\mathbf{J} = (g_S + g_L)\mathbf{J} = 2\mathbf{S} + \mathbf{L}$ is:

$$\frac{\mathrm{d}^2\sigma}{\mathrm{d}\Omega_\mathrm{f}\mathrm{d}\mathrm{E}_\mathrm{f}} = \frac{k_f}{k_i}\sum_{i,f} P(\lambda_i)\left|\langle\lambda_f \mid \sum_j e^{i\mathbf{Q}\cdot\mathbf{d}_j}\, U_j^{\sigma_i\sigma_f} \mid \lambda_i\rangle\right|^2 \delta(\hbar\omega + E_i - E_f)$$

where $|\lambda_i\rangle$ and $\langle\lambda_f|$ are the initial and final states of the sample with energies E_i and E_f respectively, $P(\lambda_i)$ is the distribution of initial states and

$$U_j^{\sigma_i\sigma_f} = \langle\sigma_f \mid b_j - m_j\mathbf{J}_{\perp j}\cdot\boldsymbol{\sigma} \mid \sigma_i\rangle$$

where $|\sigma_i\rangle$ and $\langle\sigma_f|$ are the initial and final spin states of the neutron, and $\boldsymbol{\sigma}$ are the Pauli spin matrices working on the neutron state.

From: G. Shirane et.al. ,"Neutron Scattering with Triple-Axis Spectrometer", *Cambridge Univ. Press*, 2002

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McStas components on the way

Magnetic single crystal

If $\mathbf{P} = P(\xi, \eta, \zeta) = P\hat{\zeta}$.Thus, the matrix elements of $U^{\sigma_i \sigma_f}$ can now be written

$$
\begin{aligned}
U^{++} &= b - mJ_{\perp\zeta} \\
U^{--} &= b + mJ_{\perp\zeta} \\
U^{+-} &= -m\left(J_{\perp\xi} + iJ_{\perp\eta}\right) \\
U^{+-} &= -m\left(J_{\perp\xi} - iJ_{\perp\eta}\right)
\end{aligned}
$$

where $m = \frac{r_0\gamma}{2} g f(\mathbf{Q})$ with r_0 the classical electron radius, $\gamma = 1.913$, g the Landé splitting factor and $f(\mathbf{Q})$ the magnetic form factor of a particular ion in the sample.