Erik Bergbäck Knudsen

Polarization in McStas

McStas

Simulating Polarized Neutron Scattering Experiments and Equipment with McStas

Erik Bergbäck Knudsen, DTU Physics

Mcstas “particle” model recap.

Neutron ray/package:

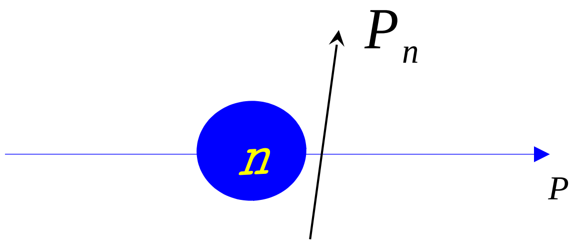
Weight: (p) # neutrons left in the package

Position: (x, y, z)

Velocity: (v_x, v_y, v_z)

Polarization: (s_x, s_y, s_z)

Time: (t)



“sub ray” level

$$P_{i,n} = 2\left(\langle \widehat{s_{x,i}} \rangle \widehat{i_{x,i}} + \langle \widehat{s_{y,i}} \rangle \widehat{i_{y,i}} + \langle \widehat{s_{z,i}} \rangle \widehat{i_{z,i}} \right)$$

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

Ray level

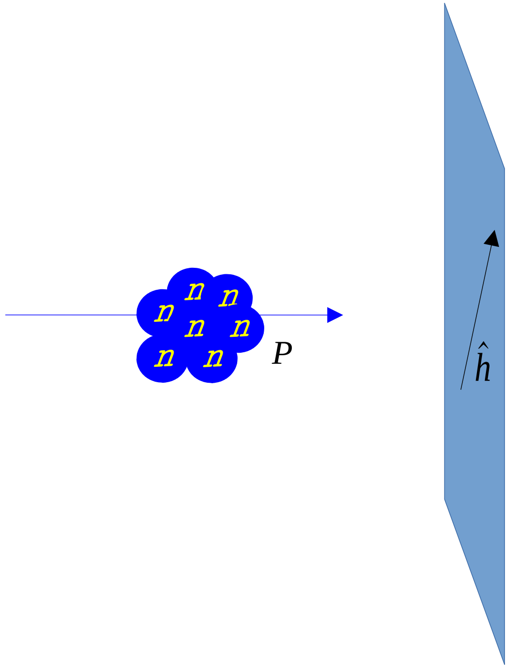
$$P_n = \frac{1}{p_n} \sum_{i}^{p} P_{i,n} ; n = raynumber$$

Beam level

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

McStas detectors/monitors

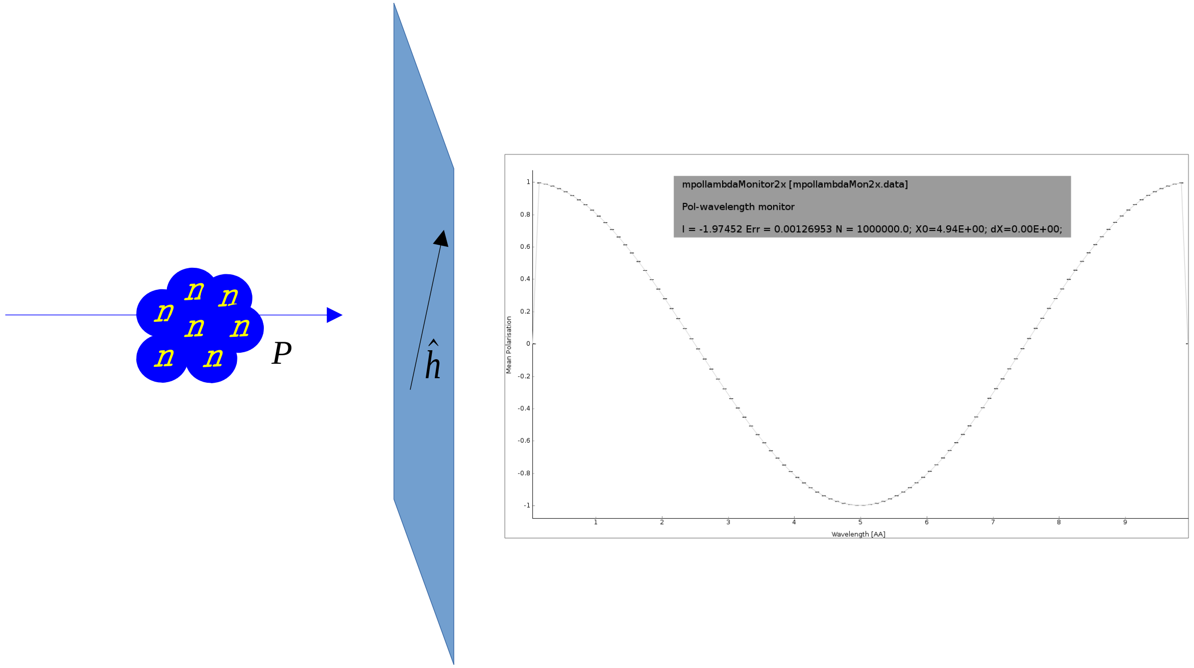
Monitoring: How and What do we monitor?



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

McStas detectors/monitors

Monitoring: How and What do we monitor?



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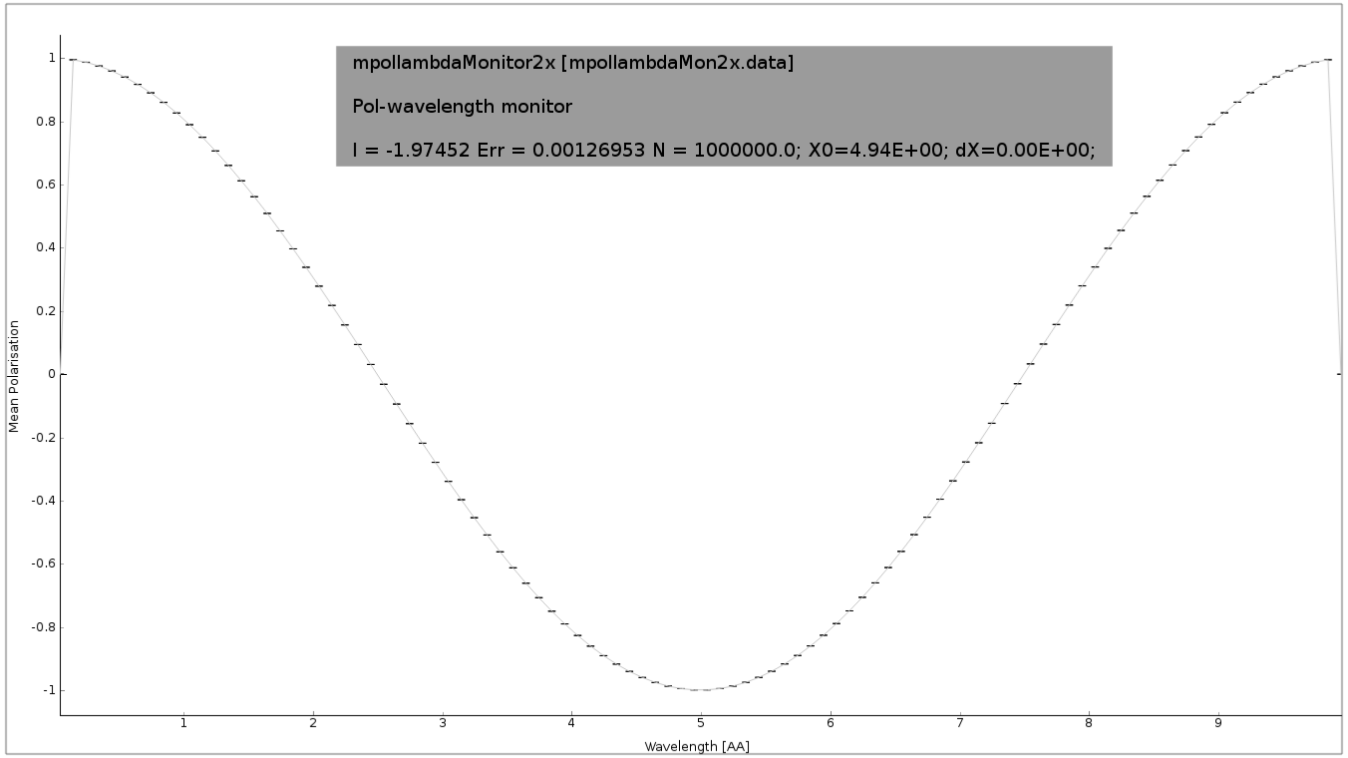
McStas detectors/monitors

Monitoring: How and What do we monitor?

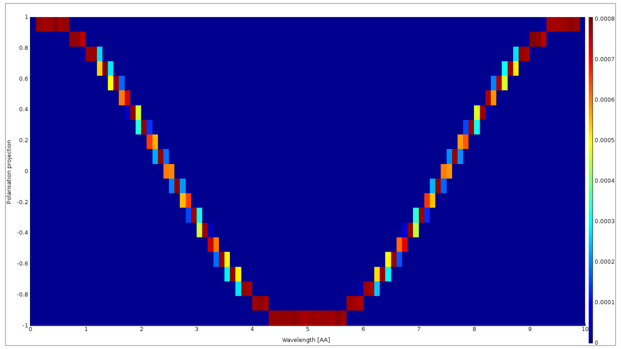


Polarization monitors

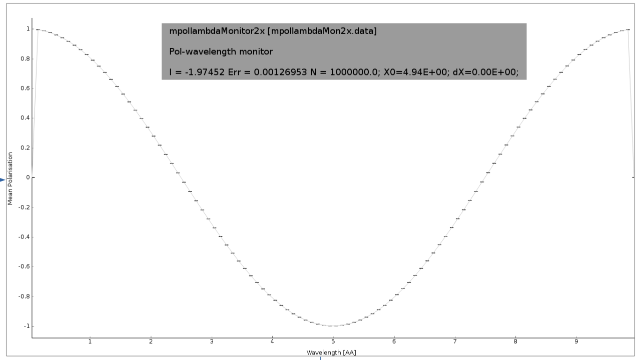
- Available monitors:
- `Pol_monitor.comp`: 0D
- `PolLambda_monitor.comp`: 2D
- `MeanPolLambda_monitor.comp`: 1D

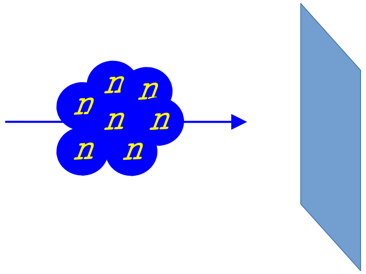
McStas polarization monitors

PolLambda_monitor



MeanPolLambda_monitor





Pol_monitor

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

Polarization components in McStas 2.7

Magnetic fields:

- Pol_FieldBox.comp
- Pol_constBfield.comp
- Pol_Bfield.comp
- Pol_Bfield_stop.comp
- Pol_triafield.comp

Monitors:

- Pol_monitor.comp
- MeanPolLambda_monitor.comp
- PolLambda_monitor.comp

Contrib:

- Foil_flipper_magnet.comp
- Single_magnetic_crystal.comp

Sample:

- Single_magnetic_crystal.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
- Pol_straight_tapering.comp
- He3_cell.comp
- RF_flipper.comp

Idealized components:

- PolAnalyser_ideal.comp
- Set_pol.comp

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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.

McStas precession algorithm

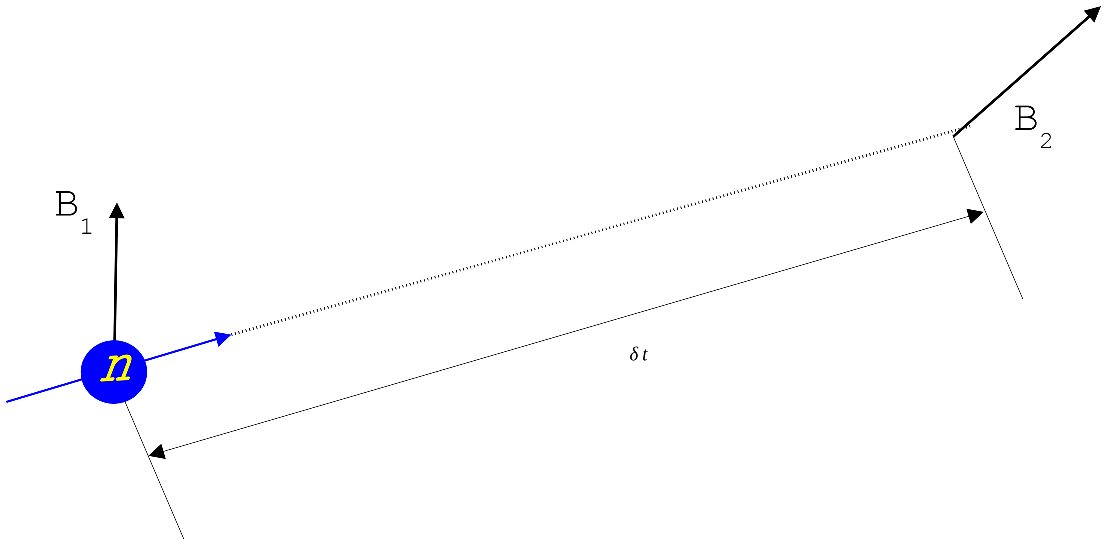
while $n_t < t_{target}$ **do**

- 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 $\frac{\mathbf{B}_1 + \mathbf{B}_2}{2}$;

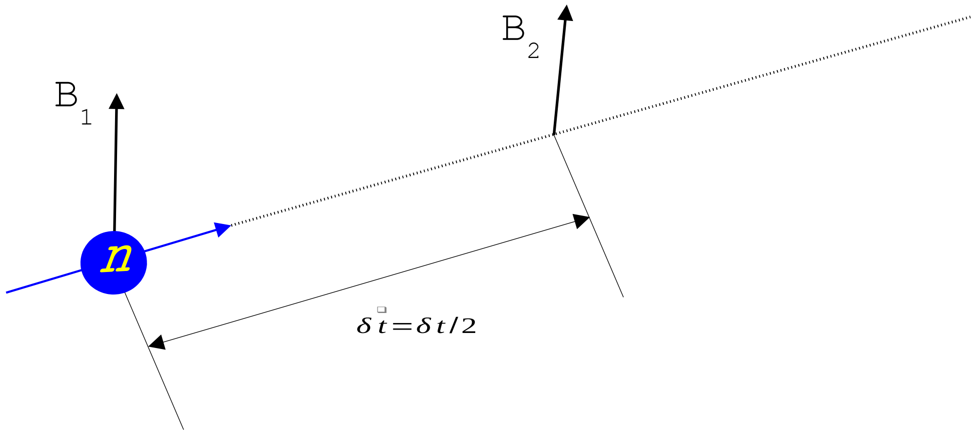
Algorithm 1: SimpleNumMagnetPrecession: Simplistic algorithm for tracking polarization of a Monte-Carlo neutron in a magnetic field. The neutron's state is stored as a position (n_x, n_y, n_z), a velocity $\mathbf{v}$, time n_t, and polarization vector $\mathbf{P_n}$.

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

McStas

McStas precession algorithm

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

store neutron;

sample magnetic field

propagate neutron: δ

sample magnet

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

restore neutron;

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

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

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

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

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

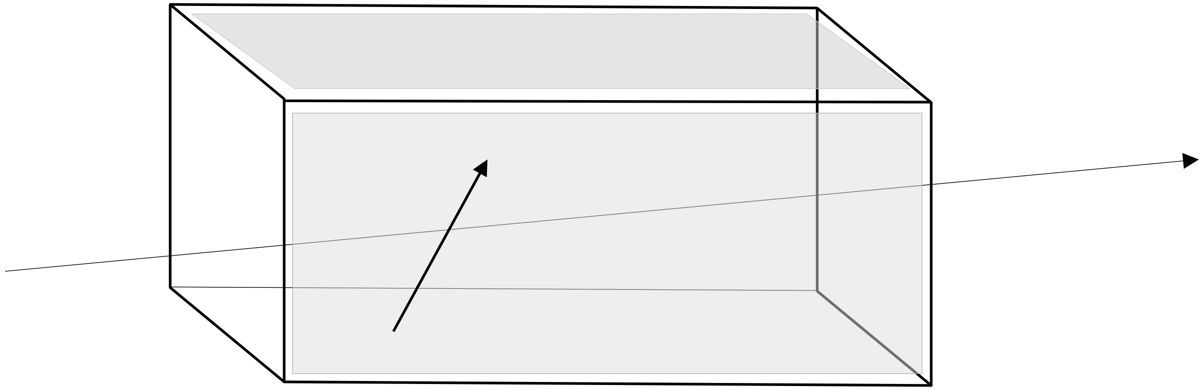
```
void mc_pol_set_angular_accuracy(double domega);
```

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

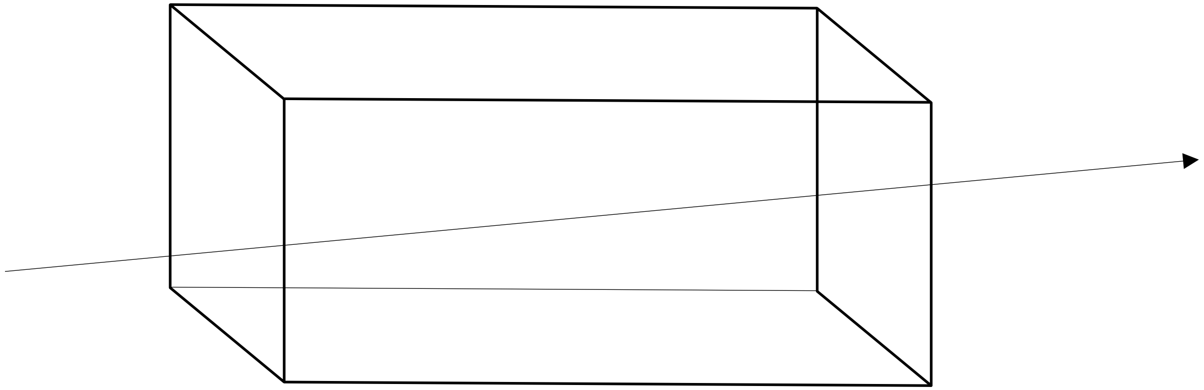
McStas magnetic fields

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



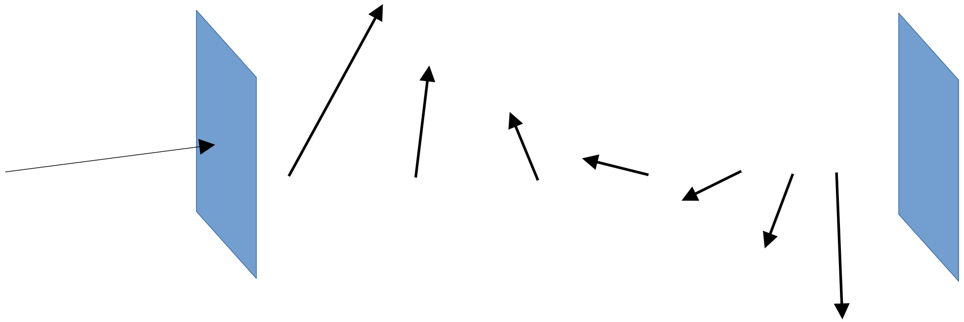
McStas magnetic fields

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



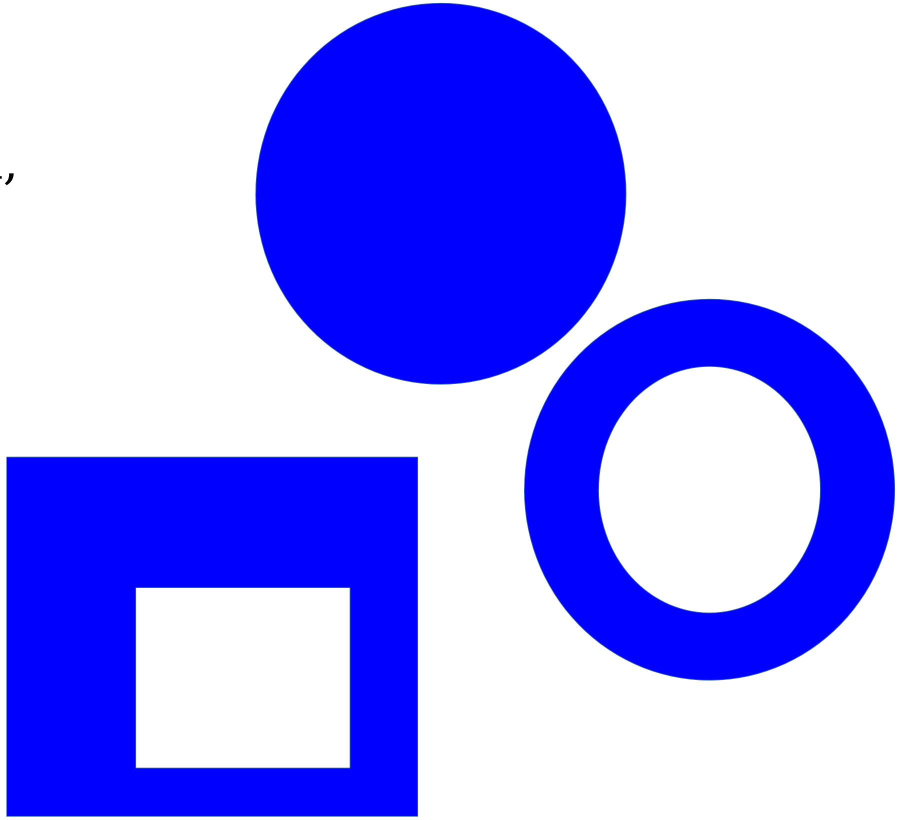
McStas magnetic fields

- `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



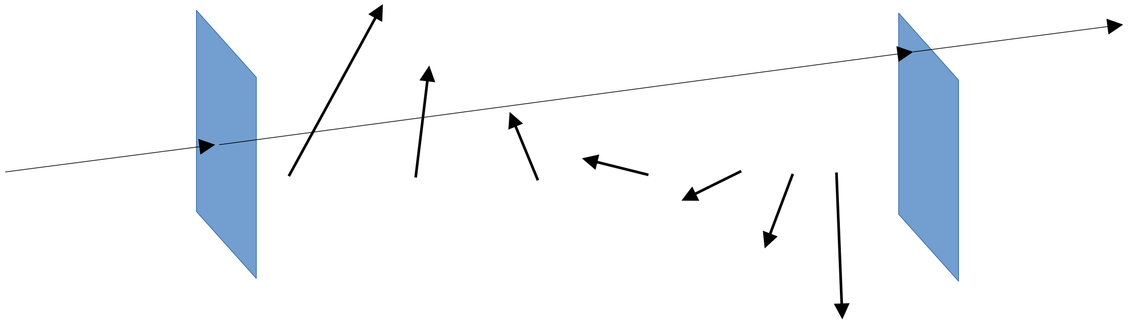
Windows can be many shapes

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



McStas Polarization Capabilities IV

- `Pol_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



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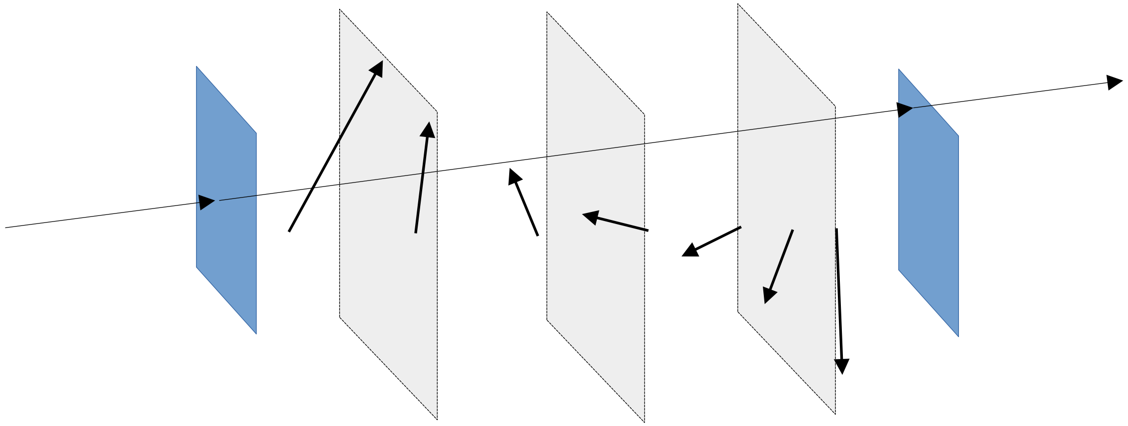
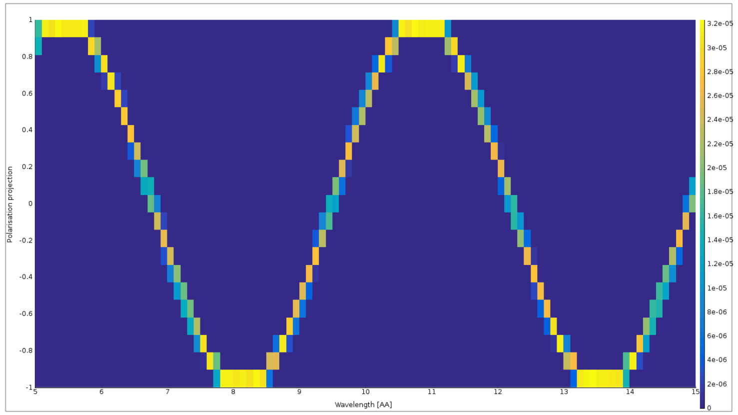
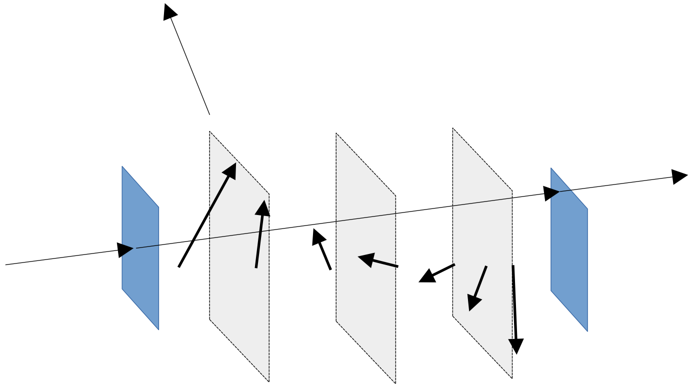
Pol_monitors along the way...



Pol_monitors along the way...





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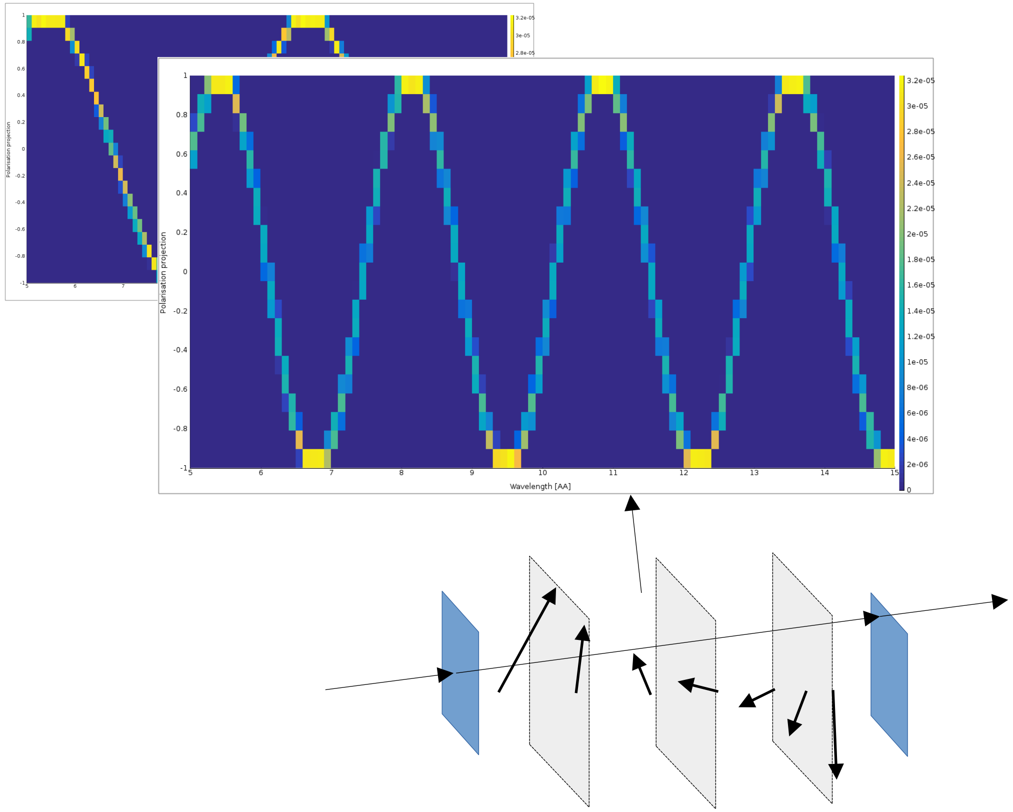
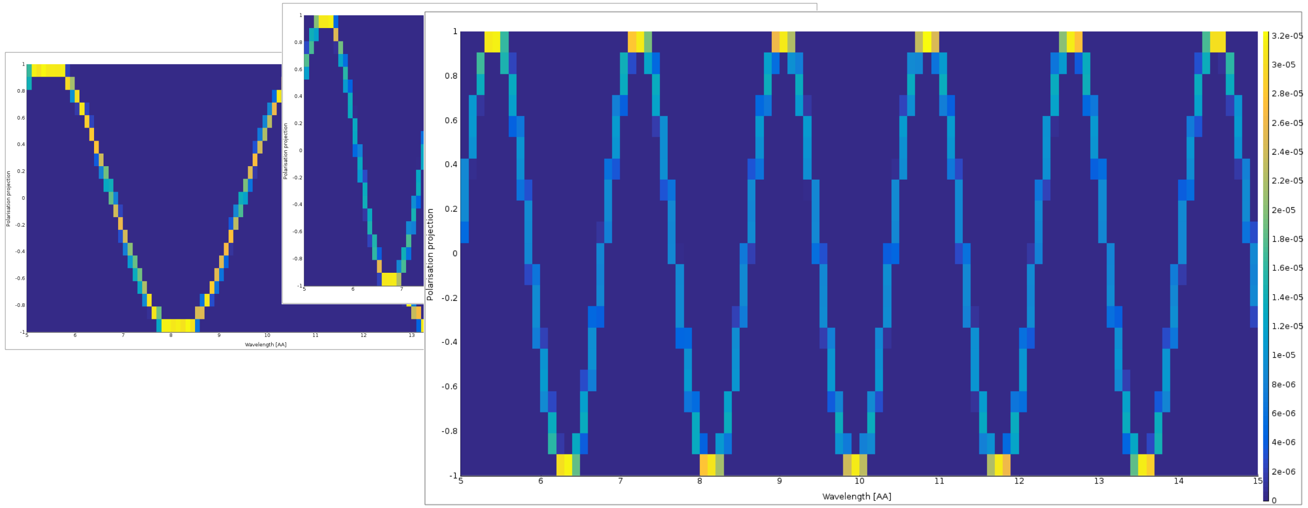
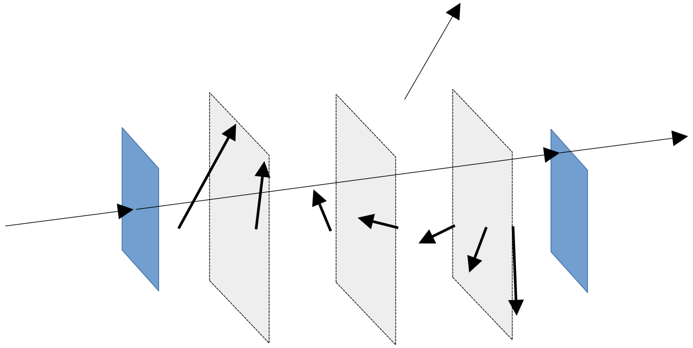
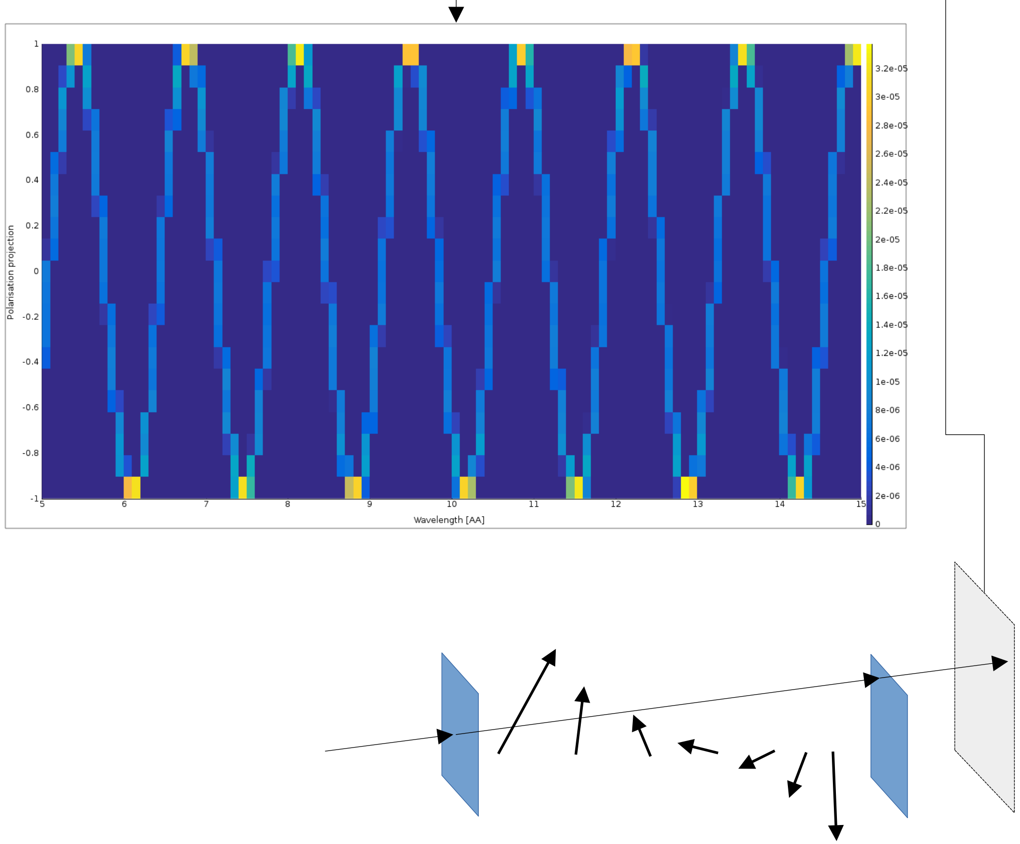


Pol_monitors along the way...

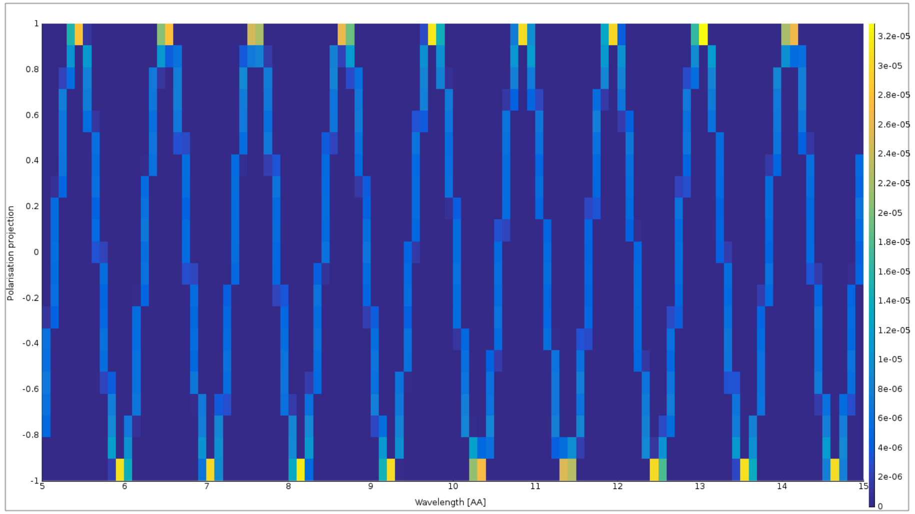


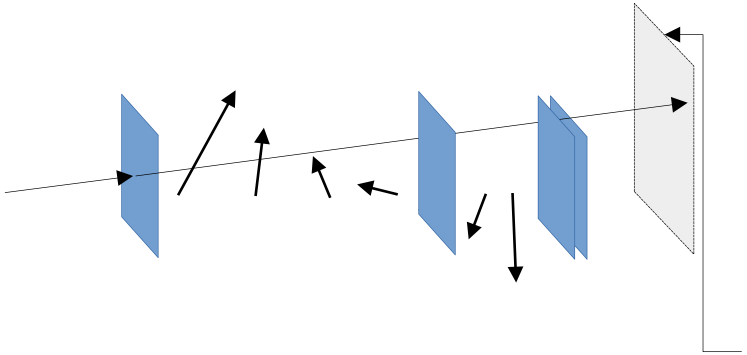


Nested fields

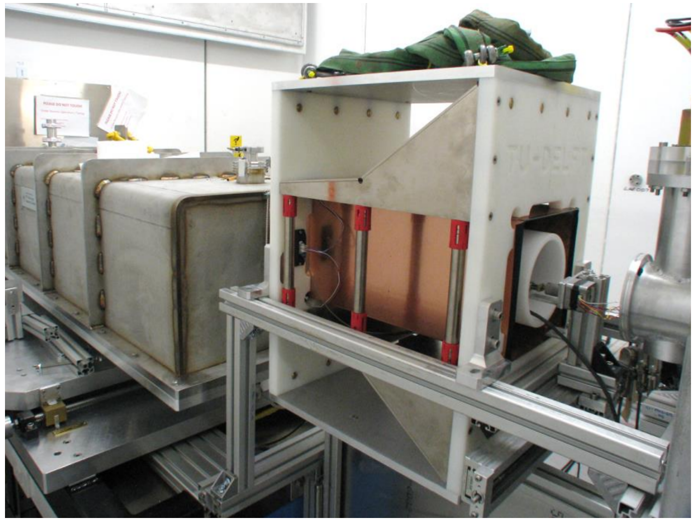


Nested fields

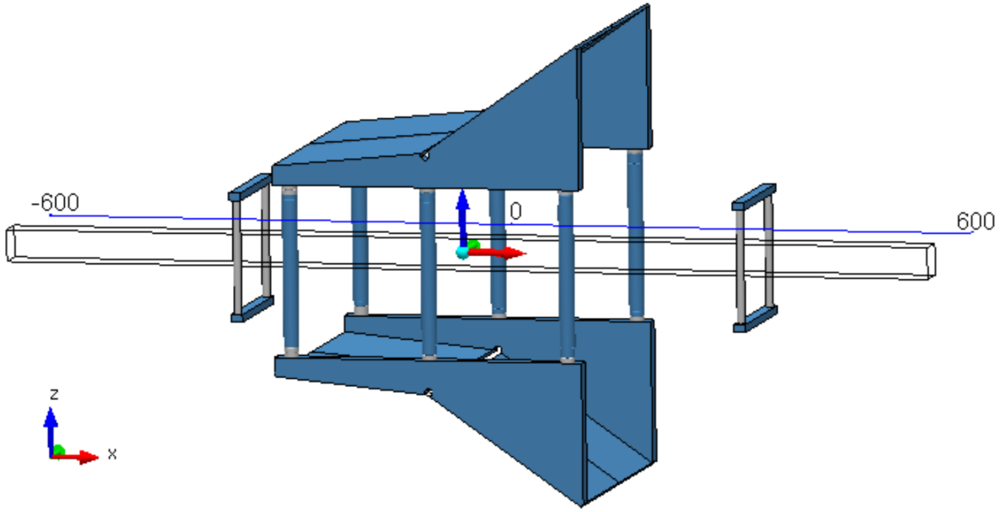




Use of Bfield to build an RF-flipper

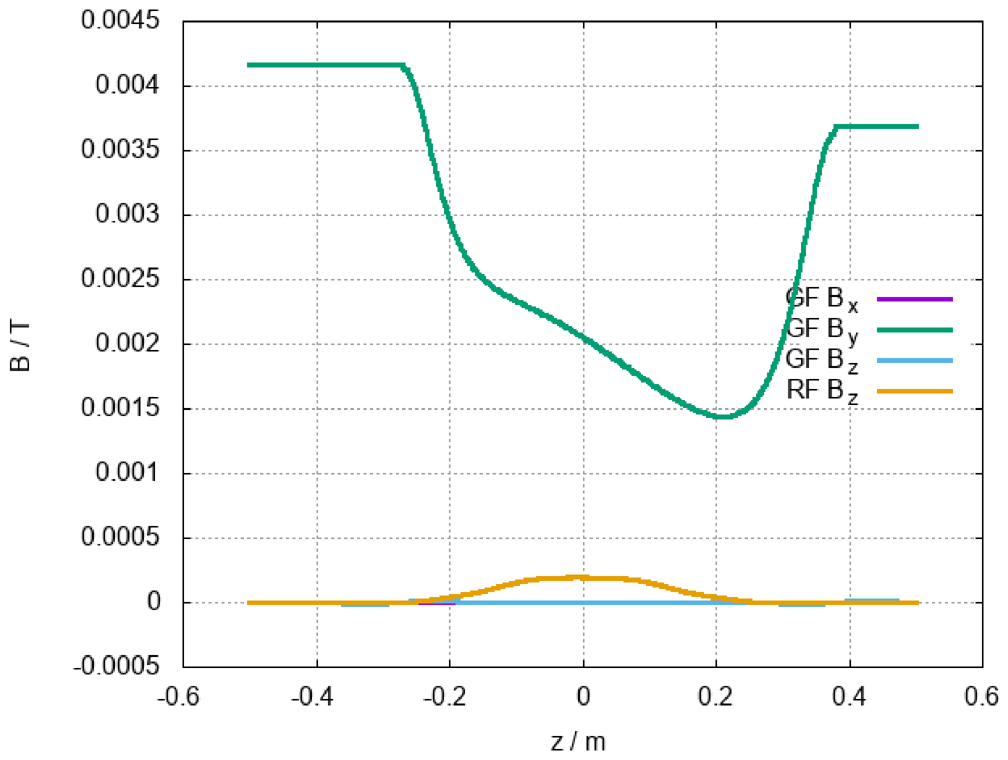


Pictures courtesy of J. Plomp & M. Thijs



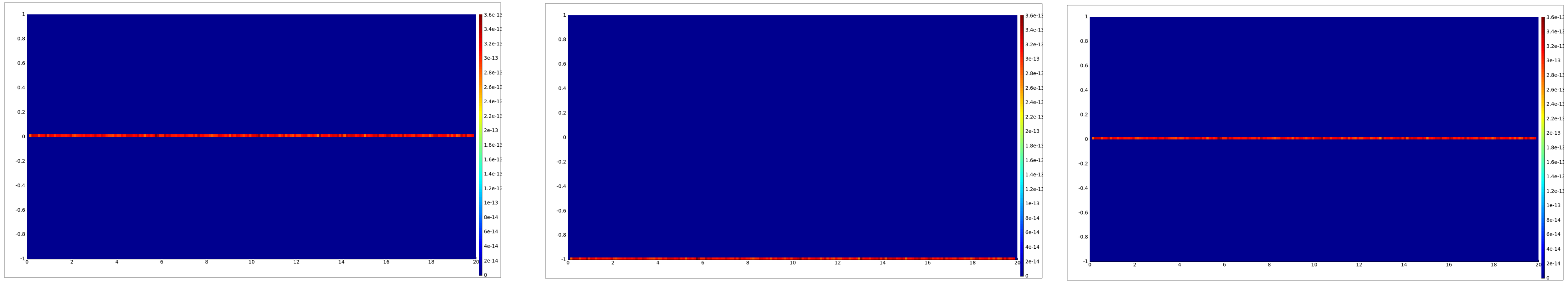
Use of Bfield to build an RF-flipper

Tabled fields where the RF field is a rotating frame.

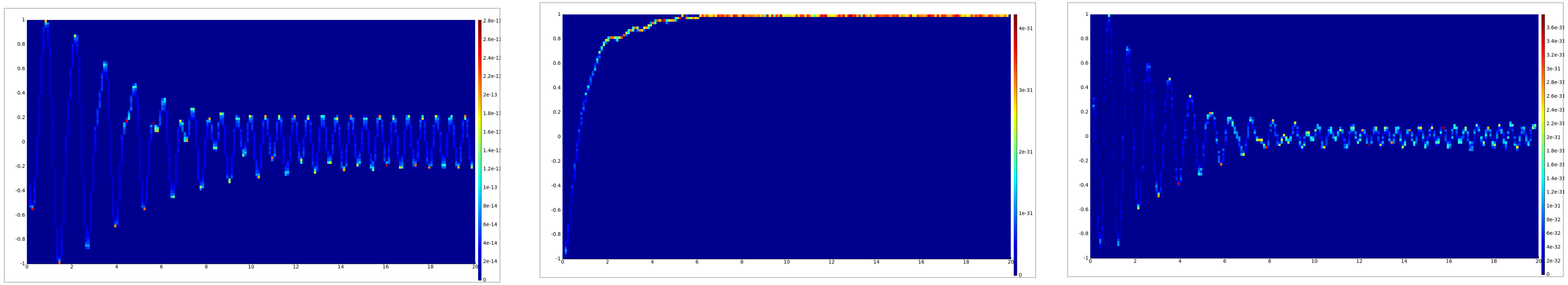


Use of Bfield to build an RF-flipper

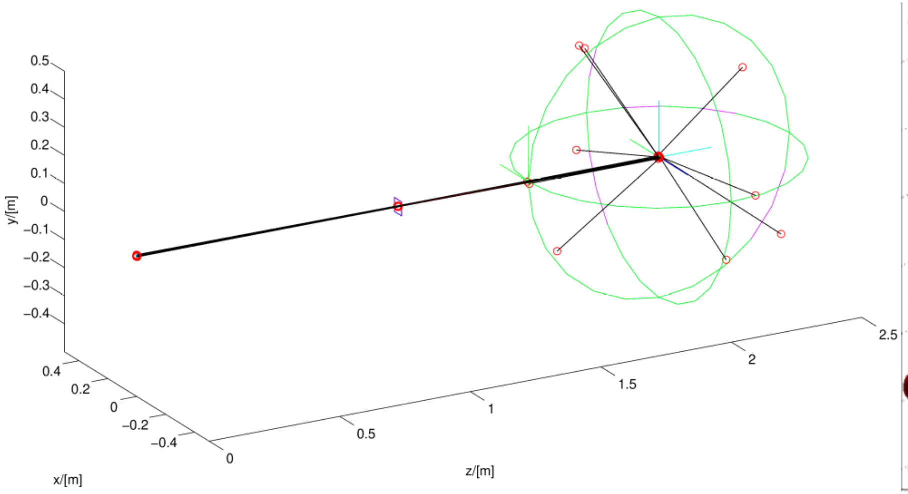
Before flipper

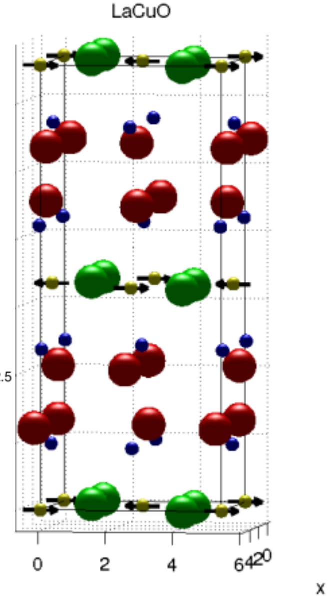


After flipper



Magnetic Single crystal

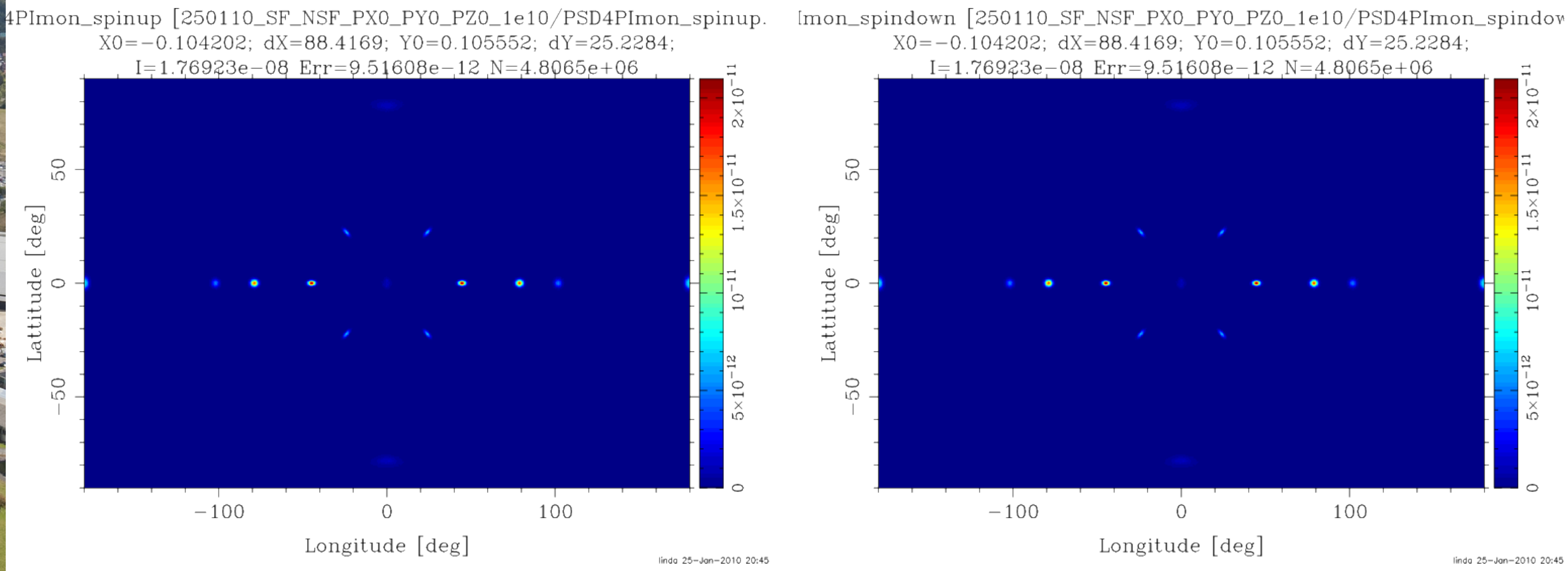




index	iontype	x	y	z	b_{coh}[fm]	g_S	S_x	S_y	S_z	g_L	L_x	L_y	L_z
1	Cu2+	0.5	0.5	0	7.718	2	0	-0.5	0	0	0	0	0
⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮	⋮

McStas component on the way

Magnetic single crystal – Unpolarized beam



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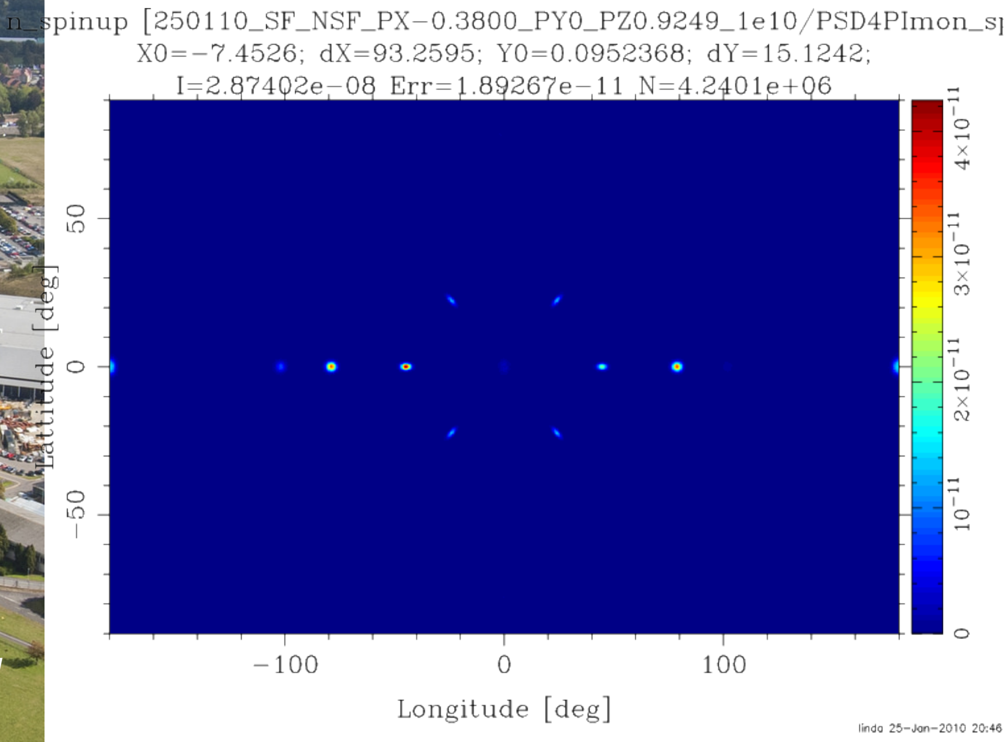

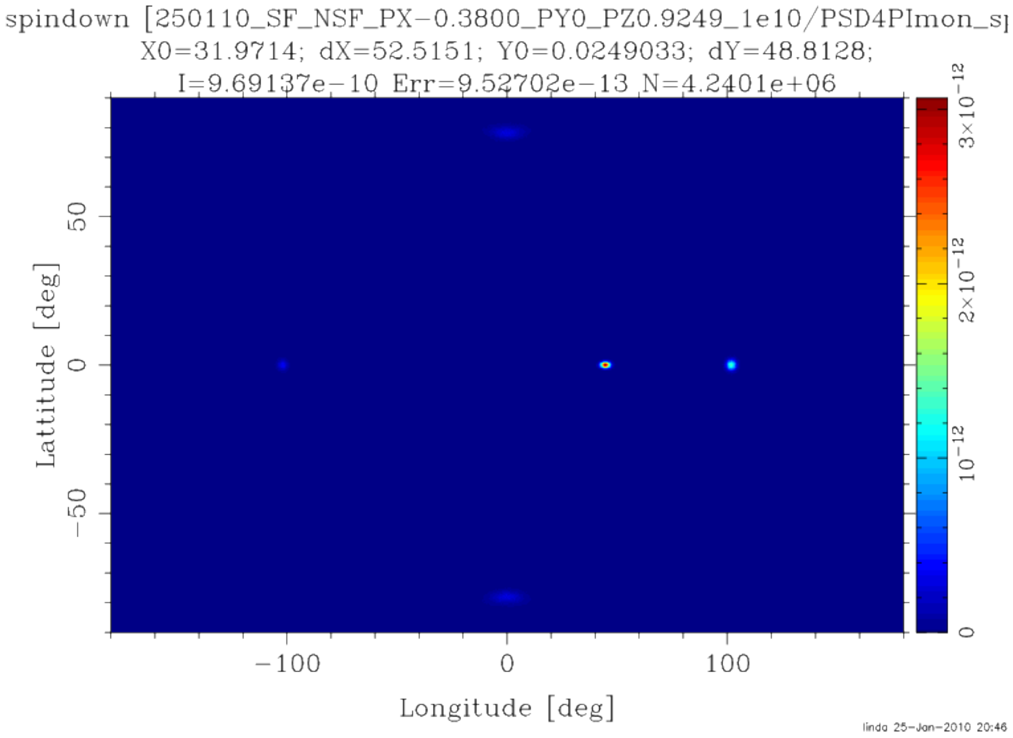

EUROPEAN SPALLATION SOURCE

DTU

McStas