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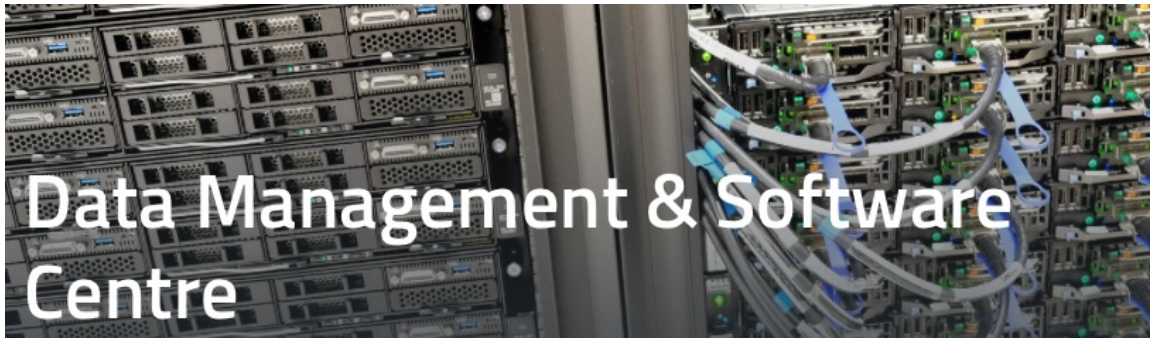


New CIS for Single-Crystal Diffraction

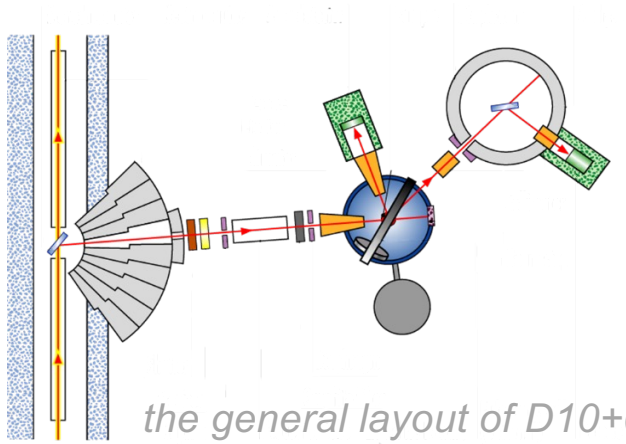
Iurii KIBALIN (CIS DMSC ESS)

STAP / October 2025

2023-2025: Responsible for D10+@ILL

Specialization of the diffractometer D10+:

- Magnetic structures in single crystals, thin films and multilayers;
- Conventional crystallography at dilution temperatures (unique for 4C-dillution), under magnetic fields, and under pressures;

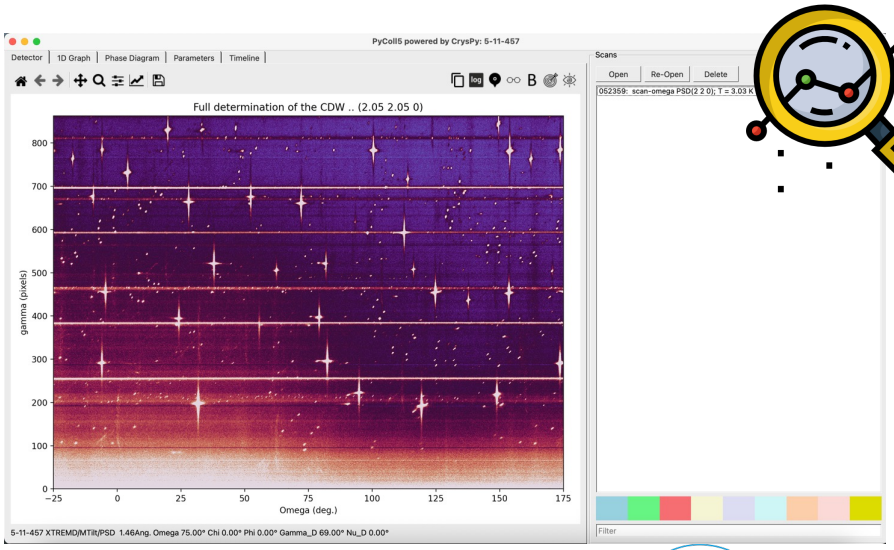


the general layout of D10+@ILL

PyColl5:

software designed for intuitive data visualization and preliminary analysis

- Compatible with data measured on D10+, D9, D23, D19, XTREMED at ILL.



https://code.ill.fr/kibalin/pycoll5

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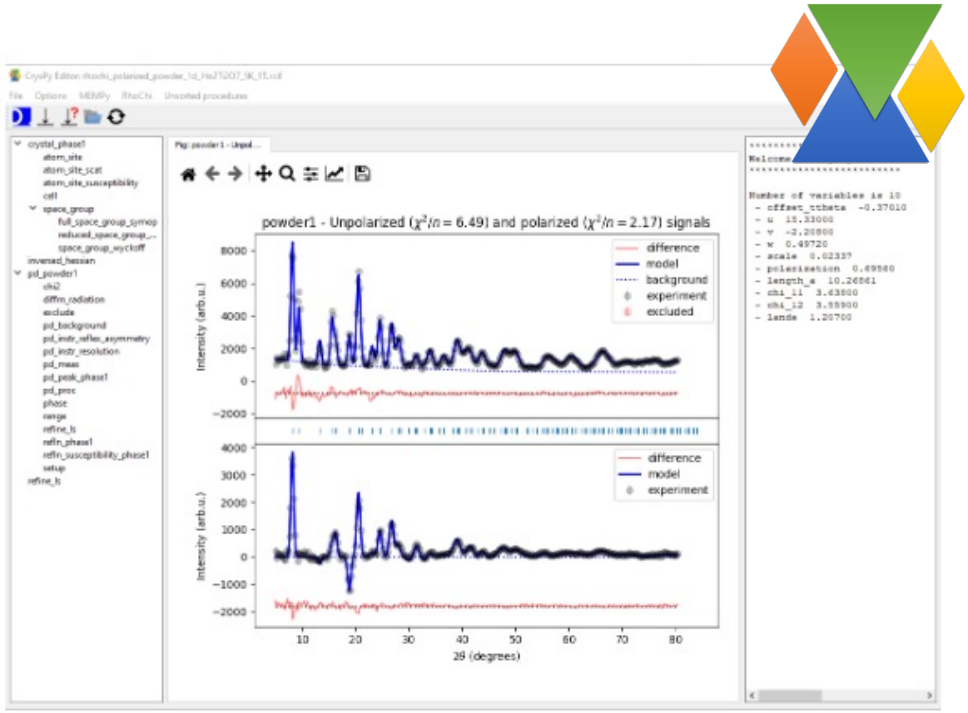
Analysis of half-polarized neutron diffraction data

The CrysPy library is an open-source program package that was originally developed *for polarized neutron diffraction* data analysis.

- The package allows the data treatment both for *powders and single-crystal* samples.
- Nuclear and (commensurate) magnetic structures refinement can be also perfomed based on *the unpolarized neutron diffraction and X-ray diffraction data*.
- CrysPy is one of the calculation engines *integrated into the EasyDiffraction* software developed by DMSC.



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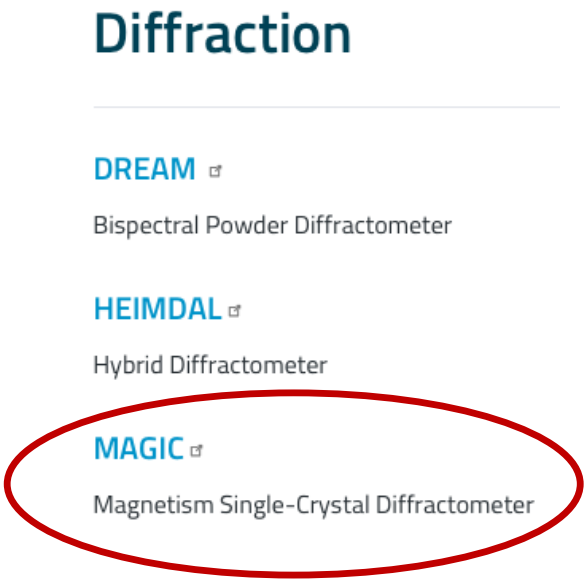
CIS for Single Crystal Diffraction

Position started September 1st 2025.

Several responsibilities among others of IDS*:

- Oversee, review, evaluate and take ownership of DMSC deliverables to relevant instruments, *specifically the full data processing pipeline;*
- Contribute to *the development of open-source software* where needed and appropriate;
- *Spend up till 20% of time on local contacting for user experiments* in alignment with instrument team;
- …



*https://confluence.ess.eu/spaces/DMSC/pages/446677876/IDS+R2A2

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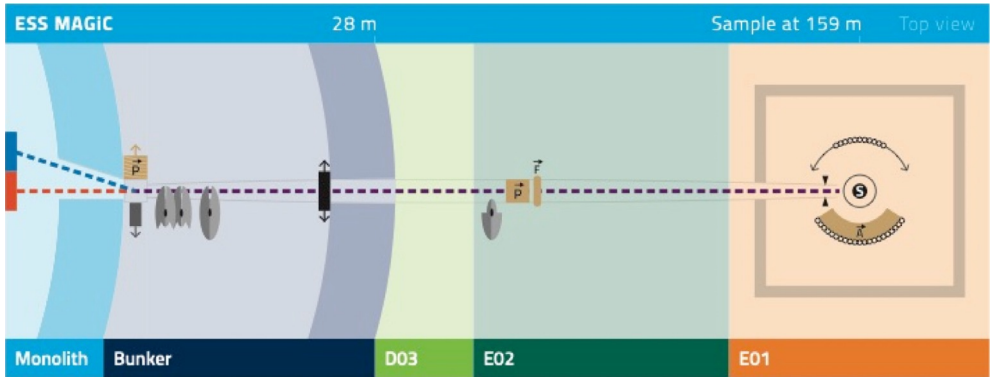
MAGiC: McStas model

a polarized single-crystal diffractometer with polarization analysis dedicated to magnetism.



McStas model is based on the model of X.Fabreges

Simplification in the current model:

- Only cold spectra
- Only unpolarized beam
- Detector A is represented as 2D banana detector

Table 11
MAGiC Quick Facts.

MAGiC Quick Facts	
Instrument Class	Diffraction
Moderator	Bispectral
Primary Flightpath	159 m
Secondary Flightpath	1 m
Wavelength Range	0.6–6 Å
Bandwidth	1.7 Å
Flux at Sample at 2 MW	1.5×10^9 n s^{-1} cm^{-2} (2.0–3.7 Å, full pulse)
Polarised Incident Beam	Permanent
Half-Polarised Detector Bank	
Q-Range	0.2–21 $Å^{-1}$
Q-Resolution $\Delta d/d$	Adjustable 1%–12%
Detector Coverage	60° [H] × 48° [V]
Polarisation Analysis Detector Bank	
Q-Range	0.2–6 $Å^{-1}$
d-spacing Resolution $\Delta d/d$	Adjustable 0.2%–4%
Detector Coverage	120° [H] × 6° [V]

Output of this McStas model:

- Event based data that can be used for data reduction pipeline (example of C60)

Andersen, K.H., D.N Argyriou, A.J. Jackson, et al. *Nuclear Instruments and Methods in Physics Research Section A: Accelerators, Spectrometers, Detectors and Associated Equipment* 957 (2020): 163402. https://doi.org/10.1016/j.nima.2020.163402.

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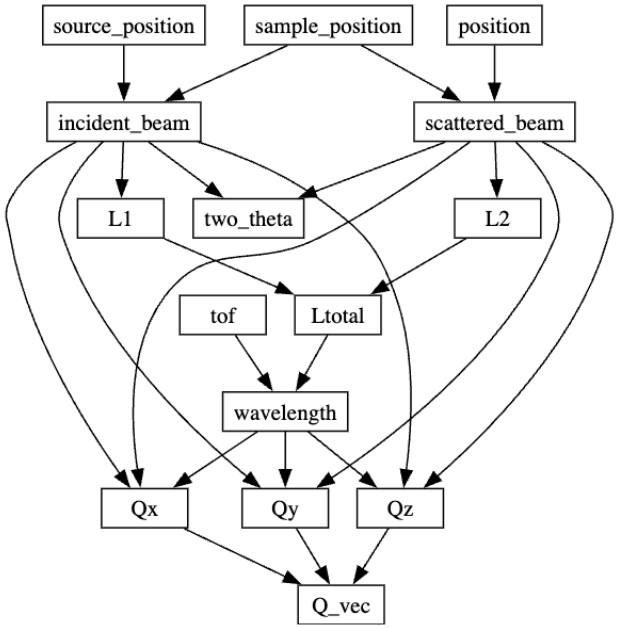
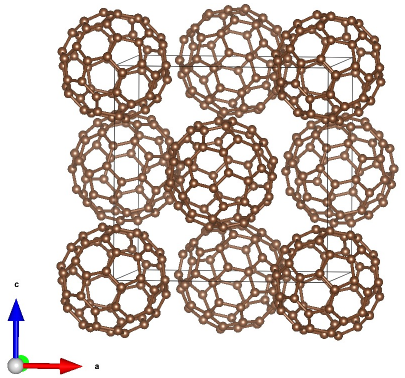
Data reduction using Scipp

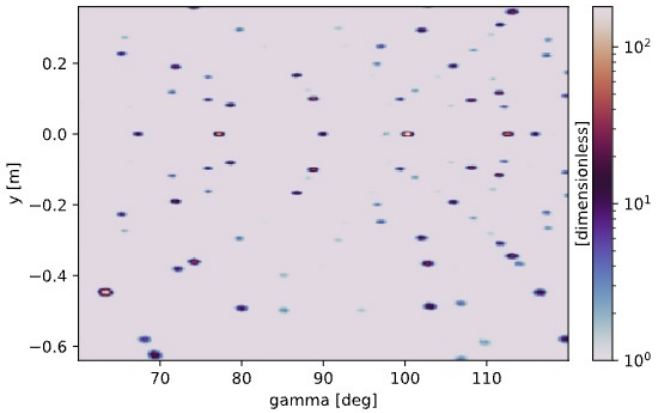
Graph to convert data to reciprocal space:



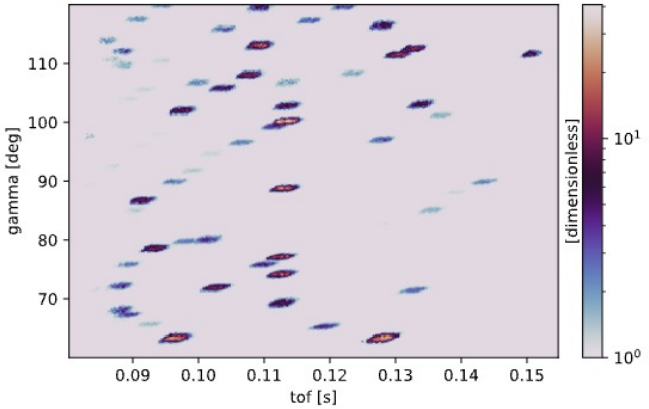
C_{60} simulated event-based data



Laue diffraction pattern



Gamma-TOF plot



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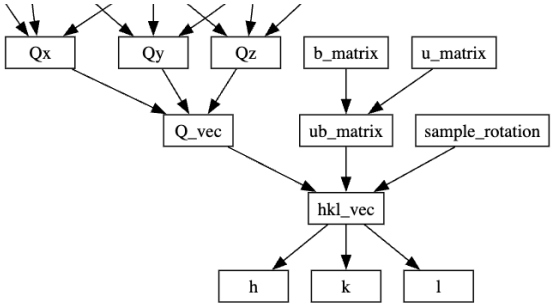
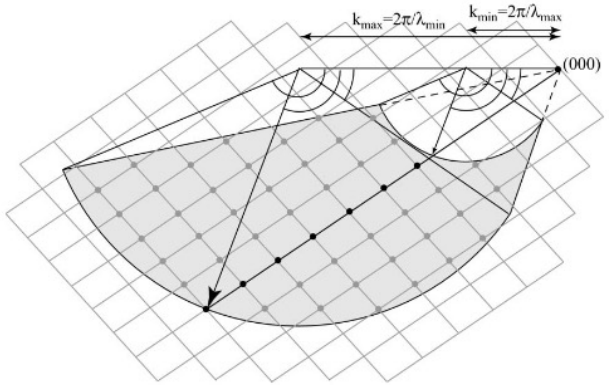
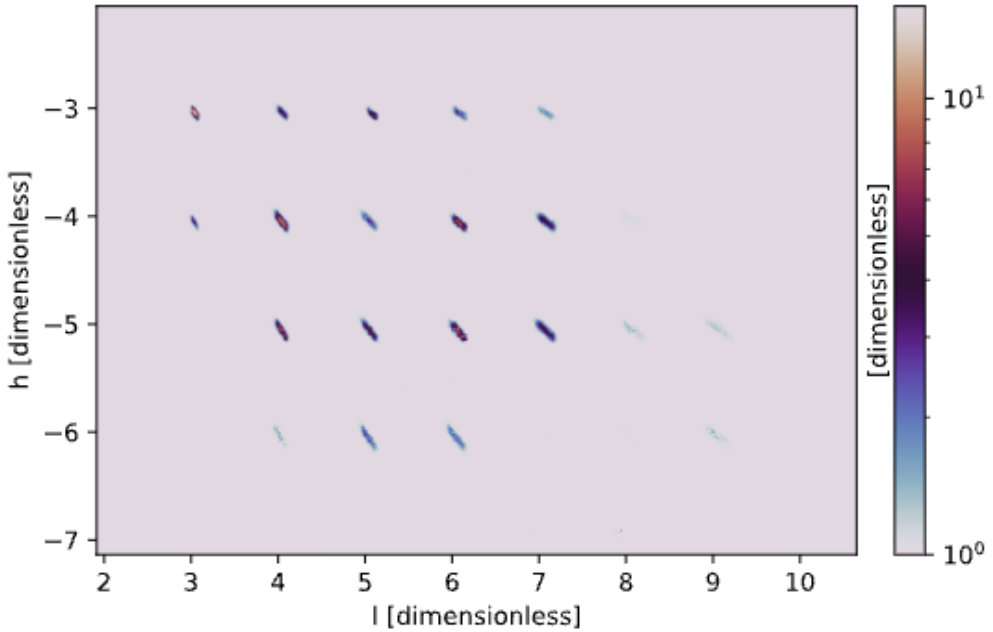
Data reduction using Scipp: HKL space

Converting to HKL space





Projection on HL-plane:
(at given UB matrix)



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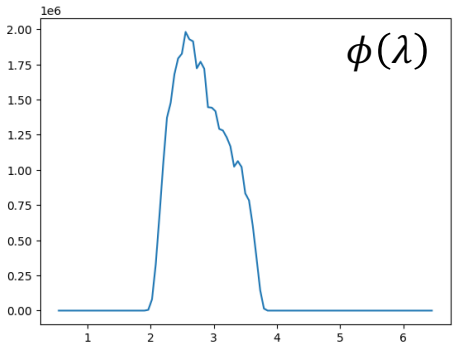
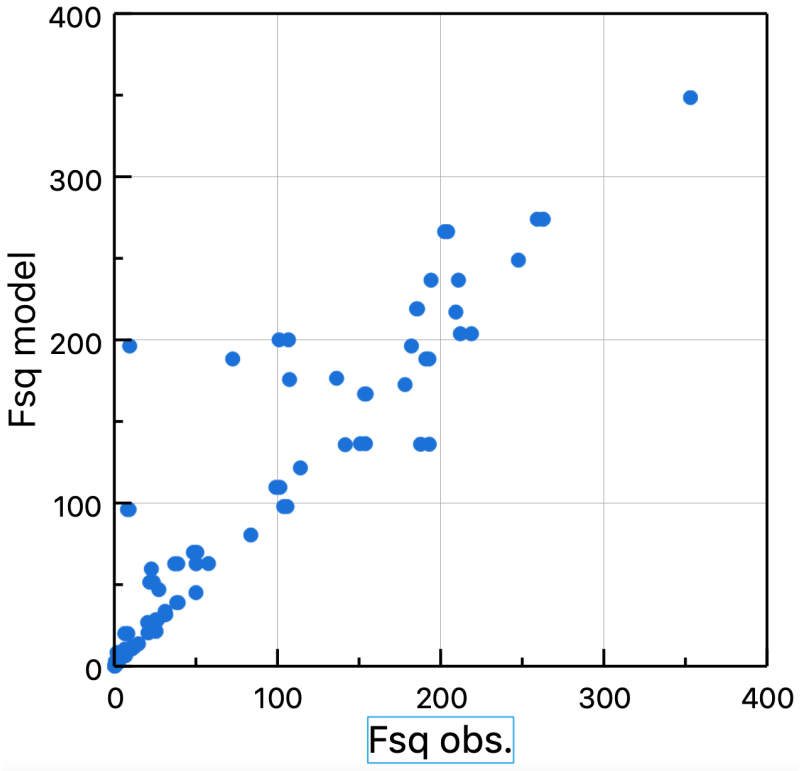
Estimated $|F_{hkl}|^2$ using Scipp

$$I_{hkl} = s \cdot \phi(\lambda)\epsilon(\lambda)A(\lambda)y(\lambda) \cdot (1+\alpha)\frac{\lambda^4}{\sin^2\theta} \cdot |F_{hkl}|^2$$



$\epsilon(\lambda) = 1$
$A(\lambda) = 1$
$y(\lambda) = 1$
$\alpha = 0$



s is the scale factor;
$\phi(\lambda)$ is the incident spectral neutron flux;
$\epsilon(\lambda)$ is the detector efficiency;
$A(\lambda)$ is the absorption correction;
$y(\lambda)$ is the extinction correction;
$\alpha = I_{TDS}/I_{Bragg}$;
2θ is the scattering angle;
F_{hkl} is the structure factor.

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Data reduction using MANTiD

MANTID

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Single Crystal Diffraction (Elastic)

In this page we describe a standard workflow for elastic single crystal diffraction data reduction at SNS. Many of these steps are encapsulated in the SNSSingleCrystalReduction algorithm. See scripts/Vates/Diffraction_Workflow.py for an example.

Contents

Loading and Processing in Detector Space

- LoadEventNexus and LoadEventPreNexus will load data into an EventWorkspace
  - For non-event data, e.g. WISH RAW files, you can use Load followed by ConvertToEventWorkspace to get an EventWorkspace.
- Use the Minus algorithm to subtract a background.

Pipeline:

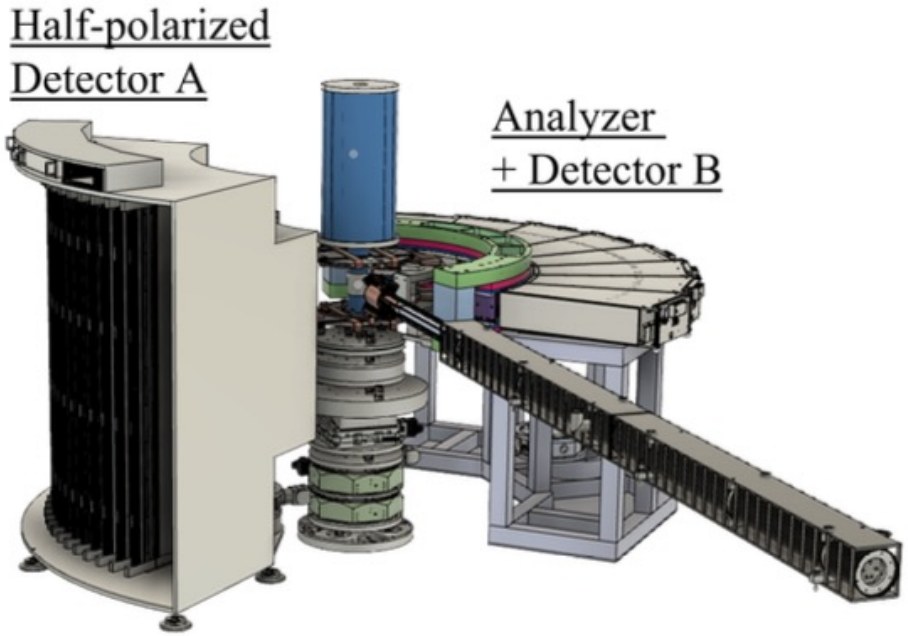
- *Finding peaks*
- *Refining UB-matrix*
- *Peaks' indexation*
- *Integrating peaks*

↓

- UB matrix and refined Unit cell parameters;
- HKL list with integrated intensities, wavelength, d-space, 2theta

Priority tasks: (i) McStas modeling

- Include polarization of neutron beam and thermal spectra in McStas model;
- Detailed McStas Model for
  - 3D Detectors on MAGiC: Detector A and Detector B;
  - Neutron Guide System on MAGiC;
  - Beam Stop and Sample Node on MAGiC.



Priority tasks: (ii) Data reduction by MANTiD and Scipp

- Transformation to Q-space: *Detector A (no analyzer)* and *Detector B (with analyzer);*
- Identification of strong peaks in reciprocal space;
- Finding the UB matrix, considering cases with *multiple grains/domains, high background* and so on;
- Integration of both strong and weak reflections based on the UB matrix;
- *Correction on absorption and extinction*.

Priority tasks: (iii) Data analysis

The workflow for the following single crystal experiments on MAGiC should be considered:

- Single-Crystal Laue TOF Diffraction;
- Half-Polarized Single-Crystal Laue TOF Diffraction;
- XYZ Polarization Analysis Laue TOF Diffraction;
- Spherical Polarimetry;
- Diffuse Magnetic Scattering.

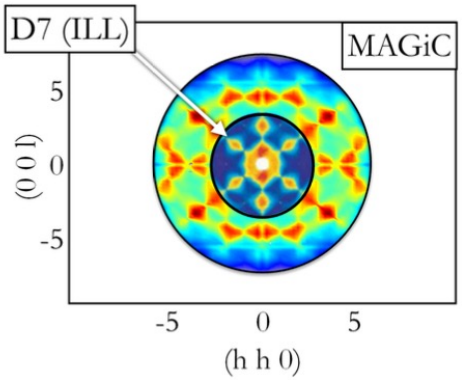


Figure 12: Simulated diffuse scattering of Ho2Ti2O7

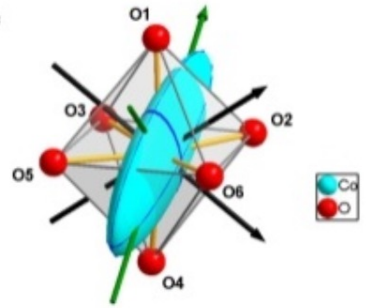


Figure 2. Co2+ magnetic ellipsoid for the complex [Co(DMF)6]2+[3].

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Conclusion

- Basic McStas Model of the MAGiC diffractometer;
- Data reduction pipeline for single crystal Laue TOF diffraction;
- Identification of priority tasks, organized into three blocks: (i) instrument modelling, (ii) data reduction, and (iii) data analysis.

Thank you for your attention!