Polarised neutron diffraction data analysis software

Andrew Sazonov, RWTH Aachen Uni & JCNS at MLZ

Motivation

- Polarised neutron diffraction techniques:
  Spherical polarimetry (SNP), Flipping-ratio (FR) measurements
- No suitable software for data analysis / magnetic structure refinement
  (full support, user friendly, graphical interface)

Available software / libraries

- Cambridge Crystallographic Subroutine Library (CCSL) based software: MagLSQ, SnpLSQ, …
  - Best support for both FR and SNP data
  - No longer being developed and has no active maintainer
  - Terminal programs without GUI (Fortran77)
- Crystallographic Fortran Modules Library (CrysFML) based software: FullProf, MagnOpt
  - Developed and maintained at ILL
  - Limited support for polarised neutron diffraction
- ShelX, Jana2006, GSAS, Topas
  - No support for polarised neutron diffraction data

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Goal

- Develop data analysis software for both instrument scientists and non-experts
- Enlarge the scientific community that uses the powerful polarized neutron diffraction techniques

Functionality

- Core functionality:
  based on crystallographic libraries CrysFML and CCSL
- Use magnetic space group symmetry for description of magnetic structures (magCIF support)
- Graphical interface:
  based on multi-platform development framework Qt
- Be open-source to allow other groups to contribute to the project

Attempts

- Applied for BMBF project 2016: Not accepted ☹
- ESS collaboration (common project, developing, maintaining, etc.)?