

# nsxtool: Data Analysis for Crystal Diffraction

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April 2017

MLZ is a cooperation between

## Overview

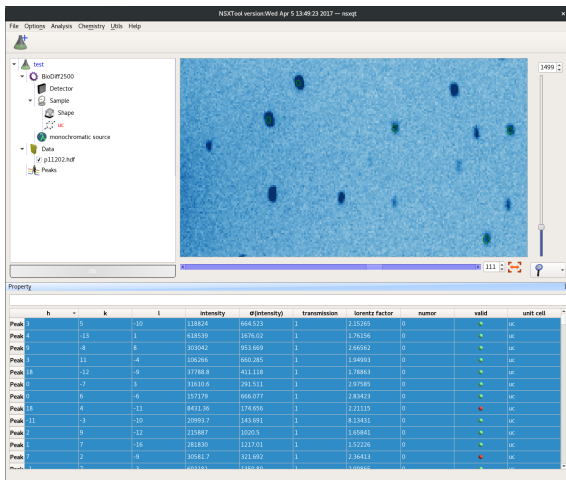
- Started in 2013 by Laurent Chapon and Eric Pellegrini (ILL)
- JCNS joined collaboration early 2016
- Two full-time developers
- Intended to replace legacy and/or proprietary software:
  - ILL: suite of instrument-specific Fortran programs
  - FRM II: HKL2000 (commercial, closed-source)
- Requirements:
  - open source
  - modern language and compiler (C++11, gcc, clang, msvc)
  - depends only on open-source third-party libraries
  - multi-platform (Linux/Mac/Windows)

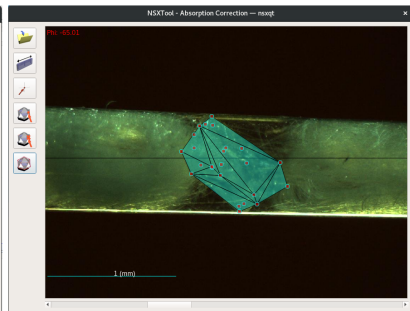
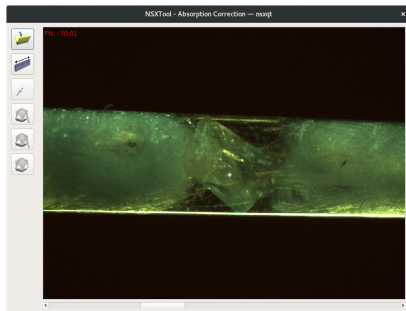
## Design

- `nsxtool` = `nsxqt` + `nsxlib`
- `nsxlib`: general library for crystal diffraction data analysis
- `nsxqt`: GUI exposing main functionality of `nsxlib`
- Modern object-oriented design: instruments, sample, source, etc. represented by abstract interfaces
- Easily modified and extended
- Third-party dependencies are open-source and actively maintained: `boost`, `eigen`, `gsl`, `hdf5`, `qt`, ...

## Features

- XML instrument definition, multiple geometries
- Automatic peak search (image filter + blob search)
- Unit cell determination and FFT auto-indexing
- Intensity integration
- Parameter refinement (unit cell, detector/sample offsets)
- Space group determination, extinction law
- Chemical formula parser for material definition
- Crystal shape determination as convex hull
- Monte-Carlo absorption correction
- Twin reflections





## WIP and Planned Features

- Import/export using nexus/hdf5 format
- Improved weak peak integration
- Intensity scaling for merged data sets
- Collection strategy
- GUI redesign/rewrite
- Python bindings for nsxlib
- Migrate from XML to YAML to improve readability
- Other instruments?