MxDC

MX Data Collector

User-friendly data collection application for MX Beamlines

Michel Fodje – CMCF
Kathryn
Scott
Shaun
Kiran
Michel
James

CMCF Team

Funding

INNOVATION.CA
NSERC
NRC-CNRC
CIHR
UNIVERSITY OF SASKATCHEWAN
Government of Saskatchewan
Canada
CMCF Software Architecture
MxLIVE

MxLIVE – Mx Lab Information Virtual Environment
- Web-based sample information management
- Meta-data archive
- Secure APIs
- Data access
- Staff Portal
- Since 2011
A set of command line utilities for automated reduction of diffraction data to “mtz”

Data Analysis Server - an RPC server for automated data analysis from MxDC.

Automated analysis of datasets from
- MX
- Powder Diffraction

Integrated with MxDC
Since 2007
MxDC – Mx Data Collector

- Experiment management,
- Interactive and automated data acquisition
- One instance per beamline
  - Configuration file
- Single-window, multi-paged GUI
  - Setup, Samples, Data, Scans, Analysis Pages
- Separate Python-based SPEC-like Beamline console for staff and commissioning
  - Since 2007
Design Principles

• **Users First!**
  - Experiment focused, NOT beamline focused
  - User friendly, intuitive & familiar GUI
  - Make common techniques easy, and complex schemes possible, without sacrificing usability.
  - Integration (Single GUI for all techniques)

• **Separation of Concerns**
  - Pluggable components
  - Versatile interfaces between components

• **Ease of deployment**
  - Focus on common functional aspect of devices relevant for experimental technique
  - Support different beamlines with different hardware devices
  - One Python Config file per beamline
X-ray Fluorescence Spectroscopy

Element: Fe, Cu, Zn, Rb, Tb, Cl, Cr, K, Br, Ar, As, Ni, Se

Excitation: 15.474 keV
Exposure: 0.5 s
Attenuation: 50%

Fluorescence

Energy: 12.667 keV
Beam Size: 300 μm
Attenuation: 0%
Dead Time: 5%
Sample: CNT-01/14/M1A1
Directory: /Users/johndoe/CNT-01_14/M1A1/mad-scan

Open Terminal
3. Mean anomalous differences in units of its standard deviation between \( F^+ \) and \( F^- \), \( \text{R.m.s.} \) are structure factor estimates obtained from the merged intensity observations in each than class.

3. Percentage of correlation between random half-sets of anomalous intensity differences.

Wilson Statistics

Twinning Analysis
FODJE

Hello, MoDC is showing two errors in the log and I don't know why. Also I am not able to do fluorescence scans. Do you know what may be wrong?

KATHRYN

Hi Michel! It looks like the fluorescence scan detector isn't connected right now.

FODJE

It's probably because we are in the middle of our shutdown. You will have to book time later once we have beam time again.

KATHRYN

Thanks, would it be possible to fix it soon? It is very crucial for my experiment.

FODJE

I also noticed that my sample is not centering automatically.

KATHRYN

Yes, one of the errors you saw is for our automated machine learning centering, so you could carry on by manually centering your samples.

FODJE

Manual centering is too hard, I like the automated one.
[michel@OPI2051-002 ~]$ broadwayd :5
Listening on /run/user/1000/broadway6.socket

(venv) [michel@OPI2051-002 ~]$ GDK_BACKEND=broadway BROADWAY_DISPLAY=:5 mxdc
MxDC (Macromolecular Crystallography Data Collector) is a software package for acquisition of Macromolecular Crystallography data and related techniques at synchrotron beamlines. MxDC has been developed since 2006 and has been the primary software for data acquisition and experiment control at the Canadian Light Source Macromolecular Crystallography beamlines. It is also used at the Pohang Light Source II in South-Korea.

### Resources

**GitHub**
https://github.com/michel4j/mxdc/

**Documentation:**
https://michel4j.github.io/mxdc/

---

**Note**

An earlier version of MxDC is described in the following publication:


[https://doi.org/10.1107/S0909049511056305](https://doi.org/10.1107/S0909049511056305)

Although developed primarily for MX beamlines, MxDC is based on an extensible generic framework that can be used to develop data acquisition systems for different types of experiments and beamlines.

### How to Use This Documentation

This documentation is divided into three sections targeted at different audiences. For MX beamline users primarily interested in using the MxDC GUI for data acquisition, it is recommended to start with the Overview section which describes the user interface. For beamline staff interested in...