



**EUROPEAN
SPALLATION
SOURCE**



NMX IDS Update

Neutron Macromolecular Crystallography

PRESENTED BY AARON FINKE

2026-04-22



The NMX Team

Who's building NMX?



Esko Oksanen
Lead Instrument Scientist



Justin Bergmann
Commissioning Instrument Scientist



Aaron Finke
Instrument Data Scientist



Zoë Fisher
Deuteration Wizard



Laís Passine (ECDC)
Controls/MXCuBE



Swati Aggarwal
Commissioning Scientist



Daniel Lundström
Lead Engineer

NMX: Neutron Macromolecular Crystallography



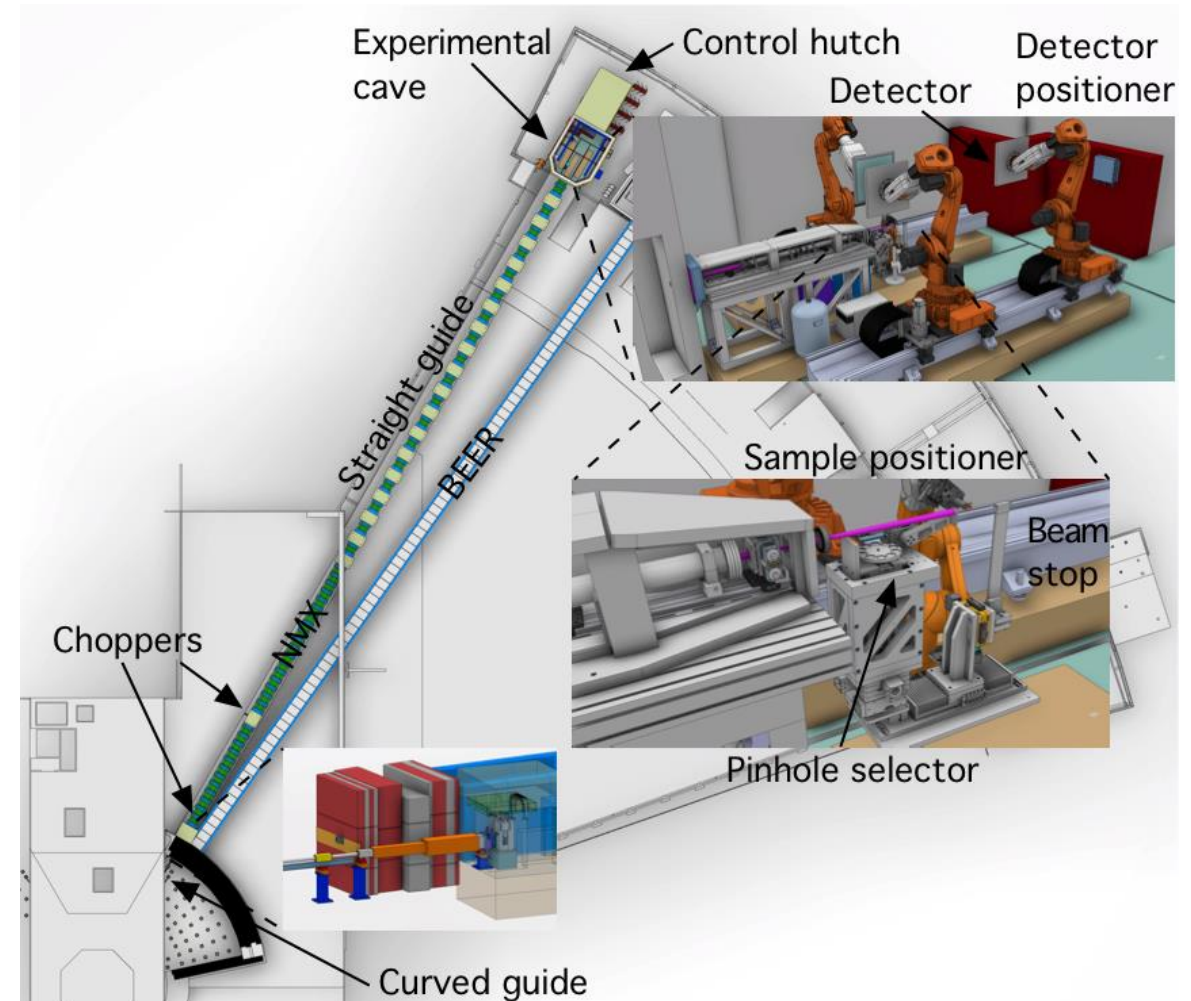
A Quasi-Laue TOF instrument for Macromolecular Crystallography

Determination of precise hydrogen atom positions in protein crystals with an innovative detector technology and robot-based goniometry.

DMSC Deliverables: ESSNMX, eventually to a complete diffraction-to-refinement pipeline using a combination of software developed at DMSC and partner institutions.

CC Goals: Processing simulated NMX data, motion tests (NICOS)

HC Goals: Beam-to-data



NMX Instrument Update

(Almost) ready for neutrons!

Accomplishments:

- Passed TG3 in Jan 2026
- Heavy Shutter SAT
- Choppers installed and tested
- Robotics Installation and Energization
- HVAC

Upcoming:

- Robotics SAT
- SAR/TG5 pushed to November
 - Biggest change: 3 detectors will be ready for HC instead of just one



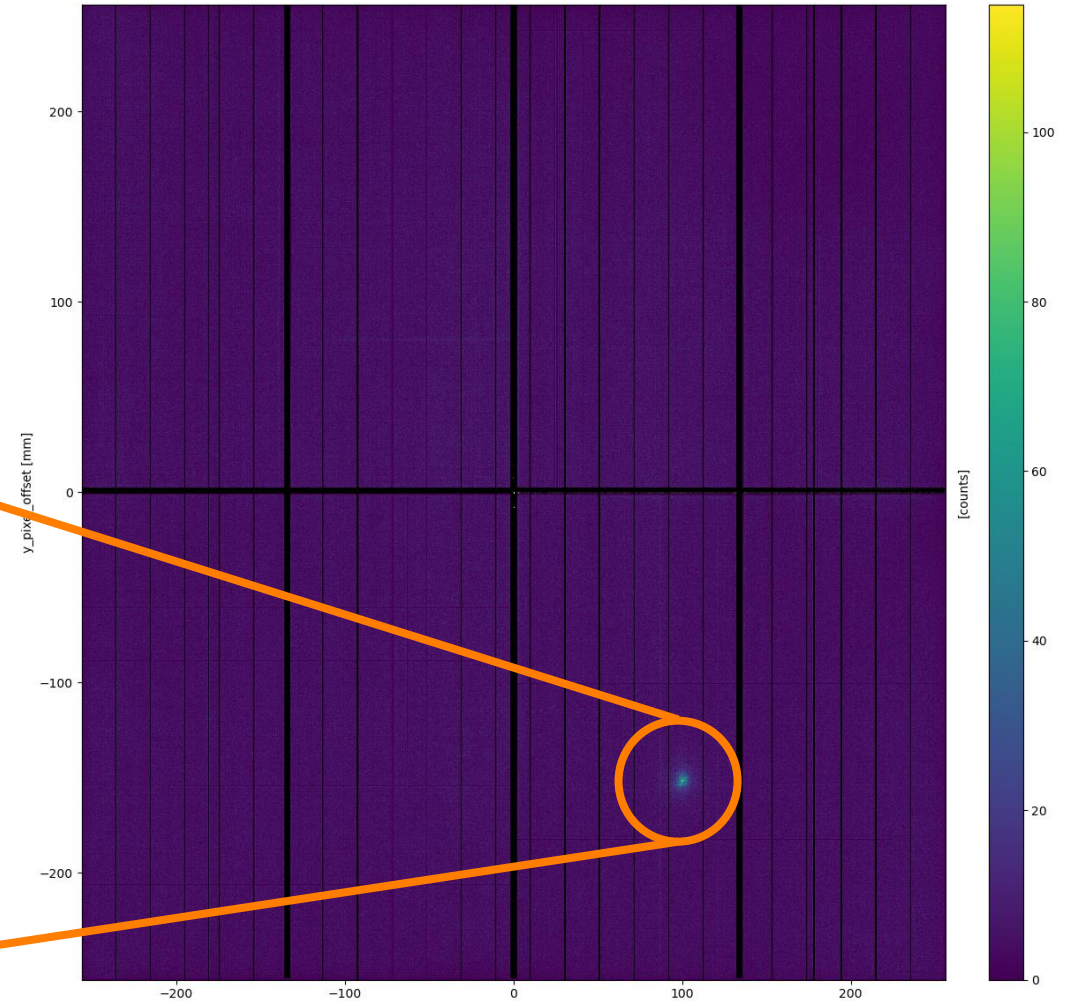
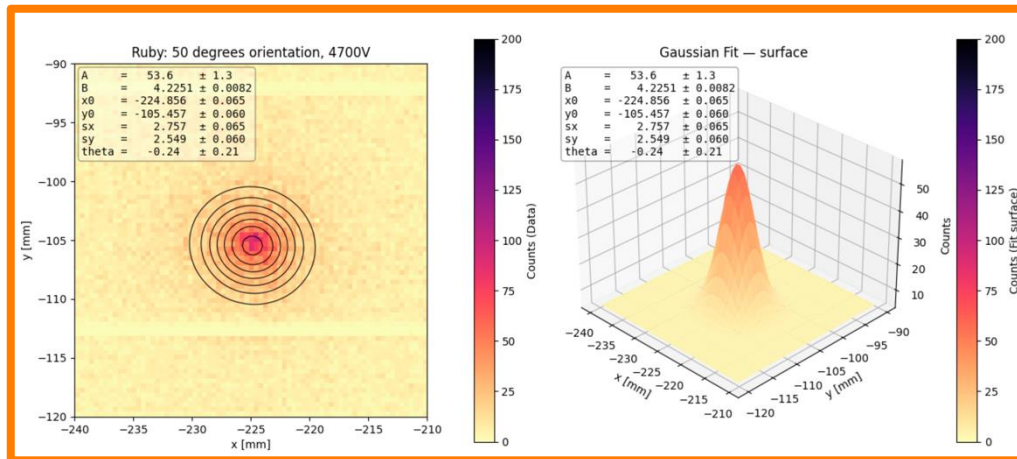
NMX Hutch with robot assembly

NMX@DMSC Update



Why test one thing when we can test everything at once?

- **First diffraction** on large detector panel (ruby, DALI beamline at ILL)
- Confirmation of successful beam-to-data pipeline with data collections at ILL, BNC
 - Detector -> RMM -> EFU -> Filewriter
 - TOF data not yet tested (maybe at J-PARC?)

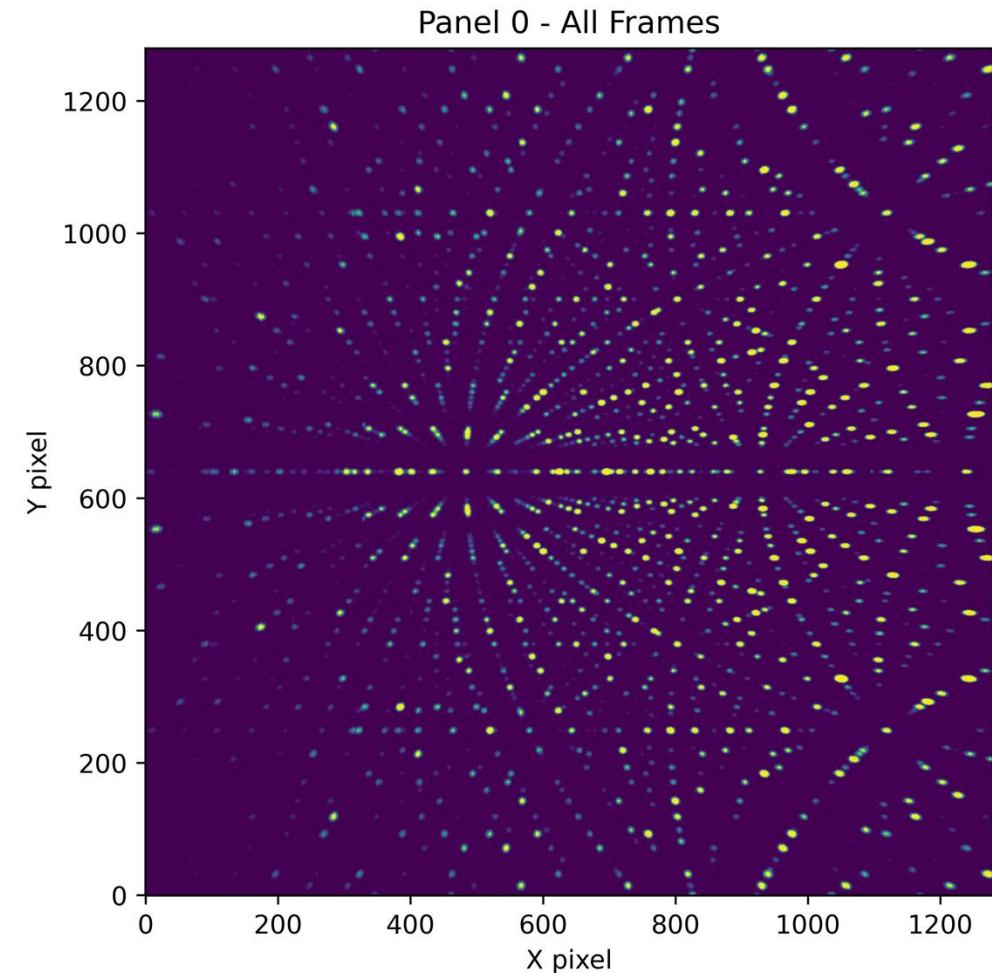


NMX@DMSC Update



How do you do neutron MX without neutrons?

- First diffraction on large detector panel (ruby, DALI beamline at ILL)
- Confirmation of successful beam-to-data pipeline with data collections at ILL, BNC
 - Detector -> RMM -> EFU -> Filewriter
 - TOF data not yet tested (maybe at J-PARC?)
- **NMX simulation paper** submitted (Acta Cryst D)
 - Preprint: bioRxiv 10.64898/2026.03.26.714568
 - Major effort between McStas, SCIPP, and NMX teams



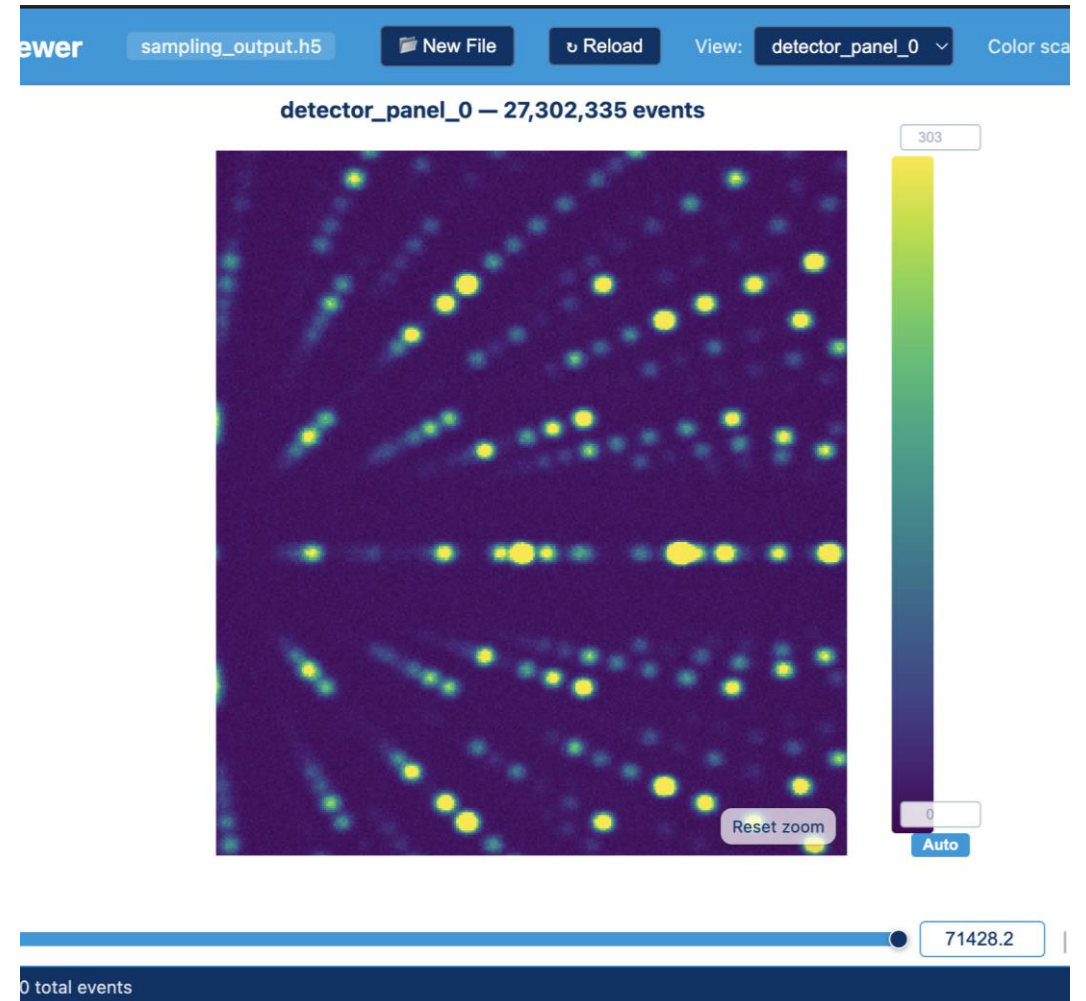
Simulated rubredoxin Laue diffraction

NMX@DMSC Update



NMX_view: A simple solution to a gap in needed tools

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 - Major effort between McStas, scipp, and NMX teams
- **NMX Event Viewer**: an H5web-based NMX event file viewer



NMX@DMSC Update

Other news

- Aaron now a member of DIALS collaboration, to ensure DIALS for Neutrons stays modernized (David McDonagh is no longer officially working on it, but is still a part of DIALS team)
- Aaron is Product Owner of VISA Working Group within DMSC
- **NMX@DMSC Day 2026**: An opportunity for the NMX group to get together and discuss topics relevant to data science and NMX

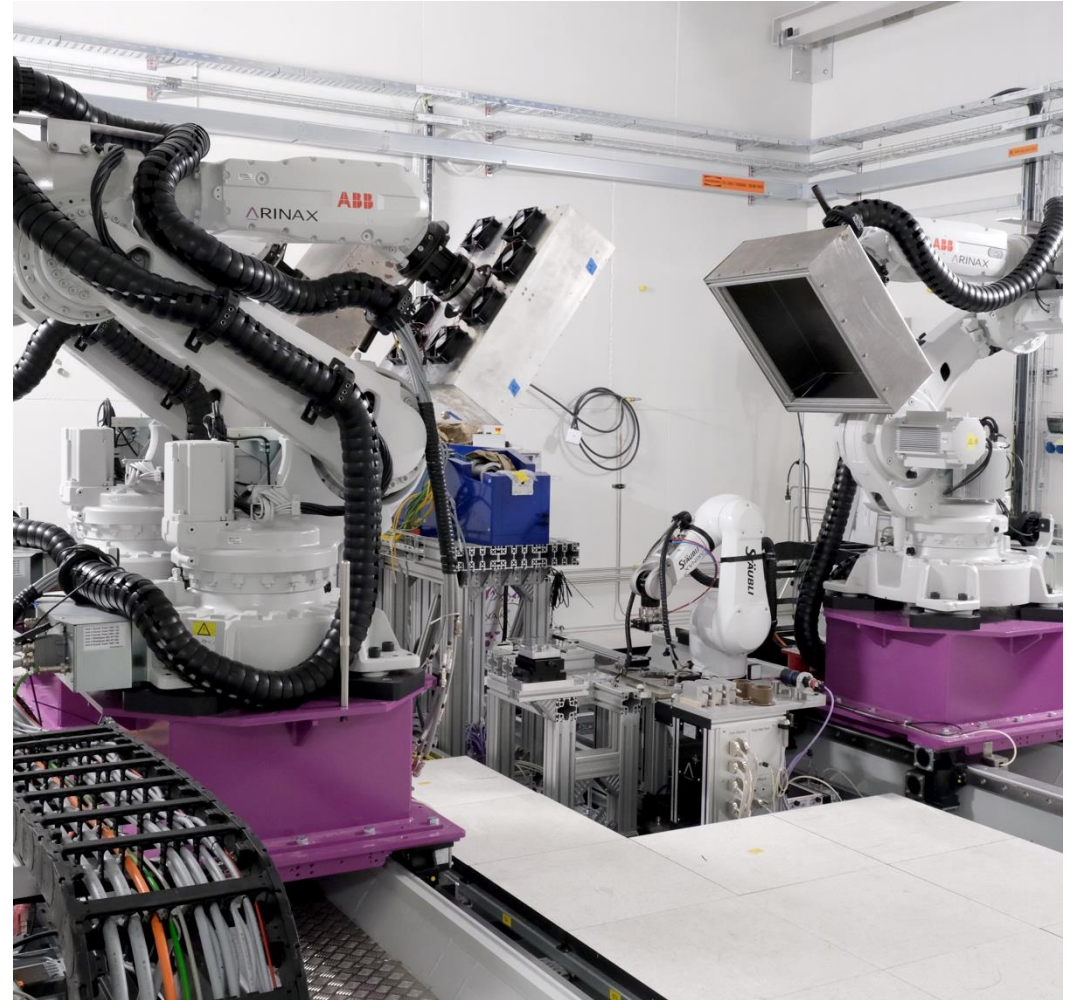


NMX@DMSC Day, 30 March 2026

NMX@DMSC

Coming up

- Help NMX pass TG5
 - All required data workflows for CC/HC is in place and ready
- NMXStrategy: Data Collection strategy and optimization for NMX
- Wavelength normalization in DIALS (to replace LSCALE/LAUENORM)
- Detector testing
- Work on streamlining automated data processing w/DIALS
- Treatment of NMX data within SciCat





Finish presentation