Materials Science and Protein Crystallography Using the MX Beamline Control Toolkit

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Plan of the Talk

- Review of MX
- XIA multichannel analyzer support
- MCS quick scan support
- Performance
- Protein crystallography
- New beamlines
- MX as device support for EPICS

What is MX?

- A portable beamline control toolkit: *Linux, Solaris, Irix, Windows, MacOS X, Cygwin, etc.*
- Designed as middleware.
- Comes with a set of servers and clients.
- Has an extensive set of device drivers: 53 motor and pseudomotor drivers, with over 250 drivers altogether.
- Easy to interface to other people's drivers.
- Easy to embed in other applications and servers.

Current Users of MX

- MR-CAT, APS Sector 10-ID *materials science*
- IMCA-CAT, APS Sector 17-ID and 17-BM *macromolecular crystallography*
- SER-CAT, APS Sector 22-ID and 22-BM *macromolecular crystallography*
- DND-CAT, APS Sector 5-BM macromolecular crystallography
- GCPCC, CAMD macromolecular crystallography

MX Portability

MX provides a way to write beamline applications that are independent of the underlying control system.

MX has been used with:

- Beamlines using only EPICS-controlled devices.
- Beamlines that do not use EPICS at all.
- Beamlines with a mix of EPICS and non-EPICS devices.
- Beamlines using other network protocols like SCIPE.
- Beamlines using vendor provided Windows DLLs.

XIA Multichannel Analyzer Support

- MX now supports the DXP-2X and Saturn MCAs from X-ray Instrumentation Associates.
- DXP-2X: A CAMAC-based MCA with 4 MCA channels per module.
- Saturn (X10P): A parallel port-based MCA.
- A Windows 98-based MX server controls the MCAs via the XIA-provided Xerxes library.
- The DXP-2X has been used by MRCAT at input count rates of up to 1.5 million counts per second per channel.

MCS Quick Scans

- MX now supports quick scans that use a multichannel scaler to buffer the data.
- Struck SIS 3801 is supported via either EPICS or directly.
- The SIS 3801 sample interval ranges from 1 µsec to 1.67 sec using its internal clock.
- It can record up to 128 K samples that can be divided between scalers as necessary.
- When used via EPICS, each scaler can have up to 4000 measurements.
- When used directly, there is no limit other than the FIFO size.

MCS Quick Scans (cont.)

- At MR-CAT, most XAFS and diffraction measurements not using an MCA are now done via quick scans.
- SER-CAT and IMCA-CAT plan to use quick scans to minimize radiation damage to crystallography samples.
- Quick scans can also use an external pulse generator as a clock instead of the internal MCS clock.
- The XIA DXP-2X MCA now has support for internal buffering of region of interest (ROI) integrals.
- MR-CAT plans to use this to measure up to 208 MCA ROI integrals per point of a quick scan.

Performance

- MX development until recently has focused on implementing necessary beamline functionality.
- Now we need to improve the performance of the control system.
- The biggest improvements are likely to be found by improving the efficiency of network communication.
- We plan to focus on improving network performance over the next several months.
- We will also explore using MX drivers in an EPICS Channel Access server.
- Perceived performance of user interfaces is also important.

Protein Crystallography with MX

MX has fairly mature support for protein crystallography related beamline control:

- Wavelength control
- Slit and filter control
- Fluorescence scans
- MAD experiment setup
- Beamline intensity optimization
- Vendor goniostat and beamline interfaces for Mar, ADSC, and Bruker.

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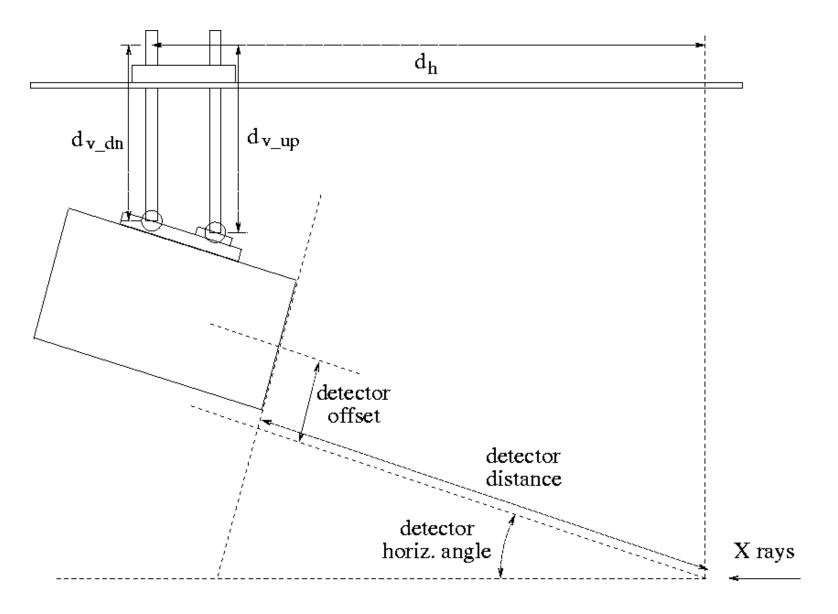
New Beamlines

- MX is now in use at several new beamlines: SER-CAT, DND-CAT, and GCPCC.
- Most of my recent crystallography development has been done for SER-CAT.
- DND-CAT and GCPCC have been relatively self supporting.

MX at SER-CAT

- SER-CAT is using Delta Tau Turbo PMACs for motor control.
- Struck VME modules are used for counter/timer support through PCI-to-VME bus interfaces.
- EPICS is only used for undulator control.
- Implemented distance, angle, and offset pseudomotors for the A-frame CCD detector support.
- Implemented MX pseudodevices for downstream BPM readout.
- Implemented beamline and goniostat interfaces for the MarCCD and Bruker Proteum CCD systems.
- SER-CAT is now making plans for increased beamline automation.

SER-CAT A-frame Detector Support



Future Plans for Crystallography

- Interfacing to robotic sample changing systems.
- Closer integration with area detector control systems.
- Batch mode sample processing.
- Remote control of data acquisition across the Internet.

MX as EPICS Device Support

- MX is designed to be easily embeddable in other applications or servers.
- EPICS IocCore has now been ported to Linux, Solaris, Win32 and RTEMS, but few device drivers exist yet.
- I plan to use the MX library and drivers as device support for EPICS.
- Code to use MX motor drivers from the EPICS motor record is currently under development.
- This will let MEDM be used to construct MX GUIs.
- It will also allow MX drivers to be used from Spec.

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