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.
Imcagui Main Window

I'm cagui M in W in d o w
MAD Experiments with Imcagui

[Image of a software interface with various options and settings for MAD experiments, including options for experiment type, periodic table elements, fluorescence detector saturation test, scan types, output directory, wavelength and energy calculations, and f' and f'' spectrum printing options.]
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

d\_v\_dn

d\_v\_up

d

detector offset

detector distance

detector horiz. angle

X rays
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.
## Acknowledgements

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