Materials Science and Protein Crystallography Using the MX Beamline Control Toolkit

William M. Lavender

Illinois Institute of Technology
Chicago, Illinois 60616

http://www.imca.aps.anl.gov/mx/
lavender@imca.aps.anl.gov

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
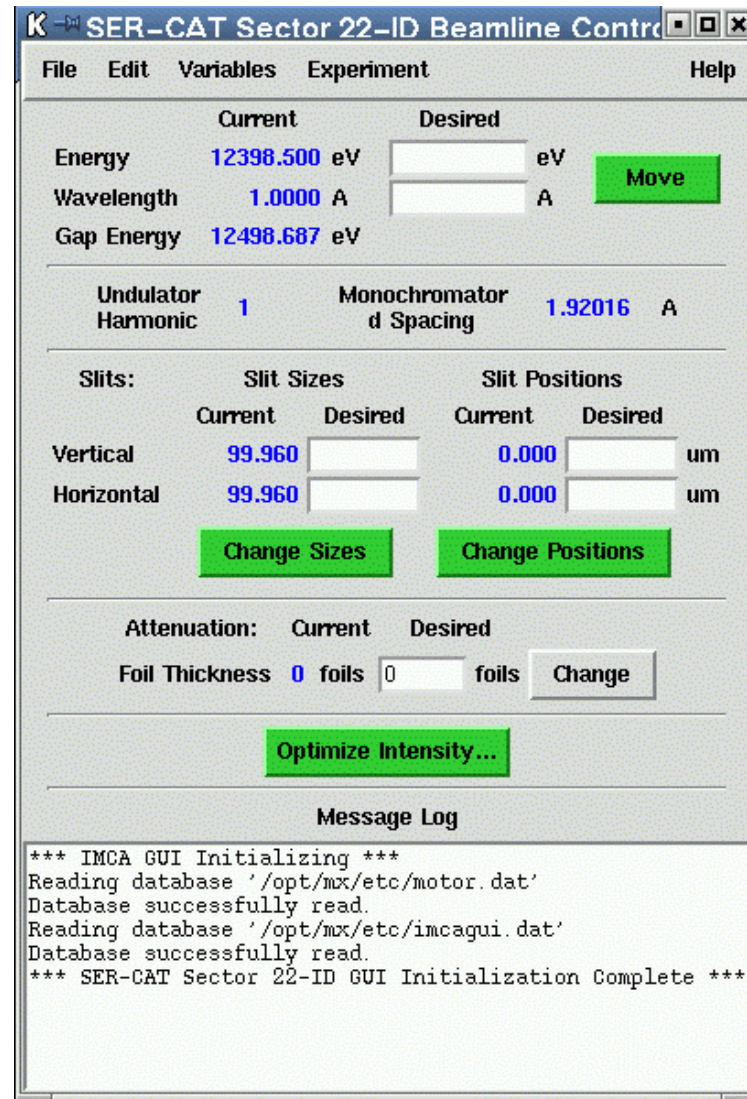
MAD Experiments with Imcagui

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_h

d_{v_dn}

d_{v_up}

detector offset

detector distance

detector horiz. angle

X rays
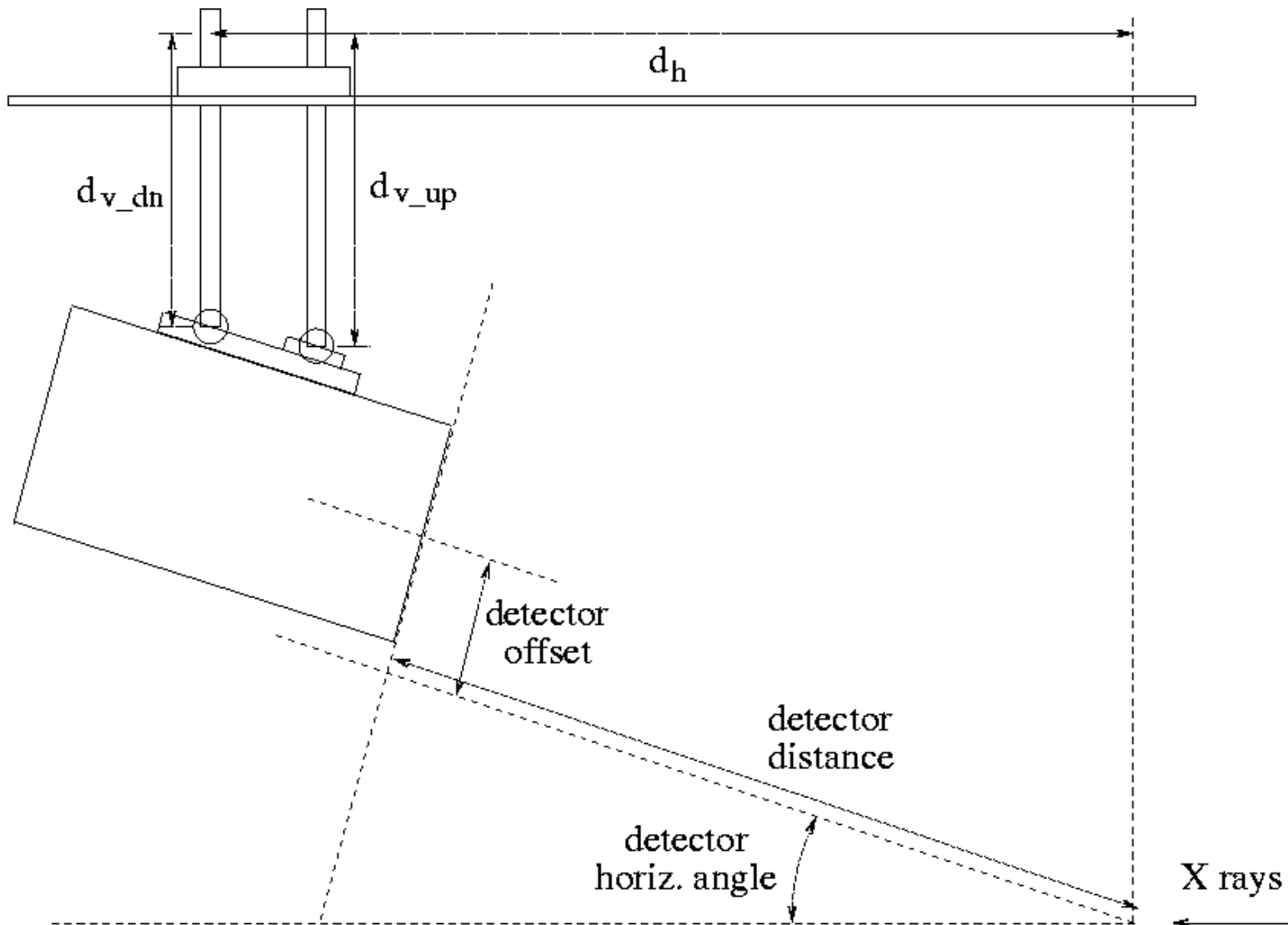
Future Plans for Crystallography

- 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