



*2007 Crystal Grid Workshop
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How Many Crystallographers Does It Take To...

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University of Minnesota X-ray Crystallographic Laboratory



XCL Instrumentation and People

- 1 SMART 1K (1995) – Looking for funding to upgrade
- 1 SMART 1000 (1999) – Looking for funding to upgrade
- 1 SMART 1K (1997) – Bought for parts for \$10K
- 1 CIMA Portal
- 1 ReciprocalNet Server
- 1 100% FTE Professional Crystallographer
- 1 50% TA for XCL and CHEM 5755 X-Ray Crystallography Course

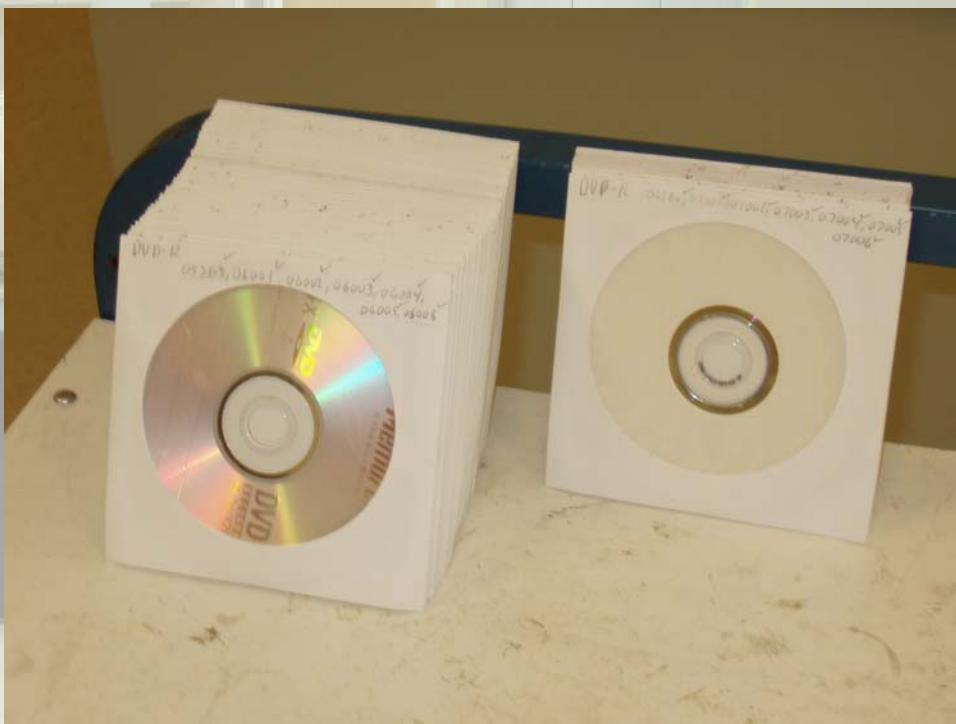
How Many Crystallographers Does It Take To...Teach The Students?

- At the University of Minnesota we offer a 4-credit hour course in X-Ray Crystallography with a laboratory.
- We have ~30 active graduate students and postdoctoral students trained at any one time.
- Since *learning* crystallography is an iterative process all active students need additional training to learn cold mounting, disorder modeling, validation and interpretation of results, etc.
- As soon as a student masters (or believes he/she has mastered) a concept, then reality comes crashing down!
- So how many crystallographers are required to support all of these students?

How Many Crystallographers Does It Take To... Keep All The Instruments Running?

- 1995 – 2007 projects total ~4000 for XCL.
- Since instituting CHEM 5755 there has been a shift from XCL staff conducting service work to students conducting their own experiments.
- In the last two years student-run experiments were ~60% of the total while using ~82% of scheduled time based on 1 instrument.
- XCL staff uses the remaining time equally for internal and external collaborators.
- Downtime over two years is about 8% of scheduled.
- The majority of downtime is due to detector problems.

How Many Crystallographers Does It Take To... Maintain The Database?



- 4-MM DAT daily/weekly backups
- DVD for raw data
- “WORK” files are kept available indefinitely
- CIMA is great for integrating raw data with metadata
- Roughly ¼TB in raw data

How Many Crystallographers Does It Take To... Manage The Laboratory?

- The day-to-day laboratory management within the XCL is challenging, but then the distractions common in public universities waste precious time.
- A great deal of effort goes into non-crystallographic activities that do not generate income.
- Working with a diverse group of users requires skill especially when it comes to using time efficiently.
- The answer to all of these questions is there are *never* enough crystallographers to do all the tasks required.
- Data management tools like automatic backups, CIMA, ReciprocalNet can streamline our work environment.

Data Security Issues

- At the University of Minnesota there is a serious effort afoot to make all sensitive data secure.
- And if you can make your sensitive data secure, then *all* data could be made secure.
- This could potentially endanger our CIMA Portal since raw and meta data is being transferred continuously between UM and IU computers and storage facilities.
- We should actively explore the issues and try to work through the problems lawyers and administrators are attempting to prevent.

CIMA Potential Development

- At the University of Minnesota we monitor the XCL with 2 cameras and each instrument's videomicroscope.
- The laboratory temperature and humidity, and chiller water temperature is monitored.
- So far we have not taken advantage of monitoring cryostat temperature.
- Potential development could monitor the X-ray generators via the B20 board RS-232 port.
- Also, monitoring crystal microscopes would have some value.
- Additional use for traditional security would have value.

XCL Minnesota 1 Wed Apr 25 23:56:16 2007



Streaming video from the lab showing both Bruker instruments

XCL Minnesota 2 Wed Apr 25 23:56:19 2007



Streaming video from the XCL



Bruker SMART 1000 video-microscope view



Bruker SMART 1K video-microscope view

Local date/time: 2007-04-25 23:54:53

LabJack U12

These values are updated approx. every 60 sec.

Times in UTC

Ambient laboratory:	21.4 C Rel. Humid. 24.7 %	2007-04-26 04:54:31Z
SMART 1000 enclosure:	21.5 C Rel. Humid. 24.6 %	2007-04-26 04:54:33Z
Water supply:	23.2 C	2007-04-26 04:54:27Z
Water return:	29.1 C	2007-04-26 04:54:27Z
Cryostream pump:	28.6 C	2007-04-26 04:54:27Z