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 instruments’ 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.
Streaming video from the lab showing both Bruker instruments

Streaming video from the XCL

Bruker SMART 1000 video-microscope view

Bruker SMART 1K video-microscope view

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