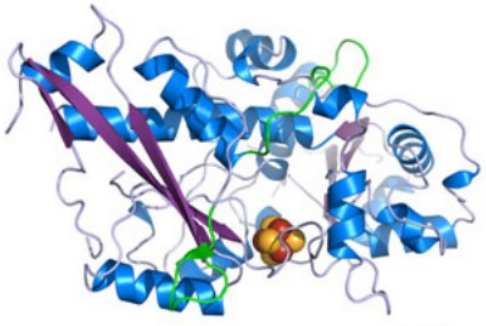
Sharing Science: SSRL Remote Lab

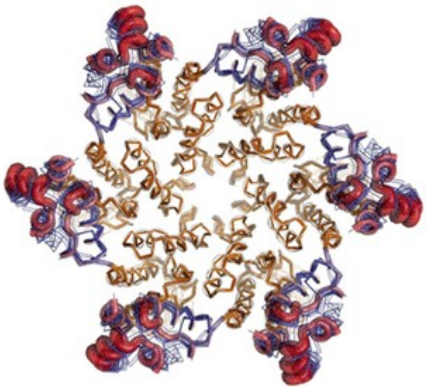
SLAC Scientific Computing Workshop
June 20-21, 2011

Collaborative Tools Session



Hydrogen Production

Membrane Transport

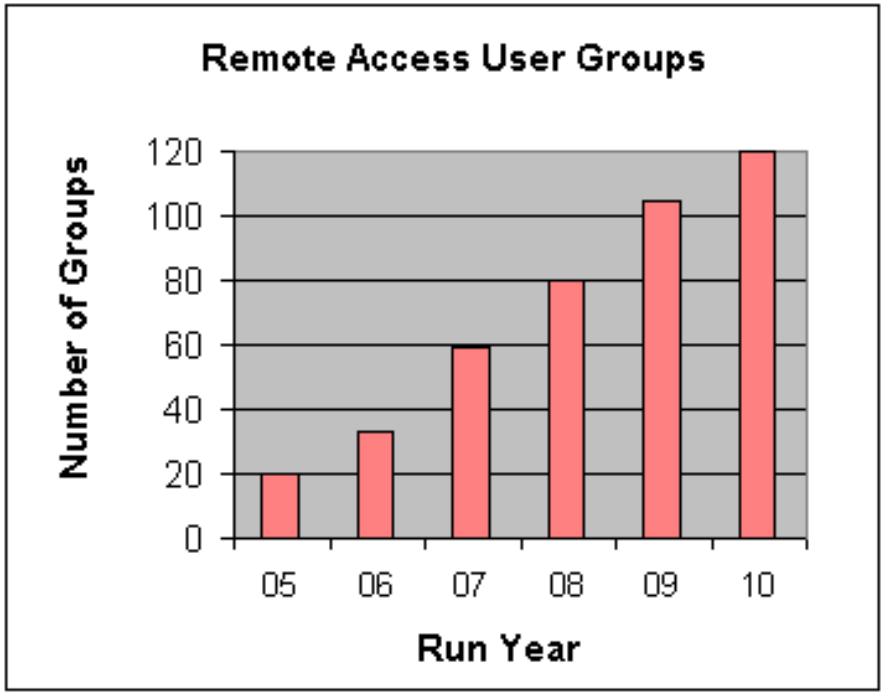


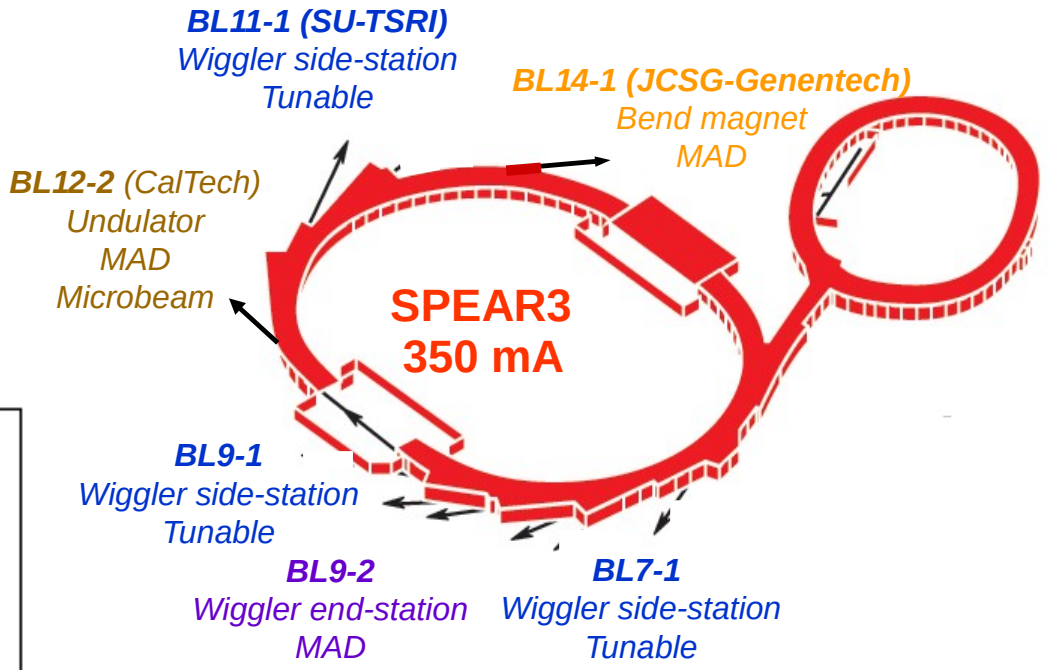
HIV

Thomas Eriksson

Macromolecular Crystallography

- 6 beamlines in operation
- 24/7, 9 months/year
- 126 user groups 2010
- ~550 experiment starts
- More than 95% remote



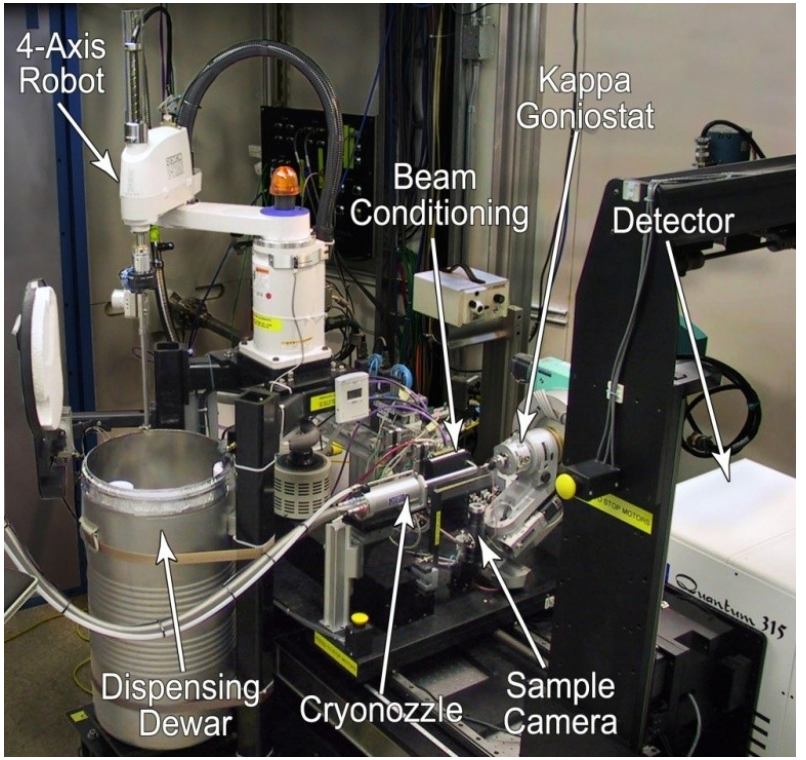


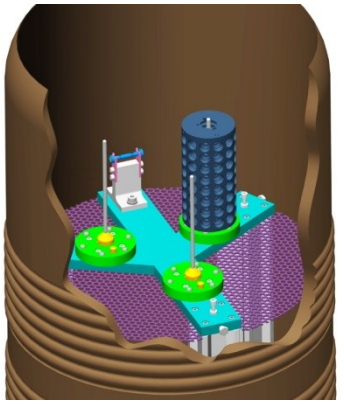
Joint Experiment

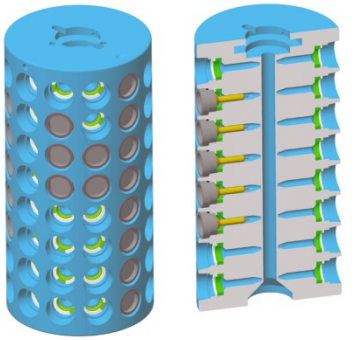
- The idea came up a little before 2000.
- An Experiment is often a collaboration between Biology and Crystallography oriented groups. Not always at the same lab or same university.
- The PI did not want to spend the night at the synchrotron, but wanted to make sure his/her grad students were not sleeping at the beamline.
- A Joint Experiment really needed to be a Remote Experiment.
- Slow at the start, a lot of things need to work flawlessly for a successful remote experiment.
- First, the beamline has to be completely automated.
- Second, it needs to be easy to join the experiment from anywhere.

Automation - 1

- Hardware
  - Robotic sample mounting
    - Sample cassettes holding 96 samples
    - 3 cassettes in dewar
    - Cassettes and tools to add samples under LN2 are provided free
  - Motorization of every motion on the beamline
  - Video feeds of sample and other critical components

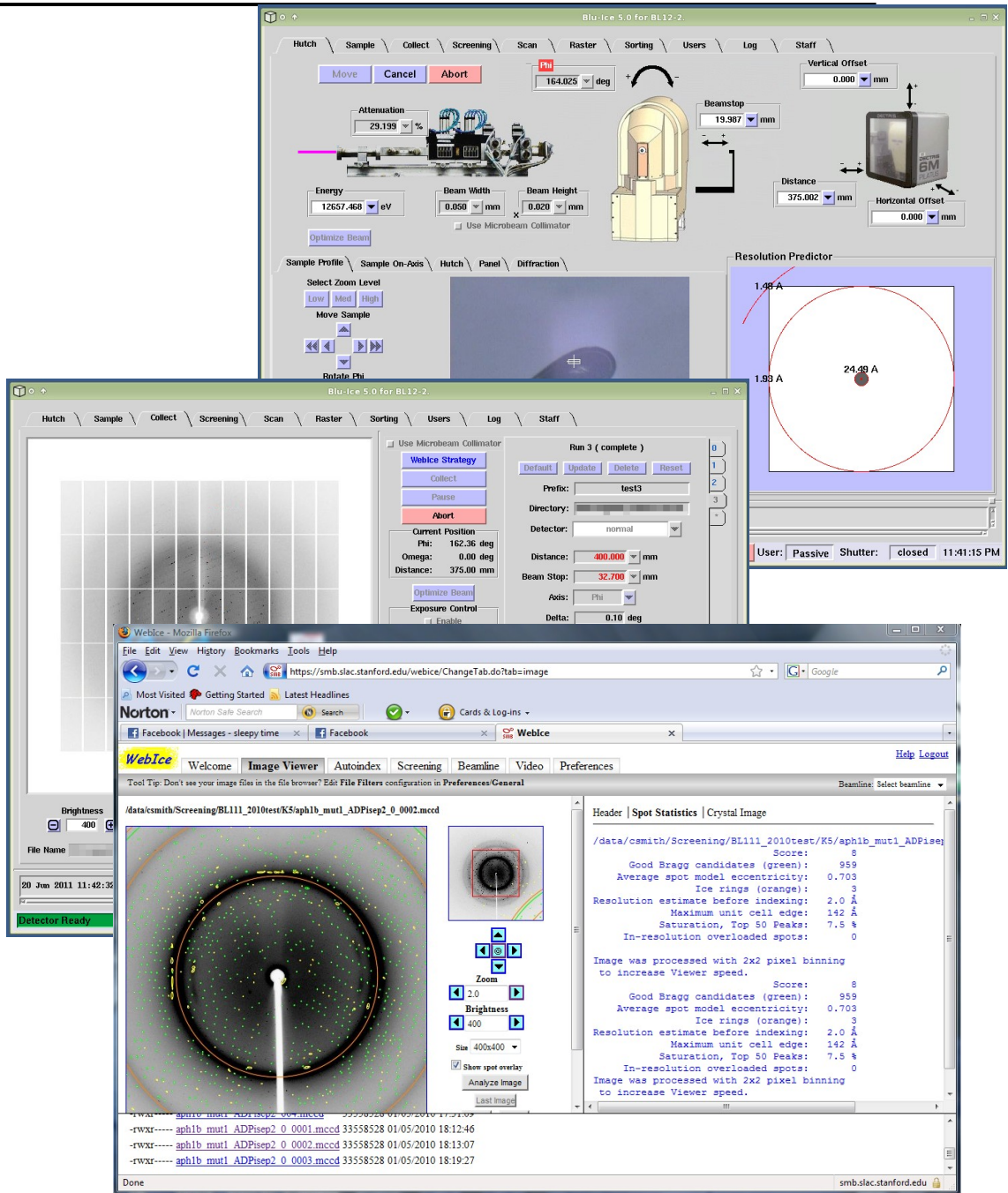






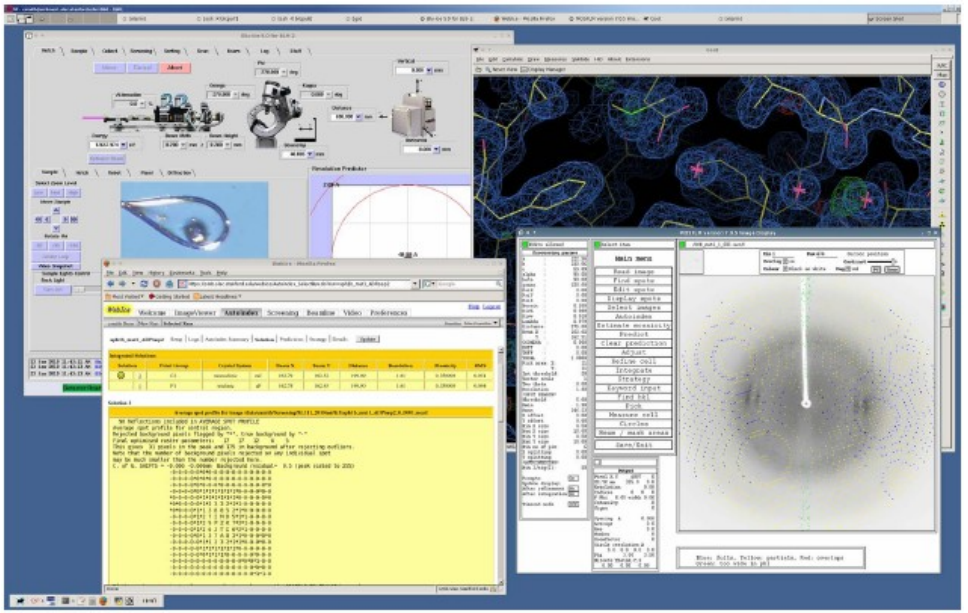
Automation - 2

- Software
  - Bluice/dcss beamline control system
    - Complete control over every aspect of the beamline
    - Sample screening, scoring
    - Data collection strategy
  - Webice – browser based
    - Slightly less functionality on the experiment control side
    - Adds initial data analysis
  - Any number of clients can connect to a beamline at the same time, provided the connecting account is authorized at the time slot.



Remote Beamline Desktop

- NX Server from NoMachine.com
  - Client is free
  - Available for Windows, Linux, OS X
  - Usable at slow network speeds
  - Robust - can reconnect to a lost session



- Users from all over the world, from California to New Zealand
- Huge decrease in cost for the user (shipping vs. airfare)
- Excellent tool for training new users, local and remote.

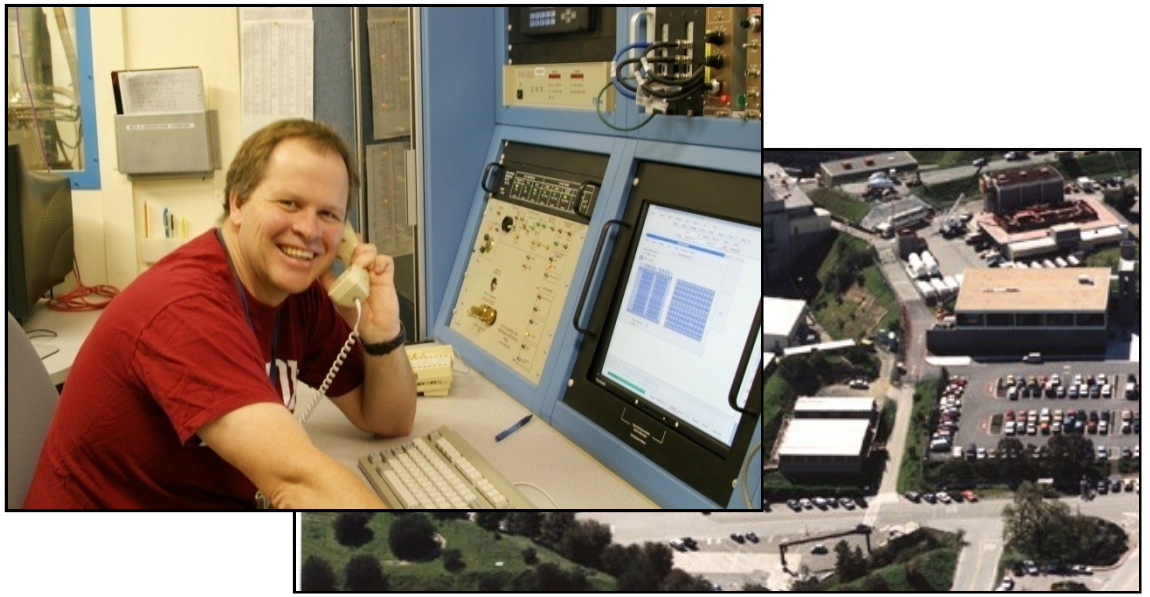
User Services

- Dewar shipping templates to/from SSRL, notification of arrival and LN2 condition. Return after experiment.
- Top up of LN2 for dewars on site.
- Upload of sample information to database for cassettes.
- Built-in “IM” interface in Blu-Ice for communication between users monitoring the same experiment.
- Simulation mode of Blu-Ice allows connecting to a virtual beamline for training purposes.
- The NX client has a session shadow feature that allows staff to give hands on help to remote users.

The Cost Advantage

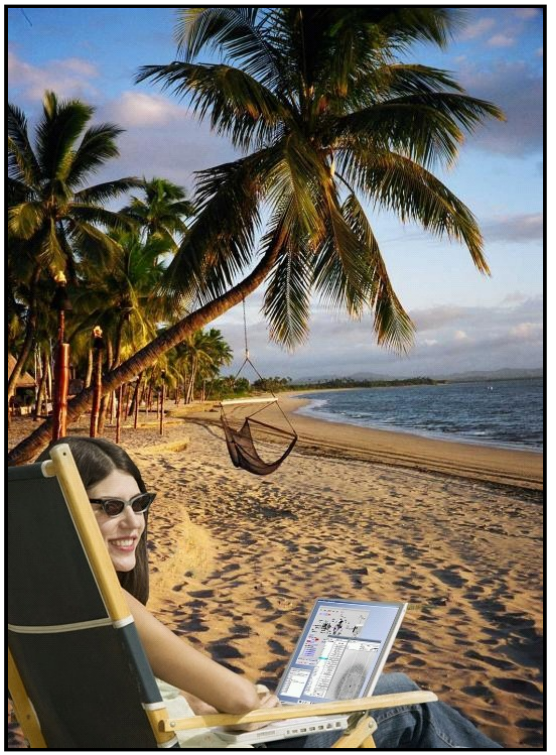
onsite data collection
(group from Huntsville, AL)

Airfare	$432.90
Meals	$191.25
Lodging	$195.00
Taxes	$19.50
Rental car	$148.00
Parking	$24.00
Total (per person)	$1010.65
Total (3 people)	$2735.95



remote data collection

Cassette Kit (incl. cassette and tools)	free
Courier ship dewar)	$200.00 (to



Typical Remote User

User Feedback

User quotes/testimonials:

“Remote access is a tremendously efficient and effective way to collect data - it has greatly widened the possible projects that we can undertake. For our lab it has become an essential tool”

“Regarding remote access, it has definitely provided more opportunities to collect data and to teach new students on how to collect good data. We would not go back to the non-remote method unless this option becomes unavailable”

“SSRL is heaven on earth for crystallography. It is always wonderful to be there for experiments, but in practical terms, the remote access, and completely integrated beam line control, robotic screening, and computational environment, greatly stimulates collaborations and many more experiments with crystals. The remote access capability greatly expands the opportunity for training, and maximizes the use of beam time. SSRL beam lines are completely unique in the world; a few other synchrotrons have remote access, but it does not work smoothly and efficiently as at SSRL”

“I feel that remote access has vastly improved the quality of the data we collect. Since we are not tired from traveling, human error is decreased. In addition, as a PI, remote access allows me to 'stalk' students and passively observe their collection after they are trained. This still allows them to be independent, but gives me a way to monitor and suggest improvements”

Future Directions

- Rest-Flow – framework for organizing the data processing sequence and decision making.
- Auto-Drug - pipeline for fragment-based drug discovery
  - Samples are treated with a multitude of potentially binding compounds
  - Utilizing the Rest-Flow framework and the control system, a personalized workflow screens all samples, determines data collection strategy and process the data and suggest which samples are potential drug targets.
- Automatic structure solving during manual data collection from Blu-Ice and Web-Ice.
  - Also using the Rest-Flow framework.
- BeamlineExpress – a sample queuing system
  - Store samples at SSRL to quickly be able to use available beamtime