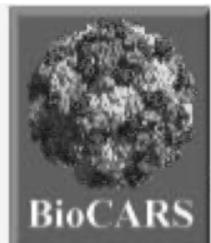


Data Collection Using Database Sequencing

Keith Brister

CARS

The University of Chicago



biocars.org

- NIH/NCRR supported resource for protein and virus crystallography managed by The University of Chicago
- Monochromatic and MAD
- BSL-2 and BSL-3 capable
- Laue
- Time-resolved Crystallography



Administrative Database

- Accounts are assigned to research groups
- Access requires group name and password (something known) as well as an "Access Key" (something owned)

BioCARS Database Registration



Principal Investigator: Keith Moffat 773-702-9950
User Administrator: Dixie Lee Franklin 630-252-0450
Scheduling/Operations: Keith Brister 630-252-0451



BioCARS Database User Registration

Please register your group to use the BioCARS User Information Database.

1. Please do not re-register
2. Select a name for your group
3. Choose a password. You will need this when entering proposal information
4. Enter a valid email address
5. Tell us who the group leader is

An access key together with a user ID will be emailed to you immediately when you press the "Register" button. Please email an email message to Keith Brister.

Group Login Name:	<input type="text"/>
Group Password:	<input type="password"/>
Email Address:	<input type="text"/>
Research Group PI Name:	<input type="text"/>
Institution:	<input type="text"/>

Please verify the group password here:
Double check email address!

BioCARS Database Login



Principal Investigator: Keith Moffat 773-702-9950
User Administrator: Dixie Lee Franklin 630-252-0450
Scheduling/Operations: Keith Brister 630-252-0451



Please log into the BioCARS User Information Database. You will be able to enter information about the people in your group, the materials you plan to bring, and fill out a proposal form.

For more information on our password or access key? Contact Keith Brister (brister@cars.uchicago.edu) or Dixie Franklin (dfranklin@cars.uchicago.edu).

Name:	<input type="text" value="brister"/>
ID:	<input type="text"/>
Access Key:	<input type="text" value="2a075c6f211c3ee1"/>
<input type="button" value="Log in"/>	

For more information? Contact Keith Brister

Group selects their own name and password

Group Name and Access Key are Stored as Cookies

CARS Proposal System (CARPS)

BioCARS User Database Menu

BioCARS User Database

Steps to Submitting an Online Proposal:

- 1) People
- 2) Samples
- 3) Chemicals
- 4) Equipment
- 5) Progress
- 6) Proposals
- 7) Trips
- 8) Publications

Questions? Contact [Keith Brister](#)

 click to verify

100 welcomePg5.v 1.4 2000/09/12 17:00:58 brister Exp 3

Name	Title	Exp
Brister_991122	Linux Transfo	
Brister_000410	Staff Training	
Brister_000410	Station Startup	
Brister_000405	Computer Mal	
1600_StartUp	4pm Start-Up	999
Brister_010320	Workshop	201
_010213	External Proposal	201
_010320	Laser Lab Set-up	exp
Brister_010328	Pinhole Alignment	expired
	test	Please Press Submit Button
Brister_020522	No User Support Available	2003-05-31

Done Adding and Editing

Questions? Contact [Keith Brister](#)

Chemicals

Trips

Act f

P

Spam- (Sta

S

Re

ANS Enter, Update, Show PUBLICATIONS!

System Propo

Funding (Staff Only)

Tools (Staff Only)

<https://biocars.org/userFrames.php3> [5/25/2002 11:13:28 AM]

Chemical Page

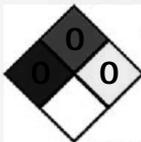
BioCARS Chemical and Gas List

Your Proposal Info	Preferences/Password	Analysis Software	Send Staff Email	Knowl Bug List	Move Detectors Late/Mono Mode	Emperor Emperor View	Run from Now	Fridge	Proposals List	Prepare	User Trip Sched Problems	Create	Bulk Email Administration	Referee Administration	Review Administration	ANSTO Referee Administration	ANSTO Review Administration	BioCARS Publications	Log Out
--------------------	----------------------	-------------------	------------------	----------------	-------------------------------	----------------------	--------------	--------	----------------	---------	--------------------------	--------	---------------------------	------------------------	-----------------------	------------------------------	-----------------------------	----------------------	---------

BioCARS User Chemicals and Gases

Name:

Chemical Formula:



Health Hazard:

Fire Hazard:

Reactivity:

Special: Oxidizing Agent Water Reactive Acid Alkali Corrosive Radioactive

Upload MSDS:

URL: editMaterial.php3, v 1.3.20000712 15:15:43 brister Exp 8

<https://biocars.org/editMaterial.php3> [5/25/2002 11:13:40 AM]

The Trip Page

BioCARS Trip Information Form

Your Proposal Info	Preferences/Password	Analysis Software	Send Staff Email	Known Bug List	Move Detectors Laser/Mono Mode	Emperor Emperor View	Run from Now Fridge Anti Fall Control	Prepare Proposals	User Trip Sched. Problems	Create	Bulk Email	Referee Administration	Review Administration	ANSTO Referee Administration	ANSTO Review Administration	BioCARS Publications	Log Out
--------------------	----------------------	-------------------	------------------	----------------	-----------------------------------	-------------------------	---	-------------------	---------------------------	--------	------------	------------------------	-----------------------	------------------------------	-----------------------------	----------------------	---------

BioCARS Trip Information Form



Principal Investigator: [Keith Moffat](#) 773-702-9950
 User Administrator: [Dixie Lee Franklin](#) 630-252-0450
 Scheduling/Operations: [Keith Brister](#) 630-252-0451



[Current Data Collection Issues](#) [Current Analysis Software](#)

Trip Name: Staff Contact:

Data Directory: [brister_0202](#)

Long Term Data Directory: [brister_0202_oil.d9q](#) [Connect to long term data storage via ftp \(ftp.spot.mcs.anl.gov:6789\)](#)

14IDB time runs from **February 27, 2002 at 8 A.M.** until **March 1, 2002 at 8 A.M.**

[Data Collection Sequences](#)

Proposals for This Trip

Proposal Name	Coming?	Title
1600_StartUp	<input type="checkbox"/>	4pm Start-Up
Brister_000405	<input checked="" type="checkbox"/>	Computer Maintenance
Brister_000410	<input type="checkbox"/>	Staff Training
Brister_000410	<input type="checkbox"/>	Station Startup
Brister_010320	<input type="checkbox"/>	Workshop
Brister_010328	<input type="checkbox"/>	Pinhole Alignment
Brister_020522	<input type="checkbox"/>	No User Support Available
_010213	<input type="checkbox"/>	External Proposal

Users Actually Coming:

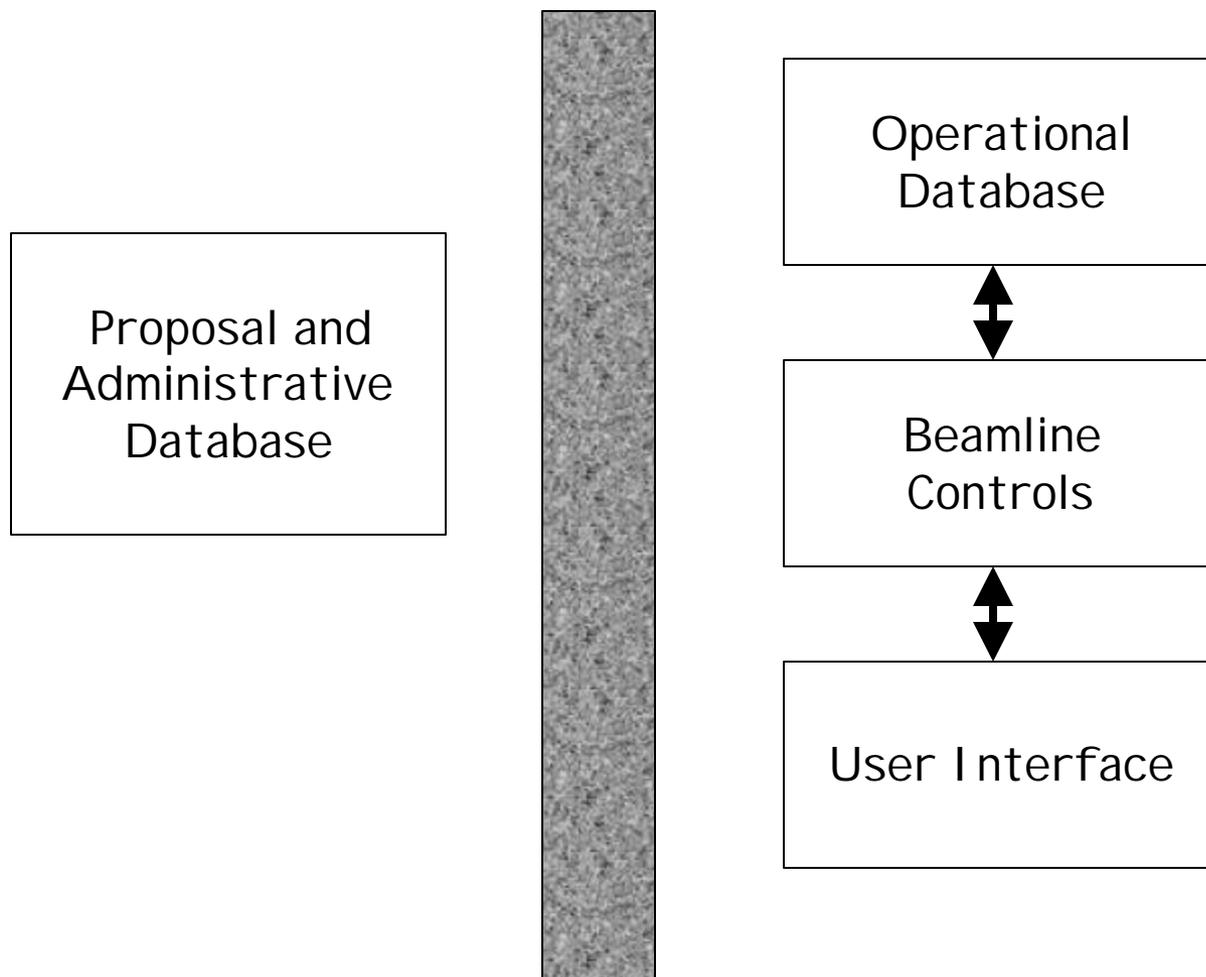
Family Given	Coming?	Arrival Date	Departure Date	Housing
Brister Keith	<input checked="" type="checkbox"/>			
Staff BioCARS	<input type="checkbox"/>			

- People Coming
- Samples Coming
- Chemicals Coming
- Access to archived data
- Set up data collection
- Run data collection

Request ESAF

<https://biocars.org/editTrip.php3> (1 of 2) [5/25/2002 11:19:46 AM]

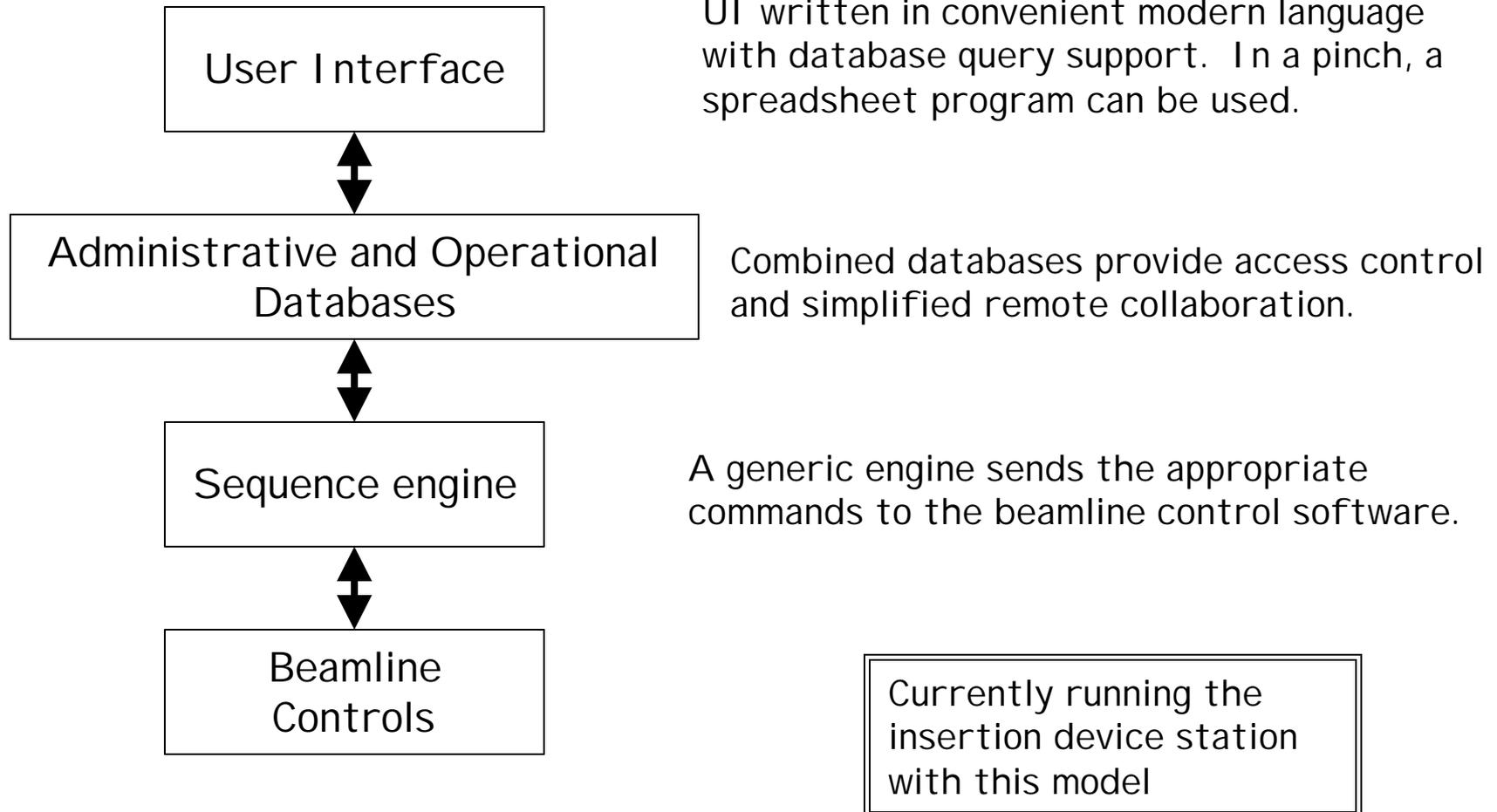
Old Beamline Control Model



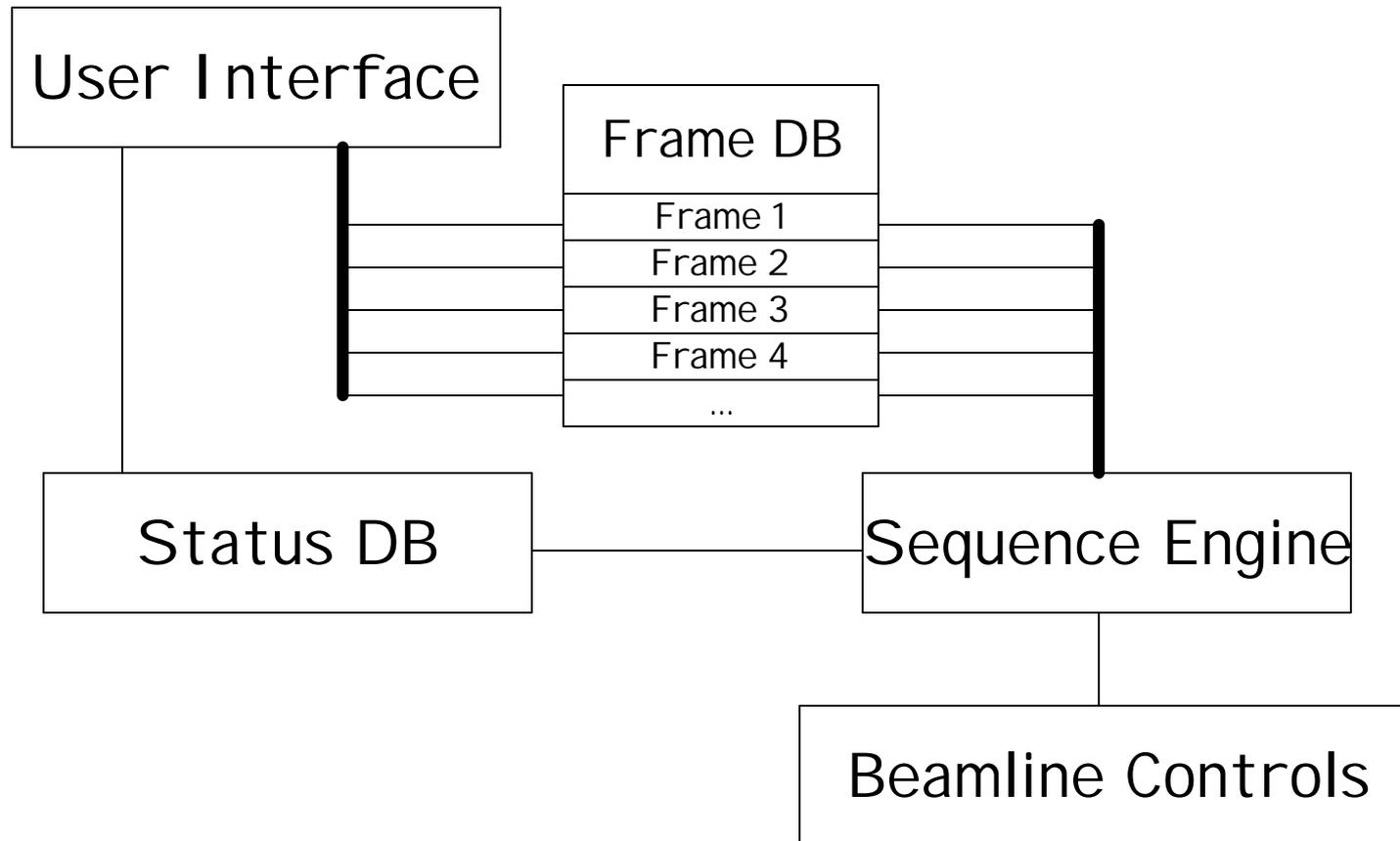
New Approach Beamline Controls and the User Interface

- The Need?
 - Interfaces require a complete knowledge of the low level beamline control code and/or the mastering of inventive interprocess communications protocols. This limits the number of people who are able to contribute to the project.
 - Although many excellent interfaces for MAD and monochromatic crystallography exist, we also need to support user experiments and staff projects for which no interface currently exists.

New Beamline Control Model



Data Sequencing Detail



Edit Page: New Sequence

The screenshot shows a web interface for creating a new sequence. It includes several sections:

- Type of Sequence:** A dropdown menu set to "Time Resolved Laue".
- Sequence to Edit:** A dropdown menu set to "New Sequence".
- *Collection Directory:** A text input field containing "/data/brister_0202".
- *File Prefix (base name):** A text input field containing "test".
- Buttons:** "Change sequence parameters" and "Delete Entire Sequence".
- Generate Frame Definitions:** A section with "Maxium number of frames to generate:" set to "300" and a "Browse..." button.
- Upload Frame Definitions:** A section with an "Upload" button.
- Outer Loop:** A section with "Take one frame with no laser" checked, "Axis:" set to "Omega", "Start Value:" set to "0", "Add" button, and "Final Value" set to "100".
- Inner Loop:** A section with "Take one frame with no laser" checked, "Axis:" set to "Pump-Probe Delay", "Start Value:" set to "1e-8", "Multiply" button, and "Number of Frames" set to "4".
- Bottom Button:** "Add data collection sequence".

Callout lines from the right side of the image point to the following elements:

- "Select type of Sequence" points to the "Type of Sequence" dropdown.
- "Select 'New Sequence'" points to the "Sequence to Edit" dropdown.
- "Enter Directory Name" points to the "*Collection Directory" text field.
- "Enter File Prefix" points to the "*File Prefix (base name)" text field.
- "Click here to generate the sequence" points to the "Add data collection sequence" button.

Monochromatic Sequence

The screenshot shows a web form for generating a monochromatic sequence. The form includes several input fields and buttons. Annotations with arrows point to specific elements:

- Type of Sequence:** A dropdown menu set to "Monochromatic Crystallography".
- Sequence to Edit:** A dropdown menu set to "New Sequence".
- *Collection Directory:** A text input field containing "/data/brister_0206".
- *File Prefix (base name):** A text input field containing "test".
- Sequence based on:** A dropdown menu set to "Use Frame Generator Below" and a "Make Copy" button.
- Generate Frame Definitions:** A section with a "Maximum number of frames to generate:" input field set to "300".
- Upload Frame Definitions:** A section with a "Browse..." button and an "Upload" button.
- Oscillation Axis:** A section with a dropdown menu set to "Omega", a "Start Value:" input field set to "-80", an "Add:" input field set to "1", and a "Final Value" dropdown menu set to "10".
- Create data collection sequence:** A button at the bottom of the form.

Annotations on the right side of the image provide instructions for each field:

- "Select type of Sequence" points to the "Type of Sequence" dropdown.
- "Select 'New Sequence'" points to the "Sequence to Edit" dropdown.
- "Enter Directory Name" points to the "Collection Directory" input field.
- "Enter File Prefix" points to the "File Prefix" input field.
- "Start first frame at this angle" points to the "Start Value" input field.
- "Increment Starting angle by this amount." points to the "Add" input field.
- "Click here to generate the sequence" points to the "Create data collection sequence" button.

Time-resolved Loops

Outer Loop

Take one frame with no laser

Axis:

Start Value:

Inner Loop

Take one frame with no laser

Axis:

Start Value:

Time-resolved sequences may have one or two loops. For each value of the outer loop the entire inner loop is generated. In this example we start with $\omega=0^\circ$ and go to 100° in steps of 10° . For each value of ω , one frame with no laser excitation is taken followed by 4 frames with the laser delayed by 1×10^{-8} , 1×10^{-7} , 1×10^{-6} , and 1×10^{-5} seconds.

If an inner loop is not desired, select "none" for the inner loop axis.

Defined Time-resolved Sequence

Type of Sequence: Time Resolved Laue

Sequence to Edit:

*Collection Directory:

*File Prefix (base name): test

55 Frames Defined

Frame	Status	File Name	Before	Commands	Expose	After
1	Ready	test_001	omega=0;bo03=0;flDelay=1E-08;	snap dir="\$seqDir" file="\$fFileName" cmd="fl2";	bo03=1;sleep t=11;	
2	Ready	test_002	omega=0;flDelay=1E-08;	snap dir="\$seqDir" file="\$fFileName" cmd="fl2";		
3	Ready	test_003	omega=0;flDelay=1E-07;	snap dir="\$seqDir" file="\$fFileName" cmd="fl2";		
4	Ready	test_004	omega=0;flDelay=1E-06;	snap dir="\$seqDir" file="\$fFileName" cmd="fl2";		
5	Ready	test_005	omega=0;flDelay=1E-05;	snap dir="\$seqDir" file="\$fFileName" cmd="fl2";		
6	Ready	test_006	omega=10;bo03=0;flDelay=1E-08;	snap dir="\$seqDir" file="\$fFileName" cmd="fl2";	bo03=1;sleep t=11;	
7	Ready	test_007	omega=10;flDelay=1E-08;	snap dir="\$seqDir" file="\$fFileName" cmd="fl2";		
8	Ready	test_008	omega=10;flDelay=1E-07;	snap dir="\$seqDir" file="\$fFileName" cmd="fl2";		
9	Ready	test_009	omega=10;flDelay=1E-06;	snap dir="\$seqDir" file="\$fFileName" cmd="fl2";		
10	Ready	test_010	omega=10;flDelay=1E-05;	snap dir="\$seqDir" file="\$fFileName" cmd="fl2";		
11	Ready	test_011	omega=20;bo03=0;flDelay=1E-08;	snap dir="\$seqDir" file="\$fFileName" cmd="fl2";	bo03=1;sleep t=11;	
12	Ready	test_012	omega=20;flDelay=1E-08;	snap dir="\$seqDir" file="\$fFileName" cmd="fl2";		
13	Ready	test_013	omega=20;flDelay=1E-07;	snap dir="\$seqDir" file="\$fFileName" cmd="fl2";		
14	Ready	test_014	omega=20;flDelay=1E-06;	snap dir="\$seqDir" file="\$fFileName" cmd="fl2";		
15	Ready	test_015	omega=20;flDelay=1E-05;	snap dir="\$seqDir" file="\$fFileName" cmd="fl2";		
16	Ready	test_016	omega=30;bo03=0;flDelay=1E-08;	snap dir="\$seqDir" file="\$fFileName" cmd="fl2";	bo03=1;sleep t=11;	
17	Ready	test_017	omega=30;flDelay=1E-08;	snap dir="\$seqDir" file="\$fFileName" cmd="fl2";		
18	Ready	test_018	omega=30;flDelay=1E-07;	snap dir="\$seqDir" file="\$fFileName" cmd="fl2";		

To delete an entire sequence, confirm YES and click here.

If needed, enter new directory and press "Change sequence Parameters"

Click here to remove unexposed frames. If all frames are unexposed (or marked to retake) then you will get the Loops screen.

Download the sequence as a spreadsheet file.

Press here when ready. This only appears if you currently have beamtime.

Edit these commands if needed

Mark frames to be retaken here. This will change "Collected" back to "Ready" for the selected frames.

Run Page

Current Clock

The screenshot displays the 'Run Page' interface. At the top left, there is a small graph labeled 'Current Clock'. Below it, the status information is as follows:

- Current: 101.9 mA
- phi: -270.000 degrees
- kappa: 0.000 degrees
- omega: -42.960 degrees
- 06/28/2002 21:20:13
- Prefix: test
- File:
- Frames: 91 out of 91 exposed

A 'RUN' button is visible, with the text 'Master: Stopped' next to it. Below this, there are two buttons: 'Hide Cameras' and 'Show Cameras'. Further down, there are three input fields:

- Sequence Name (Prefix): test [Edit]
- Exposure Time (secs): 5.
- Oscillation Width (degrees): 1.0

A callout box highlights three control buttons:

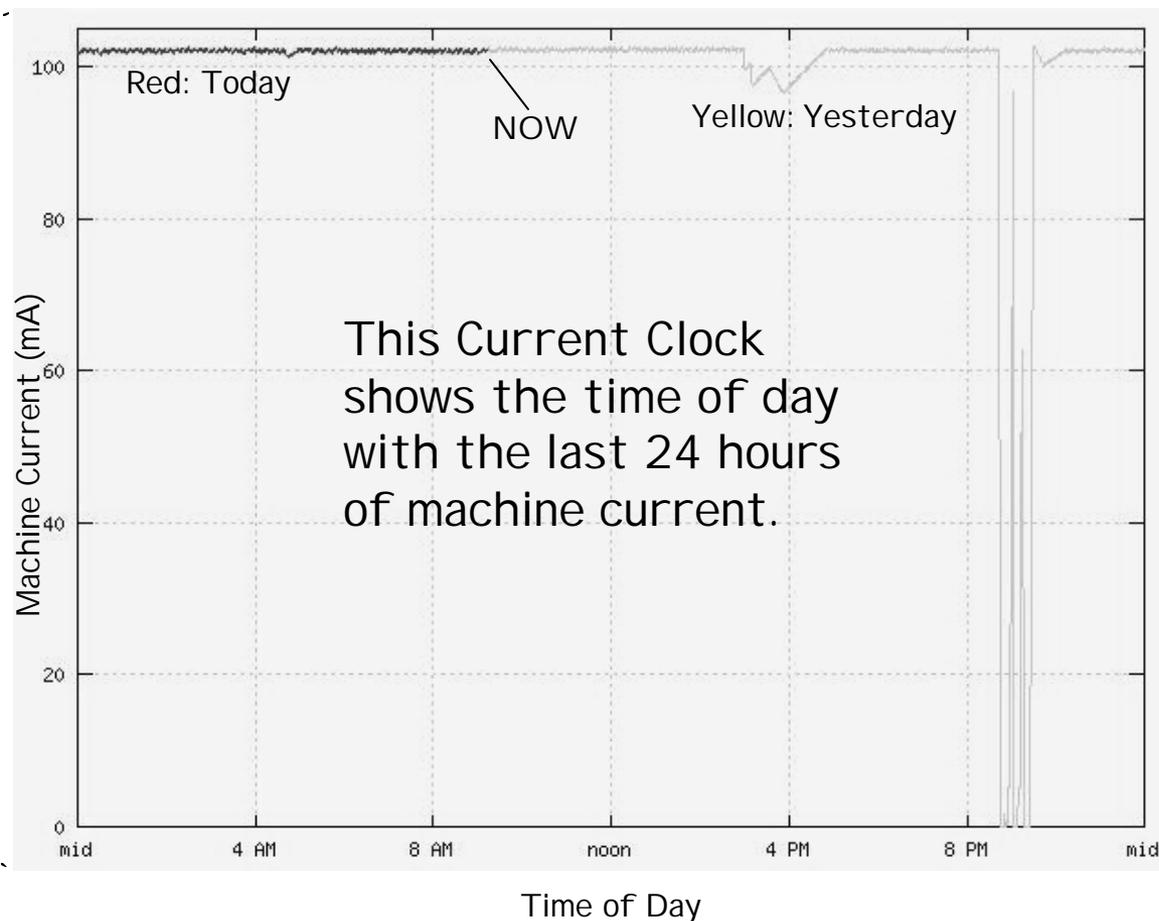
- RUN**: Start data collection
- STOP**: Stop after this frame
- Take Control**: Become Master

Hutch/Station Cameras

Select a Sequence to Run

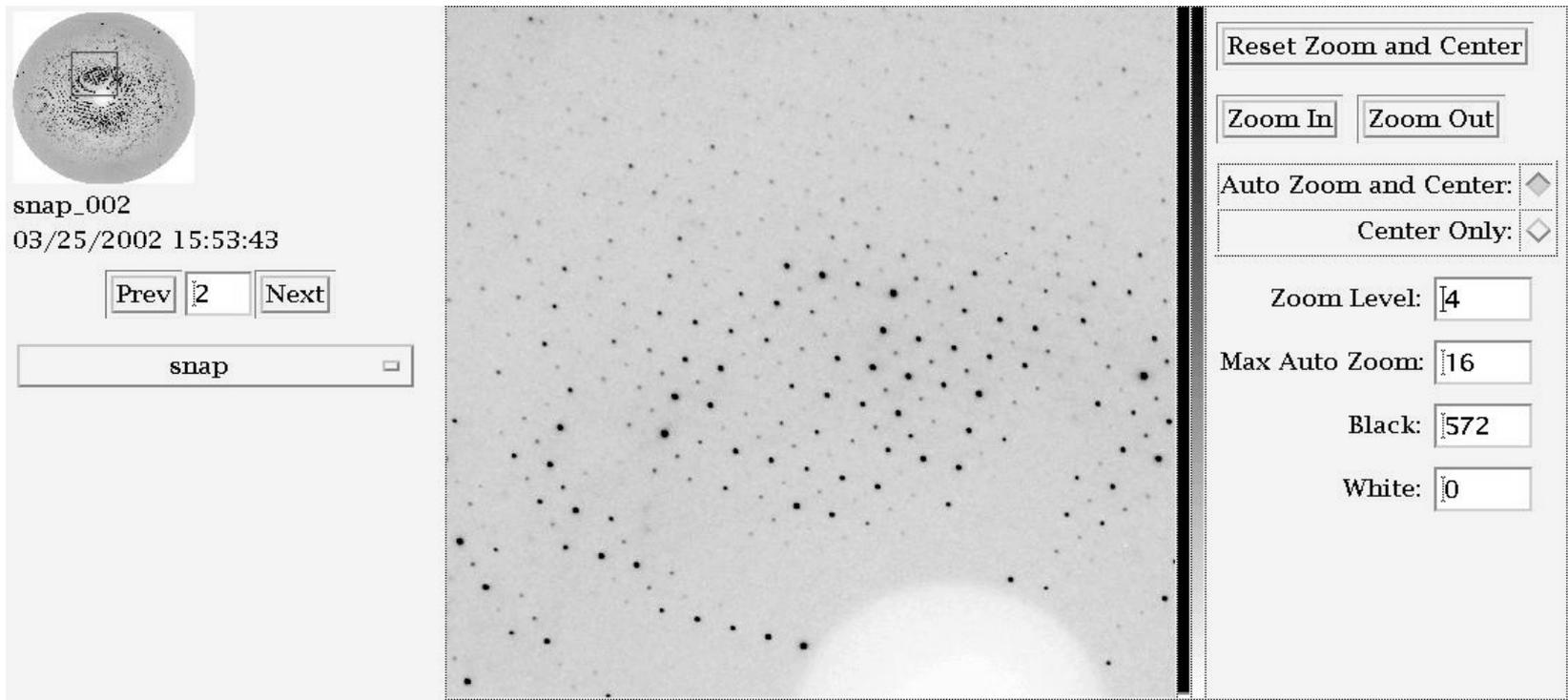
Control Run Time Parameters

Reading the Current Clock



Click small image for larger one

Remote Collaboration Tool



snap_002
03/25/2002 15:53:43

Prev 2 Next

snap

Reset Zoom and Center

Zoom In Zoom Out

Auto Zoom and Center:

Center Only:

Zoom Level: 4

Max Auto Zoom: 16

Black: 572

White: 0

Where is this going?

- Current Development
 - EPI CS interface
 - Remote access and control
 - Remote Collaborations
 - Stand-alone Detector Support (In use at GSECARS)
 - Implementation of BNL PX interface
- Support for Other Facilities
 - Generalized system in beta test (ChemMatCARS)
 - Interface to APS II system
- Open source
 - carps.sf.org (Source Forge site under construction)
- Sequence engines for non-EPI CS beamline control systems
- Interfaces for other experiments