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A WEB-BASED USER INTERFACE FOR MX1 AND MX2 BEAMLINE DATA COLLECTION AT THE AUSTRALIAN SYNCHROTRON

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SC&IT AT THE AUSTRALIAN SYNCHROTRON



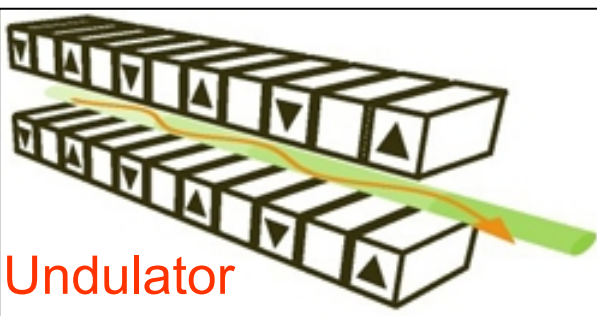
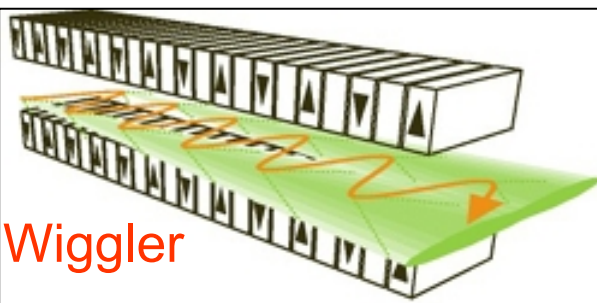
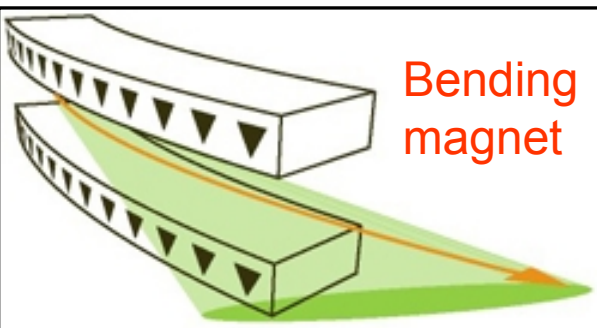
- Core IT Services
- HPC
 - MASSIVE – collaboration with Monash
- **Scientific Software Development**
 - **Automated data processing and data analysis packages**
 - **Remote access to data and instruments**

MX1/MX2 AT THE AUSTRALIAN SYNCHROTRON



Storage ring 3GeV 200mA (electrons)

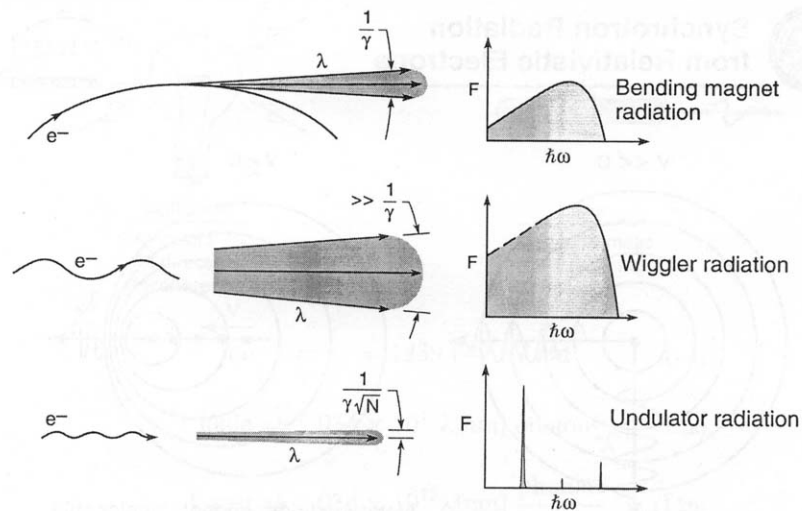
Bending magnet (MX1) – high-throughput



Medical BL



Three Forms of Synchrotron Radiation



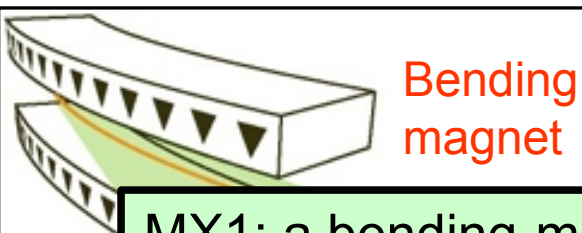
Undulator (MX2) – micro-focus

SAXS/WAXS, XFM, XAS

We have ~80% protein crystallography and ~20% chemical crystallography (more on MX1). ***We focus on user support and can-do.***

MX1/MX2 AT THE AUSTRALIAN SYNCHROTRON

Storage ring 3GeV 200mA (electrons)



Bending magnet

Bending magnet (MX1) – high-throughput

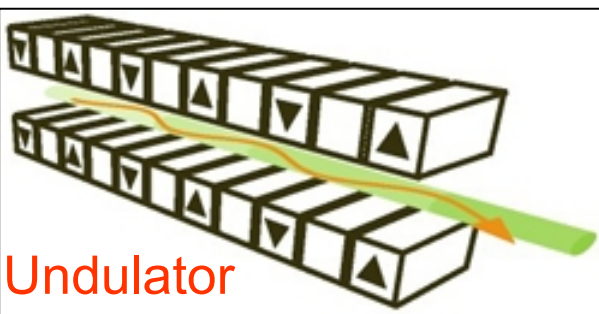
MX1: a bending-magnet crystallography beamline serving both chemical and macromolecular crystallography communities at the Australian Synchrotron

J Synchrotron Radiat. 2015 Jan 1; 22: 187–190.

<http://journals.iucr.org/s/issues/2015/01/00/ig5016/ig5016.pdf>



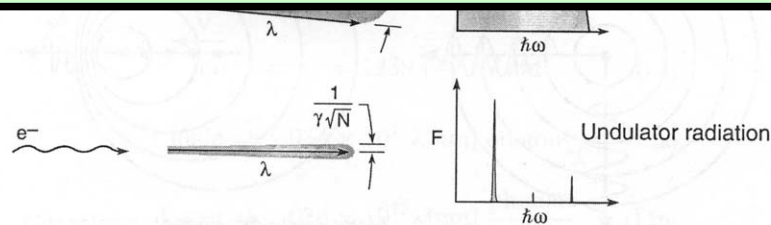
Wiggler



Undulator

Undulator (MX2) – micro-focus

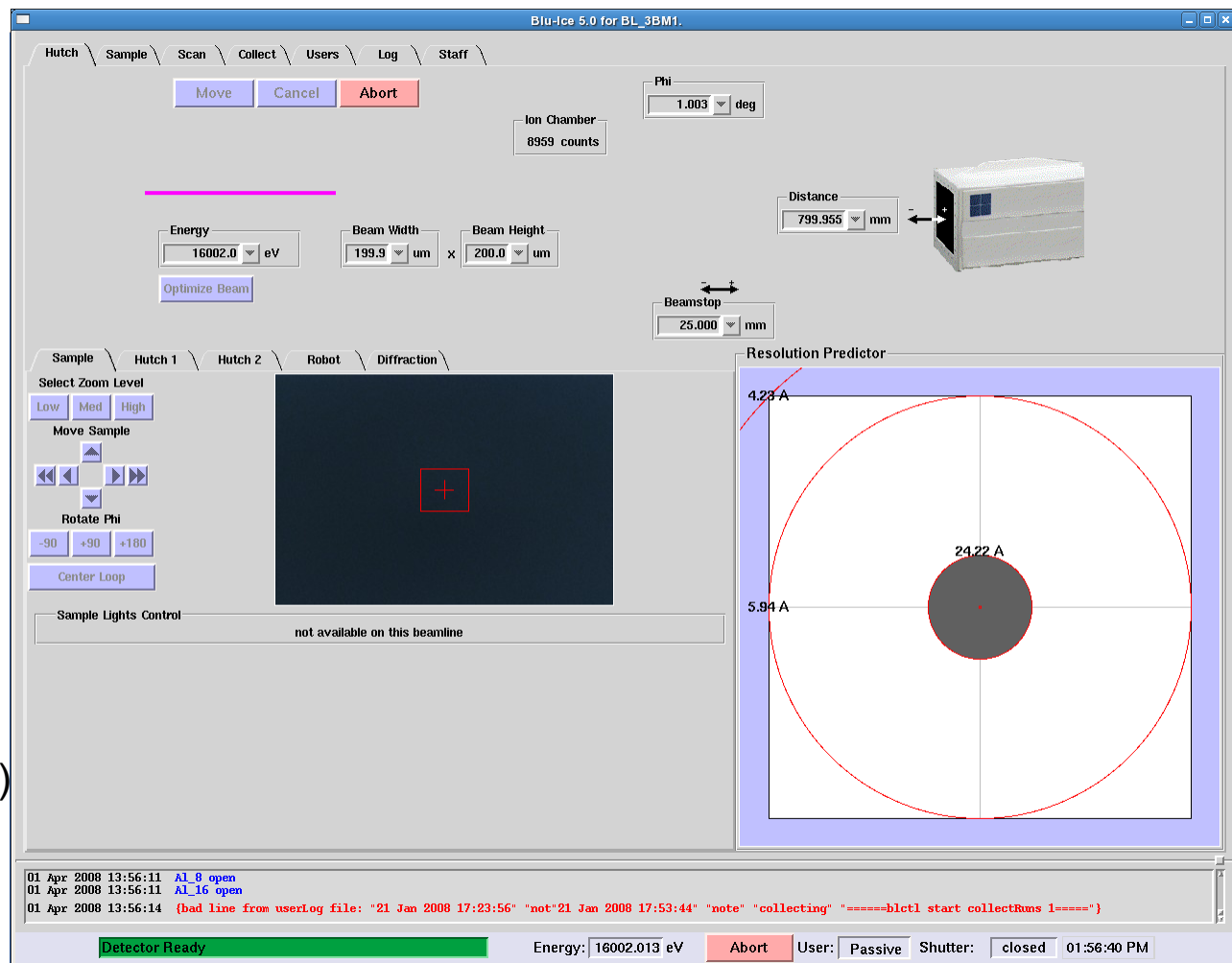
SAXS/WAXS, XFM, XAS



We have ~80% protein crystallography and ~20% chemical crystallography (more on MX1). **We focus on user support and can-do.**

BEAMLINE DATA COLLECTION UI

- ✓ Remote access via Nxclient
- ✓ Excitation scans
- ✓ Excitation vs F scans (MAD)
- ✓ Robot sample mounting
- ✓ Sample centring
- ✓ Energy change control
- ✓ Detector distance control
- ✓ Cryo temperature control (MX1)

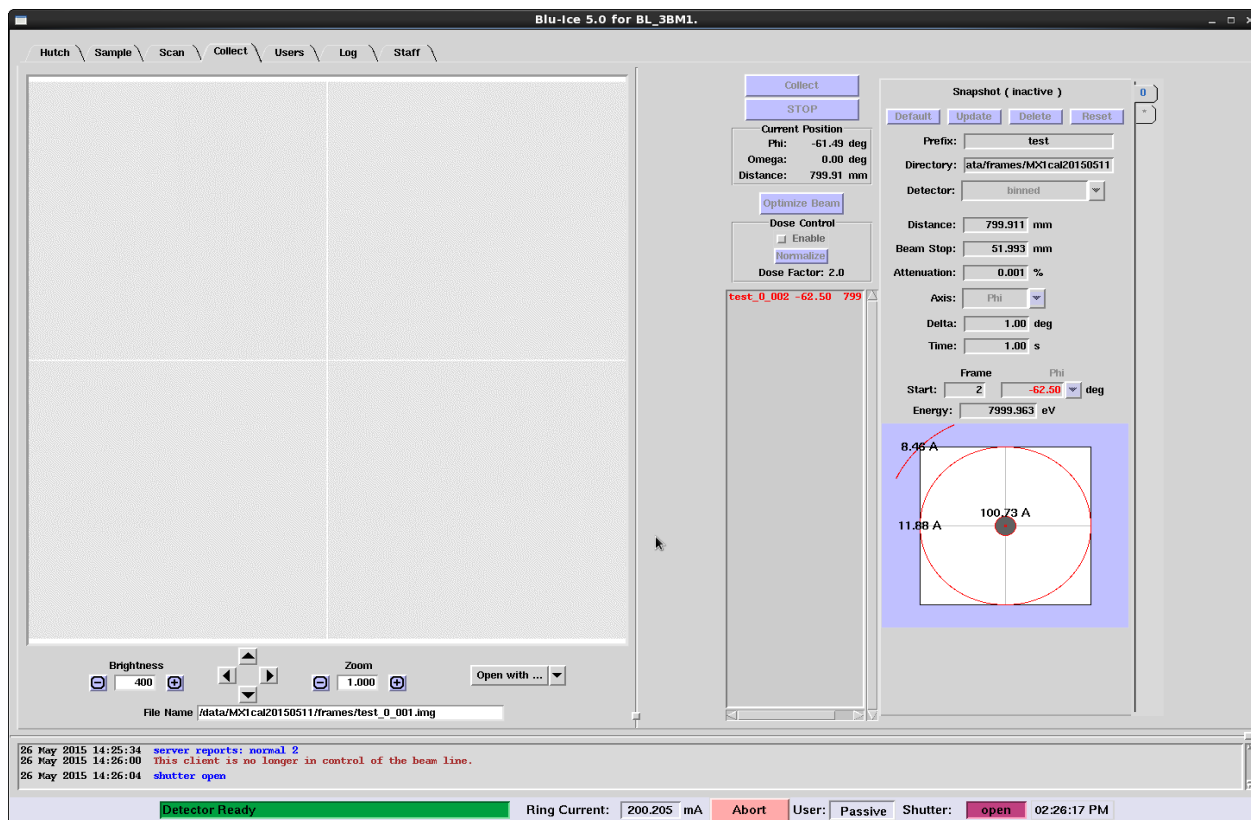


Blu-Ice

MX DATA COLLECTION - CURRENT SYSTEM

Blu-Ice

- Performance and reliability issues resulting in slower data rates and more support call-outs
- Customised, but incompatible with upstream code base.



UI PROJECT REQUIREMENTS



Yet **A**nother Integrated **B**eamline Interface for **X**stalography

- Utilise existing software infrastructure built at MX
 - Python Beamline library
 - Autoprocessing
- Replicate the functionality in Blu-Ice that is familiar to users:
 - Allow snapshots as well as datasets of longer runs
 - View the most recently collection diffraction image
 - Click to centre the sample
- Extendable: focus on collection tab but allow for addition of other functionality in a modular way

STANDARDISING THE TOOLKIT

- Python as language of choice:

- Modern language
- Good libraries



- Flask

- Lightweight Python web framework



- Redis

- Key-value store



- Javascript libraries:

- Knockout.js: MVVM javascript framework
- Bootstrap



YAIBEX IN ACTION



Collect2 - Yaibex - Mozilla Firefox

Collect2 - Yaibex

10.109.24.10:5000/collect2

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YAIBEX Home Hutch Sample Scan Collect Other

Slave

Snapshots/Datasets

New Collection

	#	File Prefix	Delta (deg)	Time (s)	Mode	Start Frame	End Frame	Start Omega (deg)	Edit	Clone	Delete
<input type="checkbox"/>	1	chem1	4	1	Dataset	1	360	91.02			
<input checked="" type="checkbox"/>	0	chem1	4	1	Snapshot	1	360	360.01			

Previous Next

Collect Stop

chem1_0_000

High Med Low

3 click centering

Current File:

Energy 17.444 Omega 181.009 Attenuation 89.97 Distance 72.162 Beam Flux 0.08 Ring Current 200.44 Shutter Closed

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YAIBEX IN ACTION



Collect2 - Yaibex - Mozilla Firefox

10.109.24.10:5000/collect2

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YAIBEX Home Hutch Sample Scan Collect Other

Table of collections

Snapshots/Datasets

New Collection

	#	File Prefix	Delta (deg)	Time (s)	Mode	Start Frame	End Frame	Start Omega (deg)	Edit	Clone	Delete
<input type="checkbox"/>	1	chem1	4	1	Dataset	1	360	91.02			
<input checked="" type="checkbox"/>	0	chem1	4	1	Snapshot	1	360	360.01			

Previous Next

Collect Stop

chem1_0_000

High Med Low 3 click centering

Current File:

Energy 17.444 Omega 181.009 Attenuation 89.97 Distance 72.162 Beam Flux 0.08 Ring Current 200.44 Shutter Closed

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YAIBEX IN ACTION



Collect2 - Yaibex - Mozilla Firefox

10.109.24.10:5000/collect2

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YAIBEX Home Hutch Sample Scan Collect Other

Slave

Snapshots/Datasets

New Collection

#	File Prefix	Delta (deg)	Time (s)	Mode	Start Frame	End Frame	Start Omega (deg)	Edit	Clone	Delete
<input type="checkbox"/> 1	chem1	4	1	Dataset	1	360	91.02			
<input checked="" type="checkbox"/> 0	chem1	4	1	Snapshot	1	360	360.01			

Previous Next

Diffraction pattern

Collect Stop

chem1_0_000

High Med Low 3 click centering

Current File:

Energy 17.444 Omega 181.009 Attenuation 89.97 Distance 72.162 Beam Flux 0.08 Ring Current 200.44 Shutter Closed

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YAIBEX IN ACTION



Collect2 - Yaibex - Mozilla Firefox

10.109.24.10:5000/collect2

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YAIBEX Home Hutch Sample Scan Collect Other

Slave

Snapshots/Datasets

New Collection

#	File Prefix	Delta (deg)	Time (s)	Mode	Start Frame	End Frame	Start Omega (deg)	Edit	Clone	Delete	
<input type="checkbox"/>	1	chem1	4	1	Dataset	1	360	91.02			
<input checked="" type="checkbox"/>	0	chem1	4	1	Snapshot	1	360	360.01			

Previous Next

Diffraction pattern

Collect Stop

chem1_0_000

High Med Low

3 click centering

Sample video feed with resolution options

Current File:

Energy 17.444 Omega 181.009 Attenuation 89.97 Distance 72.162 Beam Flux 0.08 Ring Current 200.44 Shutter Closed

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YAIBEX IN ACTION



Collect2 - Yaibex - Mozilla Firefox

10.109.24.10:5000/collect2

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YAIBEX Home Hutch Sample Scan Collect Other

Table of collections

Snapshots/Datasets

New Collection

#	File Prefix	Delta (deg)	Time (s)	Mode	Start Frame	End Frame	Start Omega (deg)	Edit	Clone	Delete	
<input type="checkbox"/>	1	chem1	4	1	Dataset	1	360	91.02			
<input checked="" type="checkbox"/>	0	chem1	4	1	Snapshot	1	360	360.01			

Previous Next

Diffraction pattern

List of file names for selected runs in table above

Sample video feed with resolution options

Collect Stop

chem1_0_000

High Med Low

3 click centering

Current File:

Energy 17.444 Omega 181.009 Attenuation 89.97 Distance 72.162 Beam Flux 0.08 Ring Current 200.44 Shutter Closed

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YAIBEX IN ACTION



Collect2 - Yaibex - Mozilla Firefox

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YAIBEX Home Hutch Sample Scan Collect Other

Table of collections

Snapshots/Datasets

New Collection

	#	File Prefix	Delta (deg)	Time (s)	Mode	Start Frame	End Frame	Start Omega (deg)	Edit	Clone	Delete
<input type="checkbox"/>	1	chem1	4	1	Dataset	1	360	91.02			
<input checked="" type="checkbox"/>	0	chem1	4	1	Snapshot	1	360	360.01			

Previous Next

Diffraction pattern

List of file names for selected runs in table above

Sample video feed with resolution options

High Med Low 3 click centering

chem1_0_000

Collect Stop

Current File:

Energy 17.444 Omega 181.009 Attenuation 89.97 Distance 72.162 Beam Flux 0.08 Ring Current 200.44 Shutter Closed

EPICS Pvs and shutter status

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YAIBEX IN ACTION



Active/Passive toggle

Table of collections

Diffraction pattern

List of file names for selected runs in table above

Sample video feed with resolution options

EPICS Pvs and shutter status

Collect2 - Yaibex - Mozilla Firefox

Collect2 - Yaibex

10.109.24.10:5000/collect2

Most Visited Centos Wiki Documentation Forums

YAIBEX Home Hutch Sample Scan Collect Other

Snapshots/Datasets

New Collection

	#	File Prefix	Delta (deg)	Time (s)	Mode	Start Frame	End Frame	Start Omega (deg)	Edit	Clone	Delete
<input type="checkbox"/>	1	chem1	4	1	Dataset	1	360	91.02			
<input checked="" type="checkbox"/>	0	chem1	4	1	Snapshot	1	360	360.01			

Previous Next

Collect Stop

chem1_0_000

High Med Low

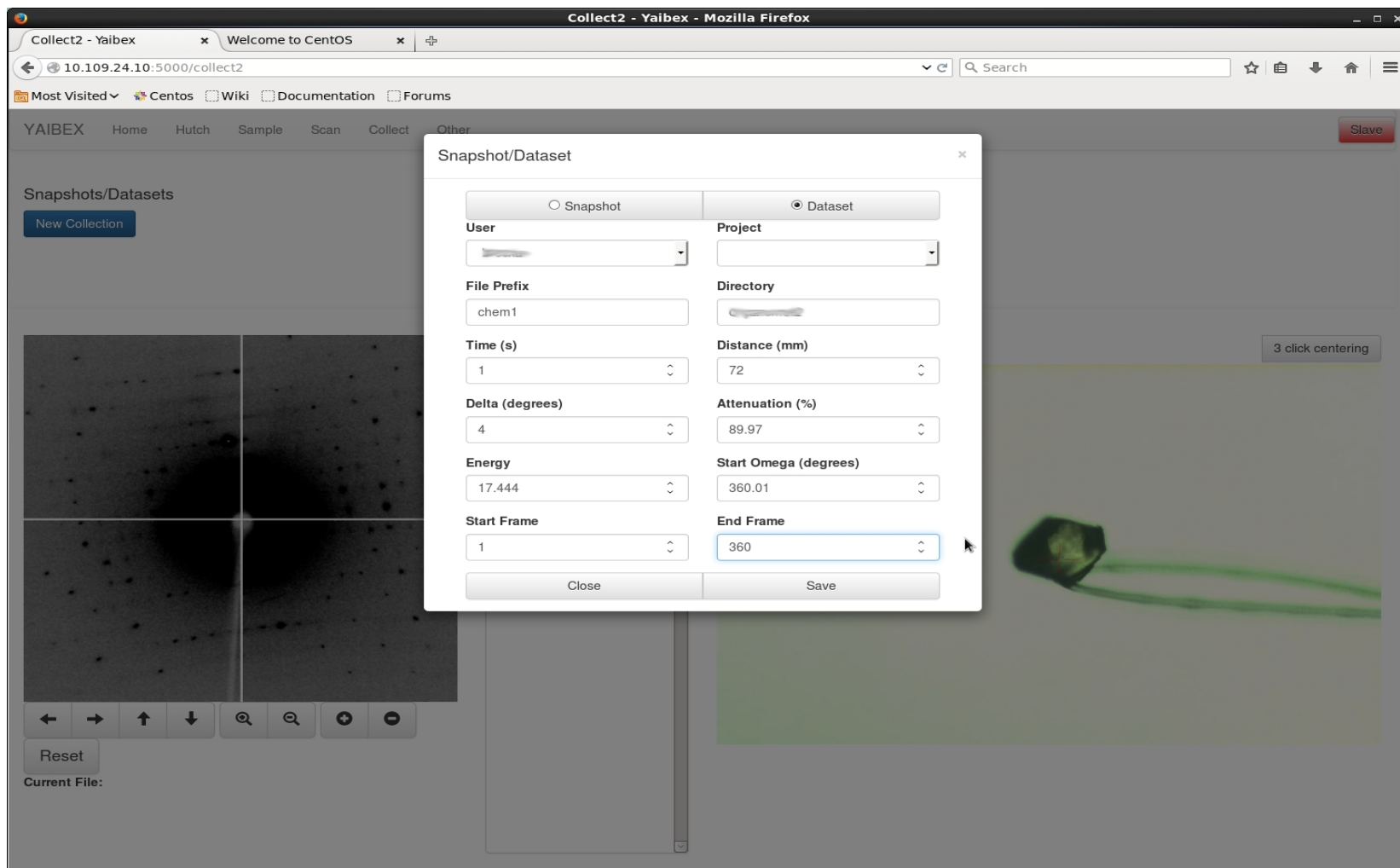
3 click centering

Current File:

Energy 17.444 Omega 181.009 Attenuation 89.97 Distance 72.162 Beam Flux 0.08 Ring Current 200.44 Shutter Closed

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YAIIBEX IN ACTION



YAIBEX IN ACTION



Single shot or dataset mode

The screenshot displays the YAIBEX web interface in a browser window. The main page has a navigation bar with links: YAIBEX, Home, Hutch, Sample, Scan, Collect, and Other. Below the navigation bar, there's a section titled 'Snapshots/Datasets' with a 'New Collection' button. The background shows a dark image with a grid overlay and a 'Reset' button. A 'Current File:' label is at the bottom left. A 'Slave' button is in the top right corner. A '3 click centering' button is visible on the right side of the main image area.

The 'Snapshot/Dataset' dialog box is open, showing two tabs: 'Snapshot' and 'Dataset'. The 'Dataset' tab is selected. The dialog contains the following fields:

- User:** A dropdown menu with a blurred selection.
- Project:** A dropdown menu with a blurred selection.
- File Prefix:** A text input field containing 'chem1'.
- Directory:** A text input field with a blurred selection.
- Time (s):** A numeric input field containing '1'.
- Distance (mm):** A numeric input field containing '72'.
- Delta (degrees):** A numeric input field containing '4'.
- Attenuation (%):** A numeric input field containing '89.97'.
- Energy:** A numeric input field containing '17.444'.
- Start Omega (degrees):** A numeric input field containing '360.01'.
- Start Frame:** A numeric input field containing '1'.
- End Frame:** A numeric input field containing '360'.

At the bottom of the dialog are 'Close' and 'Save' buttons. A green callout bubble points to the 'Dataset' tab with the text 'Single shot or dataset mode'.

YAIBEX IN ACTION



Single shot or dataset mode

Values from current EPICS PVs
or previous collections

The screenshot shows the Collect2 - Yaibex web interface. A modal dialog titled "Snapshot/Dataset" is open, allowing configuration for either a "Snapshot" or a "Dataset". The "Dataset" mode is selected. The dialog contains the following fields:

Field	Value
User	[Dropdown menu]
Project	[Dropdown menu]
File Prefix	chem1
Directory	[Dropdown menu]
Time (s)	1
Distance (mm)	72
Attenuation (%)	89.97
Energy	17.444
Start Omega (degrees)	360.01
Start Frame	1
End Frame	360

Buttons at the bottom of the dialog: Close, Save.

The background interface includes a navigation bar with links: Home, Hutch, Sample, Scan, Collect, Other. A "New Collection" button is visible under "Snapshots/Datasets". A "Slave" button is in the top right. A "3 click centering" button is near the main image area. A "Reset" button and "Current File:" label are at the bottom left.

YAIBEX IN ACTION



Collect2 - Yaibex - Mozilla Firefox

10.109.24.10:5000/collect2

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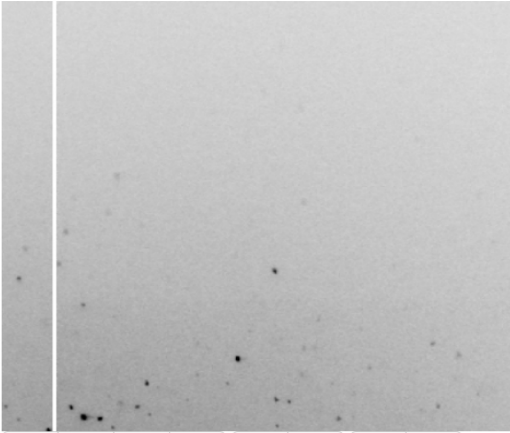
YAIBEX Home Hutch Sample Scan Collect Other Slave

Snapshots/Datasets

New Collection

	#	File Prefix	Delta (deg)	Time (s)	Mode	Start Frame	End Frame	Start Omega (deg)	Edit	Clone	Delete
<input checked="" type="checkbox"/>	1	chem1	4	1	Dataset	1	360	91.02			
<input type="checkbox"/>	0	chem1	4	1	Snapshot	1	360	360.01			

Previous Next



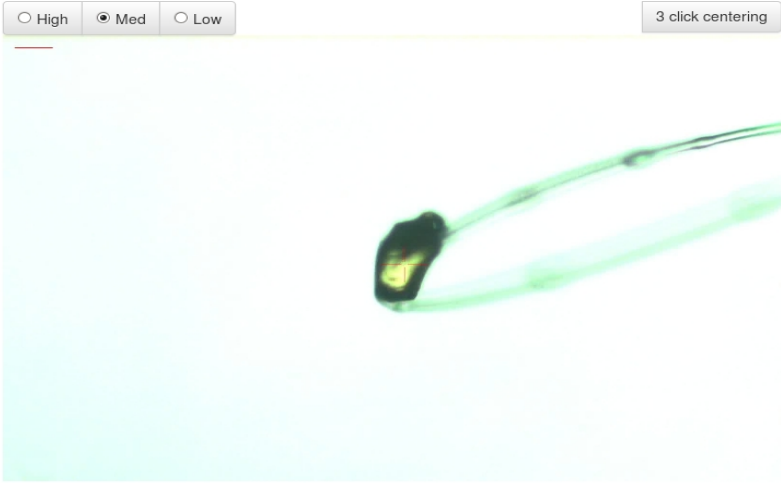
Collect Stop

- chem1_1_001
- chem1_1_002
- chem1_1_003
- chem1_1_004
- chem1_1_005
- chem1_1_006
- chem1_1_007
- chem1_1_008
- chem1_1_009
- chem1_1_010
- chem1_1_011
- chem1_1_012

← → ↑ ↓ 🔍 🔍 + -
Reset

High Med Low

3 click centering



YAIBEX IN ACTION



Select collections

Collect2 - Yaibex - Mozilla Firefox

10.109.24.10:5000/collect2

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YAIBEX Home Hutch Sample Scan Collect Other

New Collection

	#	File Prefix	Delta (deg)	Time (s)	Mode	Start Frame	End Frame	Start Omega (deg)	Edit	Clone	Delete
<input checked="" type="checkbox"/>	1	chem1	4	1	Dataset	1	360	91.02			
<input type="checkbox"/>	0	chem1	4	1	Snapshot	1	360	360.01			

Previous Next

Collect Stop

chem1_1_001
chem1_1_002
chem1_1_003
chem1_1_004
chem1_1_005
chem1_1_006
chem1_1_007
chem1_1_008
chem1_1_009
chem1_1_010
chem1_1_011
chem1_1_012

High Med Low

3 click centering

Reset

YAIBEX IN ACTION



Collect2 - Yaibex - Mozilla Firefox

10.109.24.10:5000/collect2

YAIBEX Home Hutch Sample Scan Collect Other

Select collections

New Collection

	#	File Prefix	Delta (deg)	Time (s)	Mode	Start Frame	End Frame	Start Omega (deg)
<input checked="" type="checkbox"/>	1	chem1	4	1	Dataset	1	360	91.02
<input type="checkbox"/>	0	chem1	4	1	Snapshot	1	360	360.01

Previous Next

Centre sample

Collect Stop

chem1_1_001
chem1_1_002
chem1_1_003
chem1_1_004
chem1_1_005
chem1_1_006
chem1_1_007
chem1_1_008
chem1_1_009
chem1_1_010
chem1_1_011
chem1_1_012

High Med Low

3 click centering

Reset

YAIBEX IN ACTION



Collect2 - Yaibex - Mozilla Firefox

10.109.24.10:5000/collect2

YAIBEX Home Hutch Sample Scan Collect Other

Slave

Select collections

Collection

#	File Prefix	Delta (deg)	Time (s)	Mode	Start Frame	End Frame	Start Omega (deg)	
<input checked="" type="checkbox"/>	1	chem1	4	1	Dataset	1	360	91.02
<input type="checkbox"/>	0	chem1	4	1	Snapshot	1	360	360.01

Previous Next

Centre sample

Trigger collection

Collect Stop

- chem1_1_001
- chem1_1_002
- chem1_1_003
- chem1_1_004
- chem1_1_005
- chem1_1_006
- chem1_1_007
- chem1_1_008
- chem1_1_009
- chem1_1_010
- chem1_1_011
- chem1_1_012

High Med Low

3 click centering

Reset

YAIBEX IN ACTION



Collect2 - Yaibex - Mozilla Firefox

Collect2 - Yaibex x Welcome to CentOS x

10.109.24.10:5000/collect2

Most Visited Centos Wiki Documentation Forums

YAIBEX Home Hutch Sample Scan Collect Other

Slave

Snapshots/Datasets

New Collection

	#	File Prefix	Delta (deg)	Time (s)	Mode	Start Frame	End Frame	Start Omega (deg)	Edit	Clone	Delete
<input type="checkbox"/>	1	chem1	4	1	Dataset	1	360	91.02			
<input checked="" type="checkbox"/>	0	chem1	4	1	Snapshot	1	360	360.01			

Previous Next

Zoom in diffraction image

chem1_0_000

Collect Stop

High Med Low

3 click centering

Reset

The screenshot displays the YAIBEX web interface within a Mozilla Firefox browser window. The browser's address bar shows the URL 10.109.24.10:5000/collect2. The page features a navigation menu with links for Home, Hutch, Sample, Scan, Collect, and Other. A 'Slave' button is visible in the top right corner. The main content area is titled 'Snapshots/Datasets' and includes a 'New Collection' button. Below this is a table with columns for selection, index, file prefix, delta, time, mode, start/end frames, start omega, and action icons (edit, clone, delete). The table contains two rows: one for a 'Dataset' and one for a 'Snapshot'. A green callout box with the text 'Zoom in diffraction image' points to a large diffraction image on the left side of the interface. Below the image is a control bar with navigation arrows and a 'Reset' button. To the right of the diffraction image is a 3D model of a protein structure, with a '3 click centering' button above it. The browser's status bar at the bottom shows the page title 'Collect2 - Yaibex'.

YAIBEX IN ACTION



Collect2 - Yaibex - Mozilla Firefox

Collect2 - Yaibex x Welcome to CentOS x

10.109.24.10:5000/collect2

Most Visited Centos Wiki Documentation Forums

YAIBEX Home Hutch Sample Scan Collect Other

Slave

Snapshots/Datasets

New Collection

	#	File Prefix	Delta (deg)	Time (s)	Mode	Start Frame	End Frame	Start Omega (deg)	Edit	Clone	Delete
<input type="checkbox"/>	1	chem1	4	1	Dataset	1	360	91.02			
<input checked="" type="checkbox"/>	0	chem1	4	1	Snapshot	1	360	360.01			

Previous Next

Translate diffraction image

Collect Stop

chem1_0_000

High Med Low

3 click centering

Reset

The screenshot displays the YAIBEX web interface within a Mozilla Firefox browser window. The browser's address bar shows the URL 10.109.24.10:5000/collect2. The page features a navigation menu with links to Home, Hutch, Sample, Scan, Collect, and Other. A 'Slave' button is visible in the top right. The main content area is titled 'Snapshots/Datasets' and includes a 'New Collection' button. Below this is a table with columns for selection, ID, file prefix, delta, time, mode, frame range, start omega, and actions (edit, clone, delete). Two rows are shown: one for a 'Dataset' and one for a 'Snapshot'. The 'Snapshot' row is selected. Below the table are 'Previous' and 'Next' buttons. A green callout box with the text 'Translate diffraction image' points to a large diffraction image on the left. To the right of this image is a smaller panel showing the processed image, labeled 'chem1_0_000'. Above the processed image are buttons for 'Collect' and 'Stop', and radio buttons for 'High', 'Med', and 'Low' settings. A '3 click centering' button is also present. At the bottom left of the diffraction image are navigation controls (arrows, zoom, pan) and a 'Reset' button.

YAIBEX IN ACTION



Collect2 - Yaibex - Mozilla Firefox

Collect2 - Yaibex x Welcome to CentOS x

10.109.24.10:5000/collect2

Most Visited Centos Wiki Documentation Forums

YAIBEX Home Hutch Sample Scan Collect Other

Slave

Snapshots/Datasets

New Collection

	#	File Prefix	Delta (deg)	Time (s)	Mode	Start Frame	End Frame	Start Omega (deg)	Edit	Clone	Delete
<input type="checkbox"/>	1	chem1	4	1	Dataset	1	360	91.02			
<input checked="" type="checkbox"/>	0	chem1	4	1	Snapshot	1	360	360.01			

Previous Next

Translate diffraction image

chem1_0_000

Collect Stop

High Med Low

3 click centering

Change contrast

Reset

FUNCTIONALITY SUMMARY

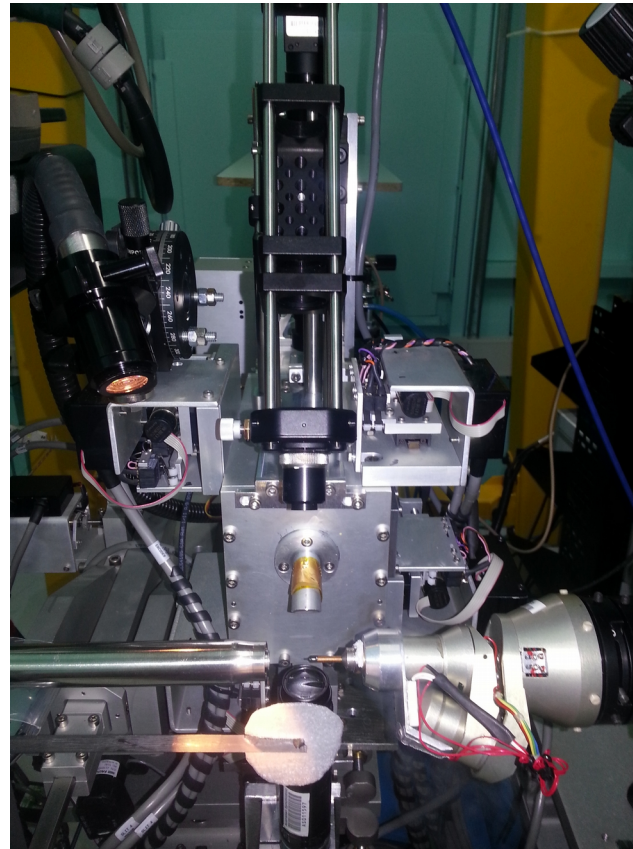
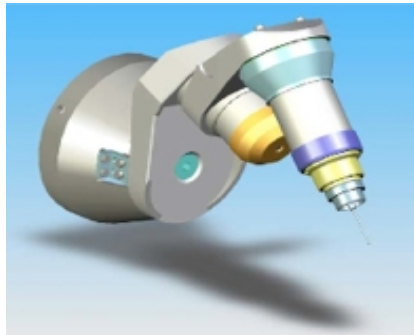


Current:

- Specify data collection parameters for both a single shot and a continuous data set
- Trigger the data collection with reporting of when the shutter is open or shut
- View live feed on sample camera ROI with click-to-centre functionality
- View epics PV values (motor values, beam current etc).
- Integrates with the current Blu-Ice instances so that only one instance can take control of the beamline, and allow switching between active and passive mode
- View the current diffraction pattern, with options to change zoom, translation and contrast.
- Integrates with autoprocessing triggering
- UI designed to work remotely on smaller laptop or tablets

FUTURE DEVELOPMENTS

- Deploy on MX2
- Other "tabs" such as hutch/sample/scan
- Integration with user portal API to fetch user, project and other information.
- Mini kappa



THANKS AND ACKNOWLEDGEMENTS



Thanks to both the SC&IT and MX teams:

David Aragao for driving the project and working with me down at the beamline.

Nathan Mudie for developing a lot of the beamline computing infrastructure YAIBEX uses.

MX beamline staff who have helped with testing and debugging.