

Data collection strategy and Data reduction in JBlueICE-EPICS

Sudhir Babu Pothineni, Nagarajan Venugopalan, Craig Ogata, Mark Hilgart
GM/CA@APS
TWG Meeting, Aug 16th 2012

Software Highlights of GM/CA@APS

- JBluice-EPICS beamline control software
- Automated screening
- Automated diffraction/fluorescence rastering for invisible crystals and to select best diffracting areas of a visible crystal
- Auto centering on visible crystals
- Automated data collection strategy
- Single site & multiple site data collection (Vector data collection)
- Automated data reduction

JBluice-EPICS: Beamline BM Version 2017.2 Build 4828

File Network Options Tools Help

Hutch Sample Screening Raster Scan Collect Analysis Users Log

Start Cancel

Attenuation: 34.98

Omega: 359.989

2-Theta: -0.000

Distance: 935.000

Energy: 12.6580

Width: 0.045

Height: 0.026

Beamstop: 30.000

Automation: Loop Centering, Crystal Centering, Stop, Enter Hutch, Optimize Beam

Sample: Low Res Sample: High Res View Hutch

LowRes Zoom: 8.00, 8.00, Rotate +-n: 1.00 deg, 180, +90 -90, +n -n

Resolution Predictor: 5.86, 8.18

APS Current: 102.1 Shutter Permit: Enabled A Shutter: N/A Endstation Shutter: Closed Endstation Secure: No

State: idle ETA: --- EMERGENCY STOP Mono: 12.658 keV IZero: 0.05 V Control: Passive Shutter: Closed

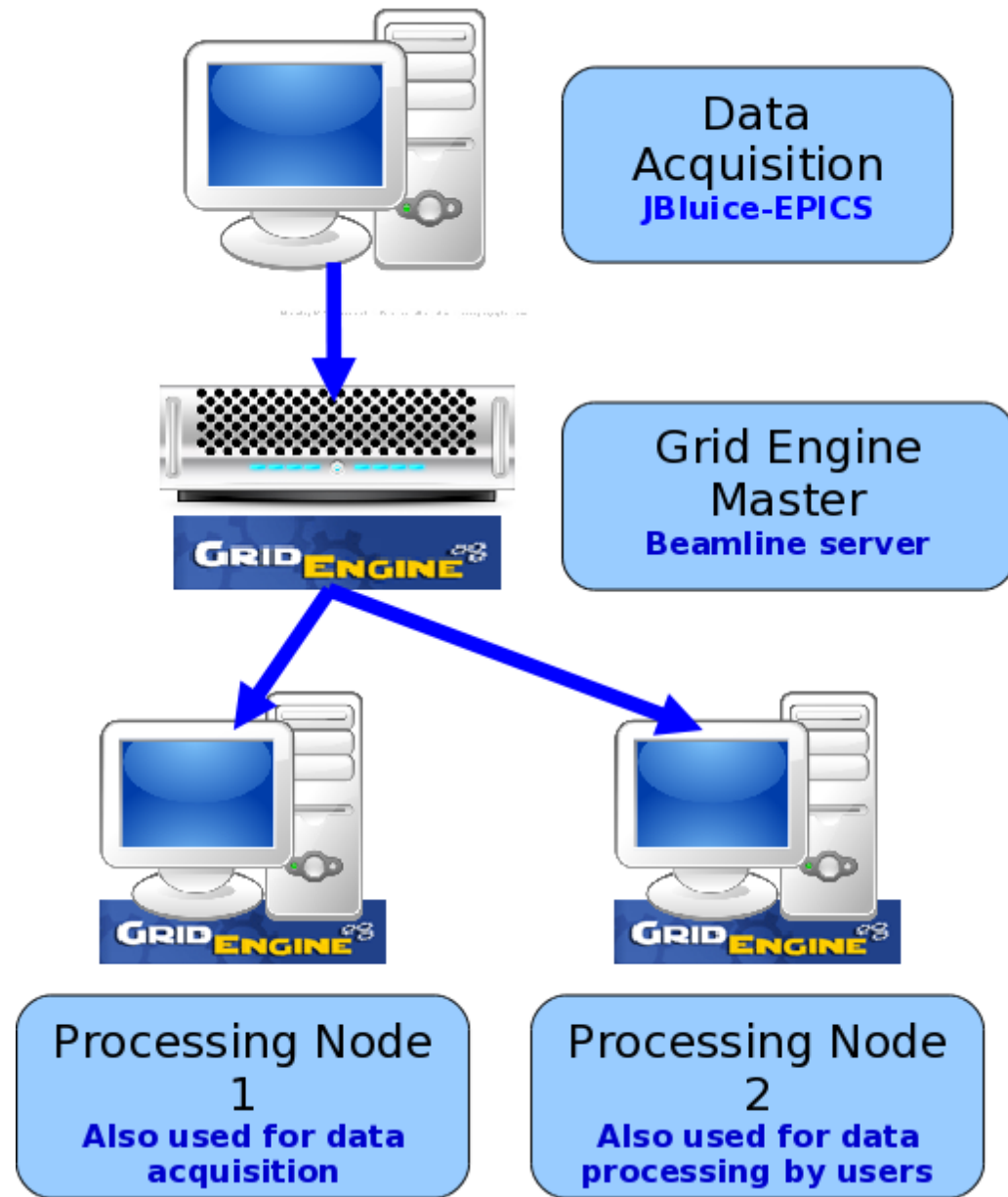
<http://www.gmca.anl.gov/jbluice-epics/>



Data Processing in JBluice-EPICS

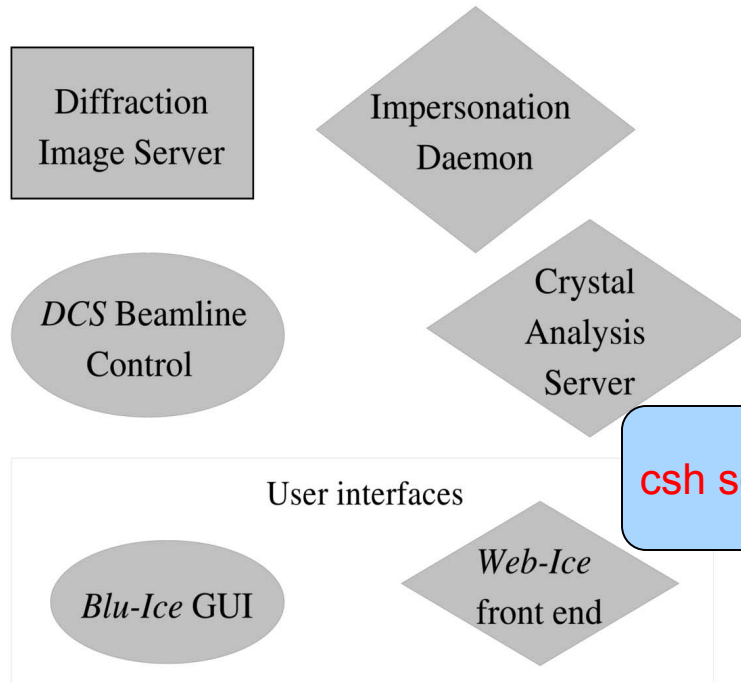
- Efficient use of available resources.
- JBluice uses Grid Engine for running strategy and data reduction jobs.
- Grid Engine is an open source batch queuing system/job scheduler.
- JBluice submits and monitors the Grid Engine jobs using DRMAA java binding and parses the result log files for quality parameters.
- Scalable to dedicated multiple node cluster.

- SSRL Webice based data collection strategy.
- XDS based data reduction

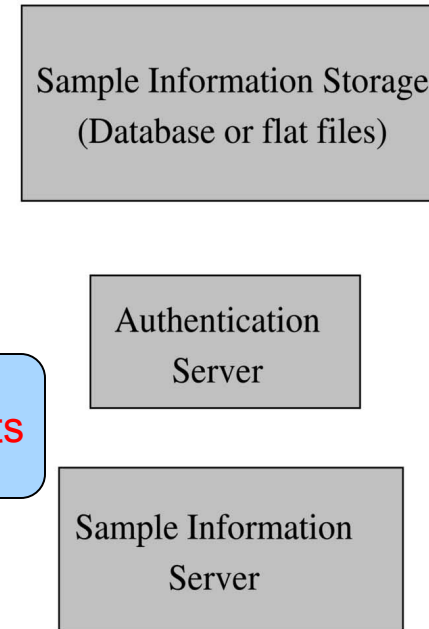


SSRL WebIce

Scalable resources (site deploys as many instances as needed)



Single-instance resources
(only one deployed per site)



csh scripts

LABELIT (autoindexing)
MOSFLM (integration)
BEST (strategy)

Web-Ice: integrated data collection and analysis for macromolecular crystallography. A. González, P. Moorhead, S.E. McPhillips, J. Song, K. Sharp, J.R. Taylor, P.D. Adams, N.K. Sauter and S.M. Soltis. *J. Appl. Cryst.* 41, 176-184 (2008).



Porting Webice to JBluice

Webice	JBluice-EPICS
Impersonation daemon, crystal-analysis server	Grid Engine
Sample information server	MySQL
Image server	Image server
JSP web interface	Java swt application interface
SSRL csh scripts for strategy calculations	Modified SSRL csh scripts for strategy calculations

- Maintenance of tomcat web server, authentication server, ssl certificates etc.. are avoided. Parallelization added.



Strategy initiated from screening tab

JBIulce-EPICS: Beamline ID-B Version 2012.2 Build 4832

File Network Options Tools Help

Hutch Sample **Screening** Raster Scan Collect Analysis Users Log

/mnt/software/common/ALS_template.xls Import spreadsheet Edit Export spreadsheet

Select	Port	CrystalID	Directory	Comment	Resolution	Score
<input checked="" type="checkbox"/>	1	A1	A1			
<input checked="" type="checkbox"/>	2	A2	A2			
<input checked="" type="checkbox"/>	3	A3	A3			
<input checked="" type="checkbox"/>	4	A4	A4			
<input checked="" type="checkbox"/>	5	A5	A5			
<input checked="" type="checkbox"/>	6	A6	A6			
<input checked="" type="checkbox"/>	7	A7	A7			
<input checked="" type="checkbox"/>	8	A8	A8			

Tasklist History

Task Progress

- A1 MountNextXtal
- A1 Paused4Center
- A1 Rotate0
- A1 Collect0
- A1 Rotate90
- A1 Collect90
- A1 Paused4Inspection

PuckType : ALS Puck A Puck B Puck C Puck D Puck E Puck F Clear Clear color code **Mounted** : none

Collection Parameters

Prefix: F15_0
Browse: /mnt/share2/sliu
Current position: Gonio = 180.901, Detector = 900.000, Attenuation = 3.002
Settings: Distance(mm): 250.000, Delta(deg): 1.0, Expose(sec): 2.0, Attenuation(factors): 20.00
Wash/Rinse by Robot: 3 wash Go

Actions

- Mount Next Crystal
- Auto Centering (Loop Crystal)
- Pause4Center
- Jpeg
- Collect Image 0 1
- Collect Image 45 1
- Collect Image 90 1
- Pause4Inspection

Robot

Ready Pause Mount Unmount Gripper Warmup

Robot Status: Current : safetyMat cleared
-1 : pause
-2 : SMR: ready

Command :

[13:06:22] NOTE: puck type ALS

APS Current: -0.0 Shutter Permit: Disabled A Shutter: Closed Endstation Shutter: Closed Endstation Secure: No
State: Idle ETA: --- EMERGENCY STOP Mono: 12.000 keV IZero: 0.02 V Control: Active Shutter: Closed

- Strategy calculation initiated automatically after collecting 2 images in screening tab.

Strategy initiated from collect tab

The screenshot displays the JBLuice-EPICS Beamline ID-D software interface, version 2012.2 Build 4803, running on Simulation Level 1*. The interface is divided into several tabs: Hutch, Sample, Screening, Raster, Scan, Collect, Analysis, Users, and Log. The 'Collect' tab is active, and the 'Strategy' sub-tab is selected. The 'Run 0 (inactive)' panel on the right shows various parameters for the current run, including Prefix, Dir, Distance, Atten., Site, Beam size, Delta, Time, Frame, and Gonio. The 'Strategy' checkbox is checked, and an orange arrow points to it. The 'Resolution Predictor' section shows a circular plot with two values: 4.19 and 5.87. The 'Run sequence >>' table lists the following data:

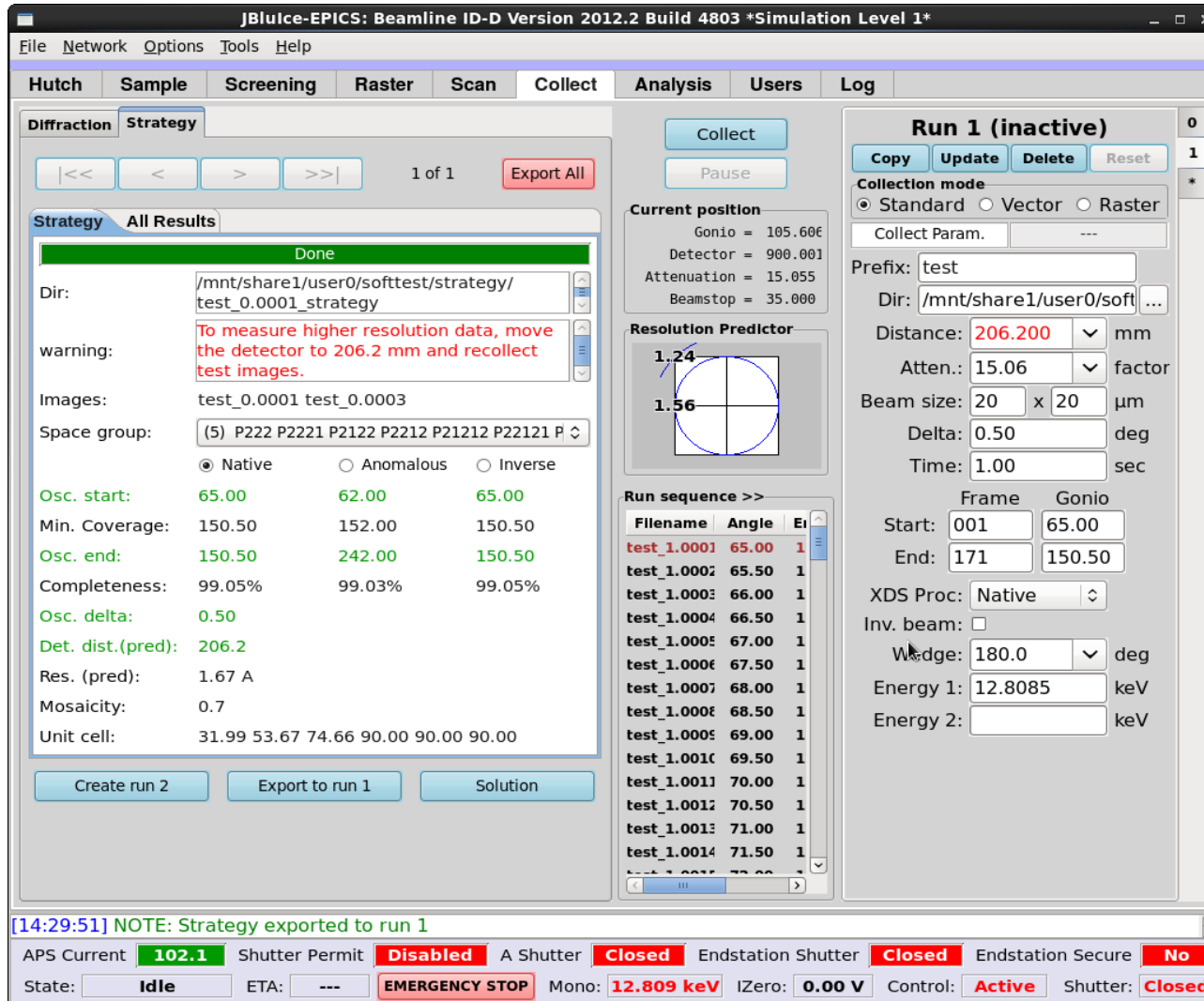
Filename	Angle	Ener
test_0.0001	14.80	12.8
test_0.0003	104.80	12.8

The status bar at the bottom indicates the following system parameters: APS Current: 102.5, Shutter Permit: Disabled, A Shutter: Closed, Endstation Shutter: Closed, Endstation Secure: No, State: Idle, ETA: ---, EMERGENCY STOP, Mono: 12.809 keV, IZero: 0.00 V, Control: Active, Shutter: Closed.

- Strategy can be initiated from collect tab '0' run for manually mounted samples



Strategy parameters



JBluice-EPICS: Beamline ID-D Version 2012.2 Build 4803 *Simulation Level 1*

File Network Options Tools Help

Hutch Sample Screening Raster Scan Collect Analysis Users Log

Diffraction Strategy

1 of 1 Export All

Strategy All Results

Done

Dir: /mnt/share1/user0/softtest/strategy/test_0.0001_strategy

warning: To measure higher resolution data, move the detector to 206.2 mm and recollect test images.

Images: test_0.0001 test_0.0003

Space group: (5) P222 P2221 P2122 P2212 P21212 P22121 P

Native Anomalous Inverse

Osc. start:	65.00	62.00	65.00
Min. Coverage:	150.50	152.00	150.50
Osc. end:	150.50	242.00	150.50
Completeness:	99.05%	99.03%	99.05%
Osc. delta:	0.50		
Det. dist.(pred):	206.2		
Res. (pred):	1.67 Å		
Mosaicity:	0.7		
Unit cell:	31.99 53.67 74.66	90.00 90.00	90.00

Create run 2 Export to run 1 Solution

Collect Pause

Current position
Gonio = 105.600
Detector = 900.001
Attenuation = 15.055
Beamstop = 35.000

Resolution Predictor
1.24
1.56

Run sequence >>

Filename	Angle	El
test_1.0001	65.00	1
test_1.0002	65.50	1
test_1.0003	66.00	1
test_1.0004	66.50	1
test_1.0005	67.00	1
test_1.0006	67.50	1
test_1.0007	68.00	1
test_1.0008	68.50	1
test_1.0009	69.00	1
test_1.0010	69.50	1
test_1.0011	70.00	1
test_1.0012	70.50	1
test_1.0013	71.00	1
test_1.0014	71.50	1

Run 1 (inactive)

Copy Update Delete Reset

Collection mode
 Standard Vector Raster

Collect Param. ---

Prefix: test

Dir: /mnt/share1/user0/soft ...

Distance: 206.200 mm

Atten.: 15.06 factor

Beam size: 20 x 20 µm

Delta: 0.50 deg

Time: 1.00 sec

Frame	Gonio
Start: 001	65.00
End: 171	150.50

XDS Proc: Native

Inv. beam:

Wedge: 180.0 deg

Energy 1: 12.8085 keV

Energy 2: keV

[14:29:51] NOTE: Strategy exported to run 1

APS Current 102.1 Shutter Permit Disabled A Shutter Closed Endstation Shutter Closed Endstation Secure No

State: Idle ETA: --- EMERGENCY STOP Mono: 12.809 keV IZero: 0.00 V Control: Active Shutter: Closed

- After strategy calculation parameters are displayed on strategy sub tab

Selecting lower symmetry spacegroup

The screenshot shows the JBluIce-EPICS software interface. The 'Strategy' tab is active, displaying a list of space groups. Space group (4) P121 P1211 is highlighted in blue, indicating it is the selected option. A warning message is visible: "To measure higher resolution data, move the detector to 206.2 mm and recollect test images." The interface also shows various parameters like "Current position", "Resolution Predictor", and "Run 1 (inactive)" settings.

Space Group List:

Space Group	Parameters
(5) P222 P2221 P2122 P2212 P21212 P22121 P21221 P212121	-->31.99,53.67,74.66,90.00,90.00,90.00
(4) P121 P1211	-->31.99,74.66,53.67,90.00,90.04,90.00
(3) P121 P1211	-->53.65,31.99,74.66,90.00,90.08,90.00
(2) P121 P1211	-->31.99,53.66,74.66,90.00,90.08,90.00
(1) P1	-->31.99,53.63,74.68,90.08,90.08,90.04

Warning: To measure higher resolution data, move the detector to 206.2 mm and recollect test images.

Current position: Gonio = 105.600, Detector = 900.001, Attenuation = 15.055, Beamstop = 35.000

Resolution Predictor: 1.24, 1.56

Run 1 (inactive) Settings: Collection mode: Standard, Prefix: test, Dir: /mnt/share1/user0/soft..., Distance: 206.200 mm, Atten.: 15.06 factor, Beam size: 20 x 20 μm, 50 deg, 00 sec, me Gonio, End: 171, 150.50

Status Bar: [14:31:27] NOTE: Strategy calculation finished. APS Current: 102.5, Shutter Permit: Disabled, A Shutter: Closed, Endstation Shutter: Closed, Endstation Secure: No, State: Idle, ETA: ---, EMERGENCY STOP, Mono: 12.809 keV, IZero: -0.00 V, Control: Active, Shutter: Closed

- Lower symmetry spacegroup can be selectable for to re-run strategy

Data Collection Strategy

- List all possible space groups from Labelit solutions.
- Solutions from same crystal symmetry are filtered.
- By default only space groups from highest symmetry are processed initially.
 - They are processed in parallel so it is faster.
- User can choose lower symmetry solution, JBluice will process and display strategy.
- User has an option to choose strategy from BEST/Mosflm.
- Displays Anomalous information, There are two options.
 - Anomalous continuous where osc. range calculated is doubled.
 - Anomalous Inverse where it will use inverse beam with 'Native' osc. range.
- Improved error/warning handling.
- All the strategy results can be saved in Excel file.
- Processing time about 30 sec (if there is index solution).



Data Reduction

- There is XDSProc option (None, Native, Anomalous) on each run on collect tab, if checked it will initiate XDS processing through Grid Engine after a dataset is collected.
- JBluice will write XDS input file XDS.INP.
- Runs XDS, POINTLESS, SCALA and TRUNCATE
- Any dataset with more than 10 images collected is automatically reduced.
- XDS runs second time with DEFPIX, INTEGRATE, CORRECT incase of failure with INSUFFICIENT PERCENTAGE of spots.
- XDS can process Anomalous data for SAD & MAD data collection.

Run 1 (inactive)

Copy Update Delete Reset

Collection mode
 Standard Vector Raster

Collect Param. ---

Prefix: test

Dir: /mnt/share1/user0/soft ...

Distance: 206.200 mm

Atten.: 15.06 factor

Beam size: 20 x 20 μ m

Delta: 0.50 deg

Time: 1.00 sec

	Frame	Gonio
Start:	001	65.00
End:	171	150.50

XDS Proc: Native

Inv. beam:

Wedge: 180.0 deg

Energy 1: 12.8085 keV

Energy 2: keV



Analysis Tab

- Display data quality parameters and plots automatically on Analysis tab.
- Direct access to XDS, SCALA, TRUNCAE logs with the click of a button.
- The scaled mtz file, and other input and intermediate files stores in a subdirectory of data.
- User can change XDS.INP and reprocess the data.

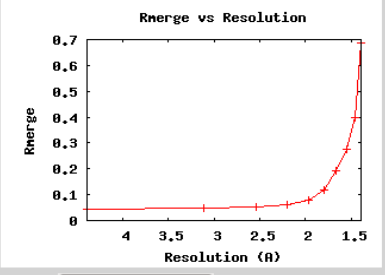
JBluice-EPICS: Beamline ID-D Version 2012.2 Build 4803

File Network Options Tools Help

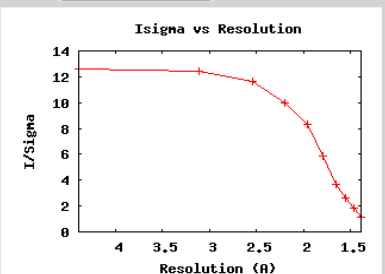
Hutch Sample Screening Raster Scan Collect Analysis Users Log

1 of 1 Export All

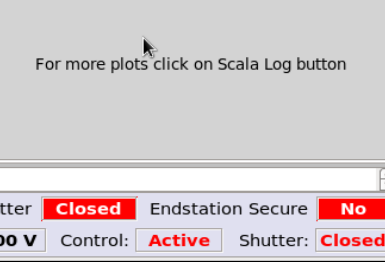
Rmerge Vs Resolution



Energy vs Resolution



I/Sigma Vs Resolution



For more plots click on Scala Log button

Data Quality All Results

Done

Sample Name: beth1_2

Dir: /mnt/staffhome/spothineni/testxsderrors//beth1_2_xds

Images: /mnt/staffhome/spothineni/testxsderrors//beth1_2.####

warning: DONE

Unit Cell: 49.61 55.26 84.24 90.00 90.00 90.00

Space Group: P 2 21 21

	Overall	InnerShell	OuterShell
Low Res.:	46.21	46.21	1.46
High Res.:	1.39	4.39	1.39
Rmerge:	0.085	0.043	0.685
Completeness:	97.4	94.7	98.1
Anom.Completeness:	93.2	91.7	94.4
Multiplicity:	4.1	3.9	4.1
Anom.Multiplicity:	2.2	2.3	2.2
I/Sigma:	9.7	24.8	1.8

XDS Log Scala Log Truncate Log

APS Current 102.4 Shutter Permit Disabled A Shutter Closed Endstation Shutter Closed Endstation Secure No

State: Idle ETA: --- EMERGENCY STOP Mono: 12.809 keV IZero: 0.00 V Control: Active Shutter: Closed



Processing time & specs

Dataset :

360 MAR ccd images

JOB= ALL

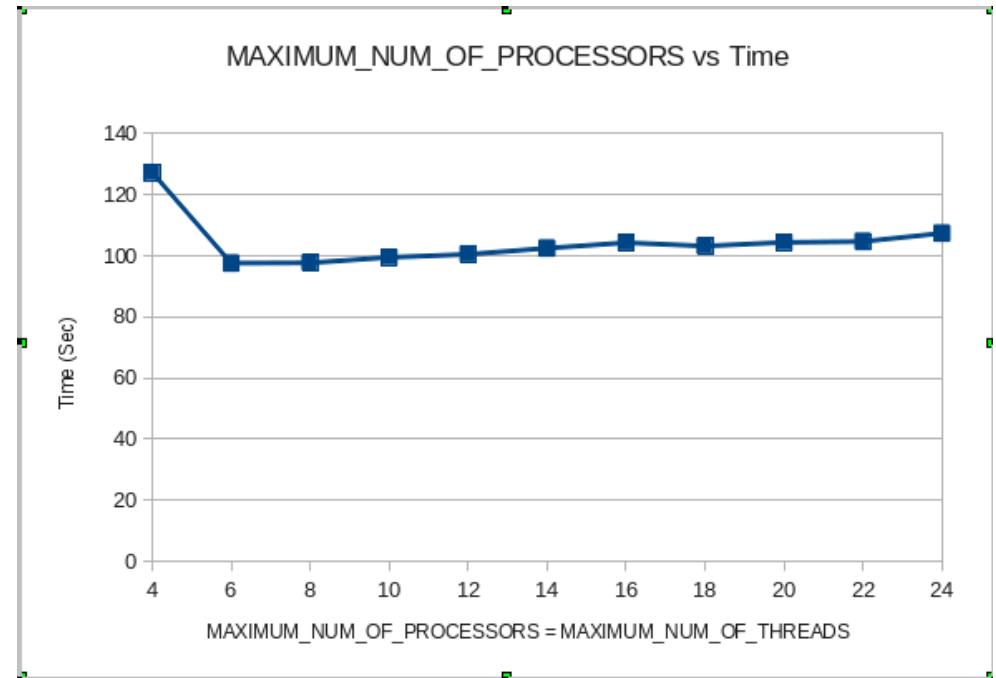
SPOT_RANGE= 1 180

MAXIMUM_NUM_PROCESSORS= 6

MAXIMUM_NUM_THREADS= 6

DELTAPHI= 5

Processing time = 97sec.



Since manual processing overlapping with auto processing on same workstations using
MAXIMUM_NUM_PROCESSORS= 4
MAXIMUM_NUM_THREADS= 4

Processing time = 127sec.

Workstation : Intel Xeon with 2 x 6 cores, hyper-threading enabled, total 24 cores.

- limitation : 32 bit.

OMP_STACKSIZE set according to number of cores.

- Ex. 64m for 24 core machine.



Future plans

- Installing dedicated machines for data processing.
- Adopting fast_dp from Diamond Light Source.
 - Error correction and reprocessing
- Running data processing in parallel to data collection.
- Processing vector data with overlaps and inverse beam.
- Processing data collected with raster sites.
- Molecular replacement for structure solution.

Thanks

JBluice-EPICS

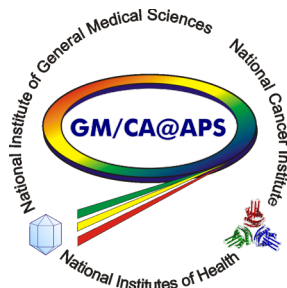
Mark Hilgart
Sudhir Babu Pothineni

GM/CA Management

Janet Smith
Robert Fischetti

Controls

Sergey Stepanov
Oleg Makarov



Crystallography

Craig Ogata
Nagarajan Venugopalan
Ruslan sanishvili (Nukri)
Michael Becker

LABELIT

Nicholas Sauter

