

Rayonix 300HS User's Guide

The new Rayonix 300HS (high speed) detector has been installed on the SER-CAT bending magnet beamline (22BM) for the start of member acceptance testing. The current plan includes the operational use of this detector beginning on Feb. 26th through the end of the current run on 22BM. The system will then be moved to 22ID for the Summer run for continued evaluation. The operational staff needs the help of our members to evaluate the performance of the new detector system, so please submit comments to John Chrzas (chrzas@anl.gov). Technical information on the detector can be found on the Rayonix website: <http://rayonix.com/products/mx-hs-series/>. The Rayonix 300HS detector has a number of advantages over our existing MAR detectors including lower read noise and significantly faster frame rates, which does support shutterless continuous rotation data collection. The purpose of this document is to educate our users on the differences between the new system and our current detectors as well how it has been integrated into sergui. This document is by no means a final version, and I will be relying on the member's feedback to make changes not only to this document but to the sergui integration as well.

What will be different?

- 1) The 300HS does not require the user to "start" marccd. The remote server (hserver) was designed to be a persistent process on the detector control computer. If the hserver is not running, then sergui will not start. We have not experienced a problem with the hserver to date, but currently, the user would need to contact the staff to restart the hserver if it fails. We are working on a method for remote validation and restart, but this will not be in place by the 26th.
- 2) The 300HS will collect continuous rotation data for all data collection runs, but will collect shuttered data for collect singles and any sergui capability such as sample rastering and helical data collection. We will be implementing continuous rotation data collection for these capabilities at a later date.
- 3) When sergui is started, the program adxv will be started in an "automated" mode which will not allow the user to load frames. If a user wants to load frames, they will need to use either marimage, mosflm, or start a different session of adxv. The "automated" adxv session will load new frames as they become available. During an active data collection run, adxv will update every 3 seconds, so far a 1 Hz data collection every third frame will be displayed. If you want to see the entire data set you can use the motion picture mode within a different session of adxv to display the entire data set.
- 4) When collecting data, the sergui standard output (located at the bottom of the screen) will indicate how long the data collection will take (for a 1 deg/sec rotation speed, this will be ~ 120 seconds for a 120 degrees of data, regardless of frame rate). During data collection sergui will be locked and non-responsive.

During the data collection the new frames will be moved to the archive directory every 3-5 seconds over a 10G fiber connection so there will be a slight delay.

How can I process my data?

As of today, the data processing programs that will support data from the new detector include cmdxdx, cmdkylin, and imosflm. Wladek Minor has been contacted, and we are in the process of securing HKL2000/denzo as another option. All data will be auto processed using cmdxdx and cmdkylin. The output of this processing will be found in subdirectories of your archive path labeled zzCmdxdx_filetemplate and zzKylin_filetemplate. If you want a more hands on approach, then mosflm is available on all SER-CAT computers including bmc83 and bmc93 by typing imosflm <>.

Here are links to tutorials on the use of imosflm:

<http://www.mrc-lmb.cam.ac.uk/harry/imosflm/ver107/quickguide.html>

<http://www.mrc-lmb.cam.ac.uk/harry/imosflm/ver107/documentation/tutorial.html>

When processing data from 22BM with imosflm, the user will need to set the beam center and change the direction of the spindles axis in Setting->Experiment:

Check "Reverse the direction of spindle axis"

Type command: ssbeamxy mar300hs

will show you the beam center for all major data processing programs.

If you have any question, just ask your user support.

What are the results of our test data?

We have collected many data sets using trypsin test samples. We have collected data using frame rates of 1 -10 Hz as well as oscillation widths of 0.1-1 degree. The data quality on these test samples has been very good. I will not go into great detail here, but if you have any questions, please contact Albert Fu (fuzq@anl.gov). The following is an xds summary is for 120 degrees of data collected at a continuous rotation speed of 1 deg/sec and a frame rate of 1Hz.

--- --- --- Brief Summary of CMDXDS Output --- --- ---

Mosaicity: 0.255

UnitCell: 54.310 58.210 66.540 90.00 90.00 90.00 P222

Warning: The space group from XDS may not be accurate!

You may check it with 'cmdkylin' or 'cmddenzo'.

statistics by Resolution Shells [range: 100.0000 1.5800]:

---	Reso	Complete	Redund	I/sigI	Rmerge	Rmeas	AnoCC	CC1/2	CC*	---
	7.07	96.30	4.02	45.95	0.0230	0.0260	0.2600	0.9990	0.9997	
	5.00	98.90	4.35	46.55	0.0240	0.0270	0.2700	0.9990	0.9997	
	4.08	99.40	4.38	48.03	0.0230	0.0260	0.2200	0.9990	0.9997	
	3.54	99.40	4.48	47.68	0.0240	0.0270	0.0800	0.9990	0.9997	
	3.16	99.60	4.51	45.07	0.0260	0.0290	0.1900	0.9990	0.9997	
	2.89	99.80	4.60	42.56	0.0270	0.0310	0.1400	0.9990	0.9997	
	2.67	100.00	4.63	37.95	0.0320	0.0370	0.1400	0.9980	0.9995	
	2.50	99.80	4.66	36.46	0.0330	0.0370	0.0900	0.9980	0.9995	
	2.36	99.90	4.67	33.97	0.0370	0.0410	0.0500	0.9980	0.9995	
	2.24	99.90	4.71	33.82	0.0380	0.0430	0.0100	0.9980	0.9995	
	2.13	99.90	4.68	30.55	0.0420	0.0470	0.0000	0.9980	0.9995	
	2.04	99.90	4.72	29.31	0.0440	0.0490	0.0200	0.9980	0.9995	
	1.96	100.00	4.70	26.06	0.0510	0.0570	-0.0200	0.9960	0.9990	
	1.89	99.90	4.74	23.61	0.0560	0.0640	0.0200	0.9960	0.9990	
	1.83	100.00	4.72	19.40	0.0690	0.0780	0.0300	0.9940	0.9985	
	1.77	100.00	4.75	17.12	0.0790	0.0900	-0.0100	0.9930	0.9982	
	1.72	99.80	4.71	15.10	0.0930	0.1050	0.0000	0.9900	0.9975	
	1.67	99.90	4.71	13.22	0.1050	0.1190	0.0100	0.9880	0.9970	
	1.62	100.00	4.71	11.45	0.1240	0.1400	-0.0200	0.9830	0.9957	
	1.58	88.10	3.59	8.78	0.1380	0.1610	0.0100	0.9740	0.9934	
	all	98.90	4.59	26.72	0.0390	0.0440	0.0400	0.9990	0.9997	

Effective Resolution Range in Reduced Data: 100.00 1.58

Rmerge:	0.0390	[0.0230,	0.1380]
Redund:	4.59	[4.02,	3.59]
Complt:	98.90	[96.30,	88.10]
I/SigI:	26.72	[45.95,	8.78]
Rmeas:	0.0440	[0.0260,	0.1610]
AnoCc:	0.0400	[0.2600,	0.0100]
CC1/2:	0.9990	[0.9990,	0.9740]
CC*:	0.9997	[0.9997,	0.9934]