

Data analysis at SACLA

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Sample data

Pump (800 nm laser)-probe (XFEL) X-ray diffraction measurement for Bi thin film

- BL: 3
- Scan motor name: “xfel_bl_3_st_2_motor_1/position” (delay stage of laser)
- Run number: 714350~714560
- Delay scan range: -2550 ~ -1650 pulse, 5 pulse step (1 pulse = 6.671 fs)
- IO signals: “xfel_bl_3_st_2_pd_user_4_fitting_peak/voltage” & “xfel_bl_3_st_2_pd_user_5_fitting_peak/voltage”
- MPCCD Background: Run# 714259
- Timing Monitor Background: Run# 713326

1. Login SACL A HPC system

1. Connect the SPring-8 network with VPN service
2. `$ssh -X (username)@xhpcfep`
3. `$qsub -I -X -l select=1:ncpus=2`

Reference

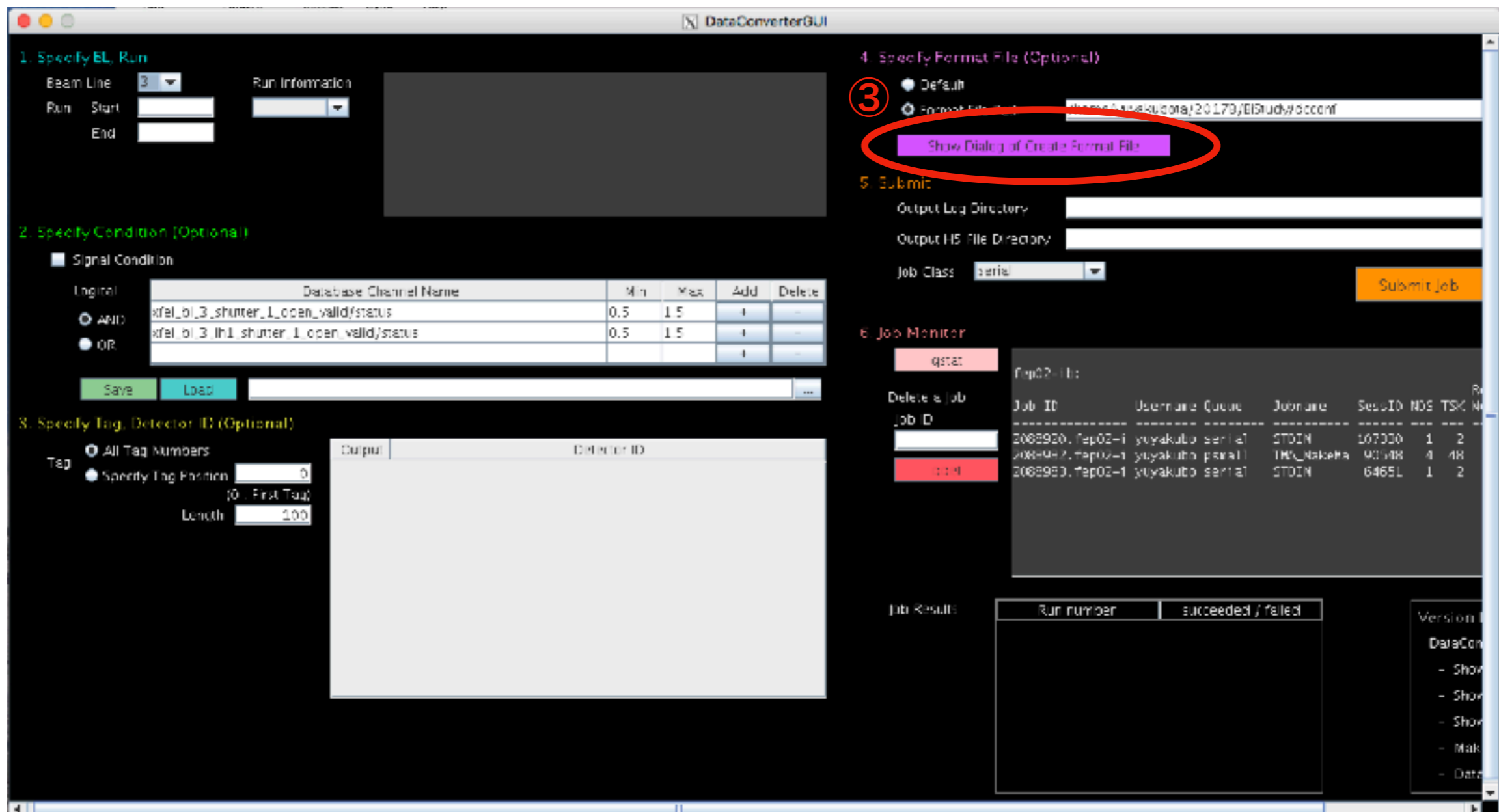
HPC Portal site (via VPN)

<http://xhpcfep.hpc.spring8.or.jp>

2. Extract data from the DB and the Storage

1. Make a configure file for DataConvert

1. \$DataConverterGUI
2. Open GUI window
3. Click Show Dialog of Create Format File



2. Extract data from the DB and the Storage

1. Make a configure file for DataConvert

4. Add signals you want
5. save your configure file

⑤

Save Load /work/wslab/ubola/sample/EI.conf

Reset to Default Format of Beam Line 1 Reset to Default Format of Beam Line 2 Reset to Default Format of Beam Line 3

Turn OFF All Check Box

Output	HS Dataset Path	Symbol
<input checked="" type="checkbox"/>	%file%/run_%run%/imperf_%de/index/detector_info/detector_name	SYN_DET_IMPERF_NAME
<input checked="" type="checkbox"/>	%file%/run_%run%/imperf_%de/index/detector_info/detector_scale	SYN_DET_IMPERF_SCALE
<input checked="" type="checkbox"/>	%file%/run_%run%/imperf_%de/index/detector_info/detector_offset	SYN_DET_IMPERF_OFFSET
<input checked="" type="checkbox"/>	%file%/run_%run%/imperf_%de/index/req_%req%/detector_data	SYN_DET_IMPERF_IMACC_TAG
<input checked="" type="checkbox"/>	%file%/run_%run%/cps_%de/index/detector_info/detector_name	SYN_DET_CPS_NAME
<input checked="" type="checkbox"/>	%file%/run_%run%/cps_%de/index/detector_info/detector_scale	SYN_DET_CPS_SCALE

Turn OFF All Check Box

Output	HS Dataset Path	Symbol	Type or DB Channel
<input checked="" type="checkbox"/>	%file%/file_info/format_type	SYN_FORMATTYPE	null
<input checked="" type="checkbox"/>	%file%/file_info/run_number_list	SYN_RUNNUMBER_LIST	null
<input checked="" type="checkbox"/>	%file%/file_info/version	SYN_DATAVERSION	null
<input checked="" type="checkbox"/>	%file%/run_%run%/event_info/tag_number_list	SYN_TAGNUMBER_LIST	null
<input checked="" type="checkbox"/>	%file%/run_%run%/event_info/time_stamp	SYN_TAGTIME	xfel-bl-3-shutter-1-open-valid/status
<input checked="" type="checkbox"/>	%file%/run_%run%/event_info/bl_szen_07/pulse_motor	SYN_PULP	null

Turn OFF All Check Box

Output	Field	HS Dataset Path (Continue from the Field column)	Symbol	Type	DB Channel
<input checked="" type="checkbox"/>	%file%/run_%run%/event_info/bl_3/fel_5/camera/camera_5_rol.coordinate.y0		SYN_SYNCDB_PLAIN	INT	xfel-bl-3-st-5-mpccd-1-rol.coordinate.y0
<input checked="" type="checkbox"/>	%file%/run_%run%/event_info/bl_3/fel_5/camera/camera_5_rol.coordinate.y0		SYN_SYNCDB_PLAIN	INT	xfel-bl-3-st-5-mpccd-1-rol.coordinate.y0
<input checked="" type="checkbox"/>	%file%/run_%run%/event_info/bl_3/fel_5/camera/camera_5_rol.coordinate.y1		SYN_SYNCDB_PLAIN	INT	xfel-bl-3-st-5-mpccd-1-rol.coordinate.y1
<input checked="" type="checkbox"/>	%file%/run_%run%/event_info/xfel-bl-3-st-2-pd-user-4_fitting_peak/voltage		SYN_SYNCDB_PLAIN	FLOAT	xfel-bl-3-st-2-pd-user-4_fitting_peak/voltage
<input checked="" type="checkbox"/>	%file%/run_%run%/event_info/xfel-bl-3-st-2-pd-user-5_fitting_peak/voltage		SYN_SYNCDB_PLAIN	FLOAT	xfel-bl-3-st-2-pd-user-5_fitting_peak/voltage

④

Select & Add DB Channel

Category: ST2 Part1: xfel_bl_3 Part2: _st_2_pd_user

2. Extract data from the DB and the Storage

1. Make a configure file for DataConvert

- Reference

http://xhpcfep.hpc.spring8.or.jp/assets/docs/DataConverterGUI_UsersManual_en.pdf

- Please use a sample configure file (including signals of I/O and delay stage)
`/work/yuyakubota/Sample/DataConvert_sample.conf`

2. Extract data from the DB and the Storage

2. DataConvert

1. \$MakeTagList -b 3 -r (Run#) -out (file name1).list
2. \$DataConvert4 -l (file name1).list -dir (directory name) -o (file name2).h5

To use your config file, please add a command option “-f”.

```
$DataConvert4 -l (file name1).list -dir (directory name) -o (file name2).h5 -f  
(config file name)
```

- Reference

MakeTagList: http://xhpcfep.hpc.spring8.or.jp/assets/docs/MakeTagList_UsersManual_en.pdf

DataConvert: http://xhpcfep.hpc.spring8.or.jp/assets/docs/DataConvert4_UsersManual_en.pdf

- Examples of results for Run# 714350
/work/yuyakubota/Sample/714350.list and 714350.h5

2. Extract data from the DB and the Storage

Sample of HDF file (714350.h5) for Run# 714350

image data

image data of MPCCD

delay stage

delay stage

PD user 4

Bi (111) diffraction spot

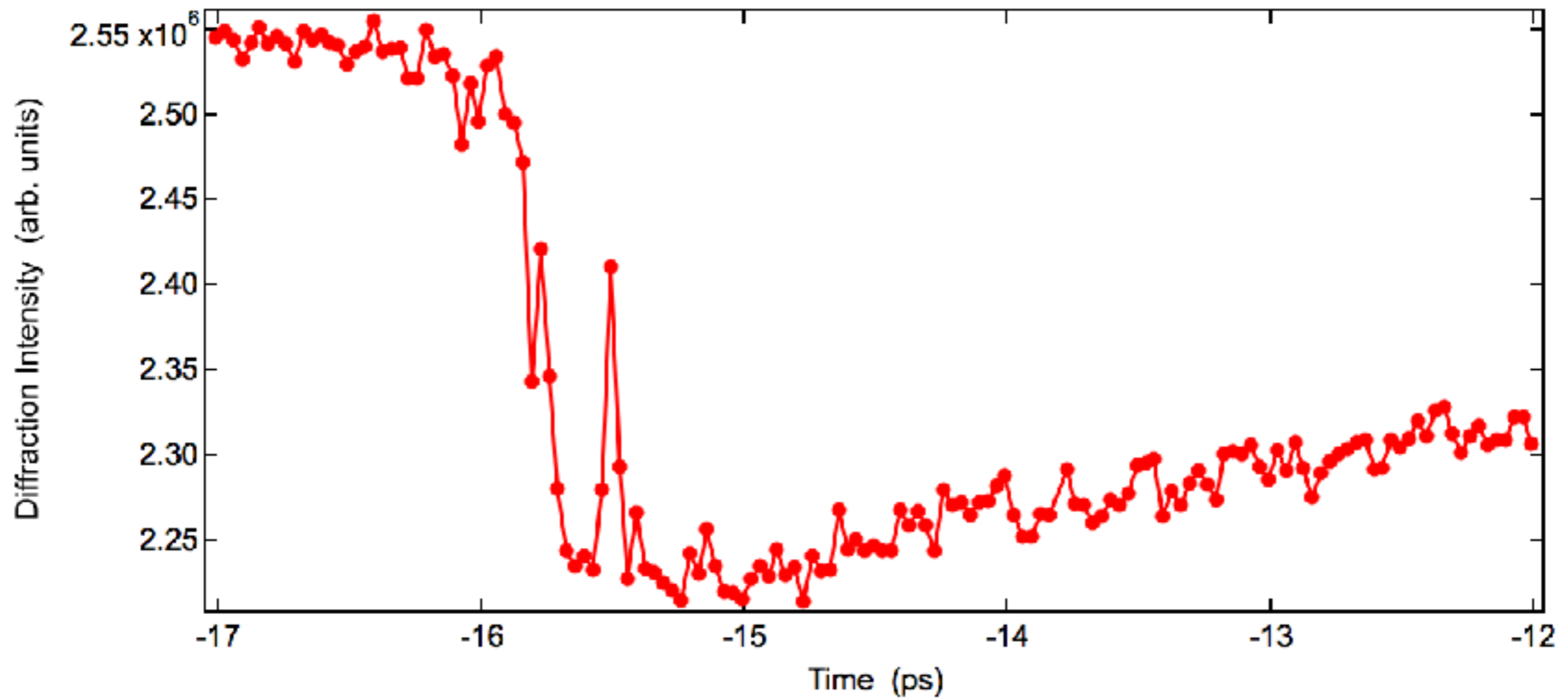
IO

0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24
-1350.0	7335.0	2330.0	7335.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0

0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24
0.0	0.02222394	0.0	0.0200811	0.02189226	0.02482196	0.0075900	0.0	0.0	0.0373153	0.0271066	0.0	0.0	0.0140773	0.0112001	0.00274035	0.0080229	0.0212074	0.0067601	0.0173449	0.0309511	0.0	0.008727	0.038087	

3. Result of the scan

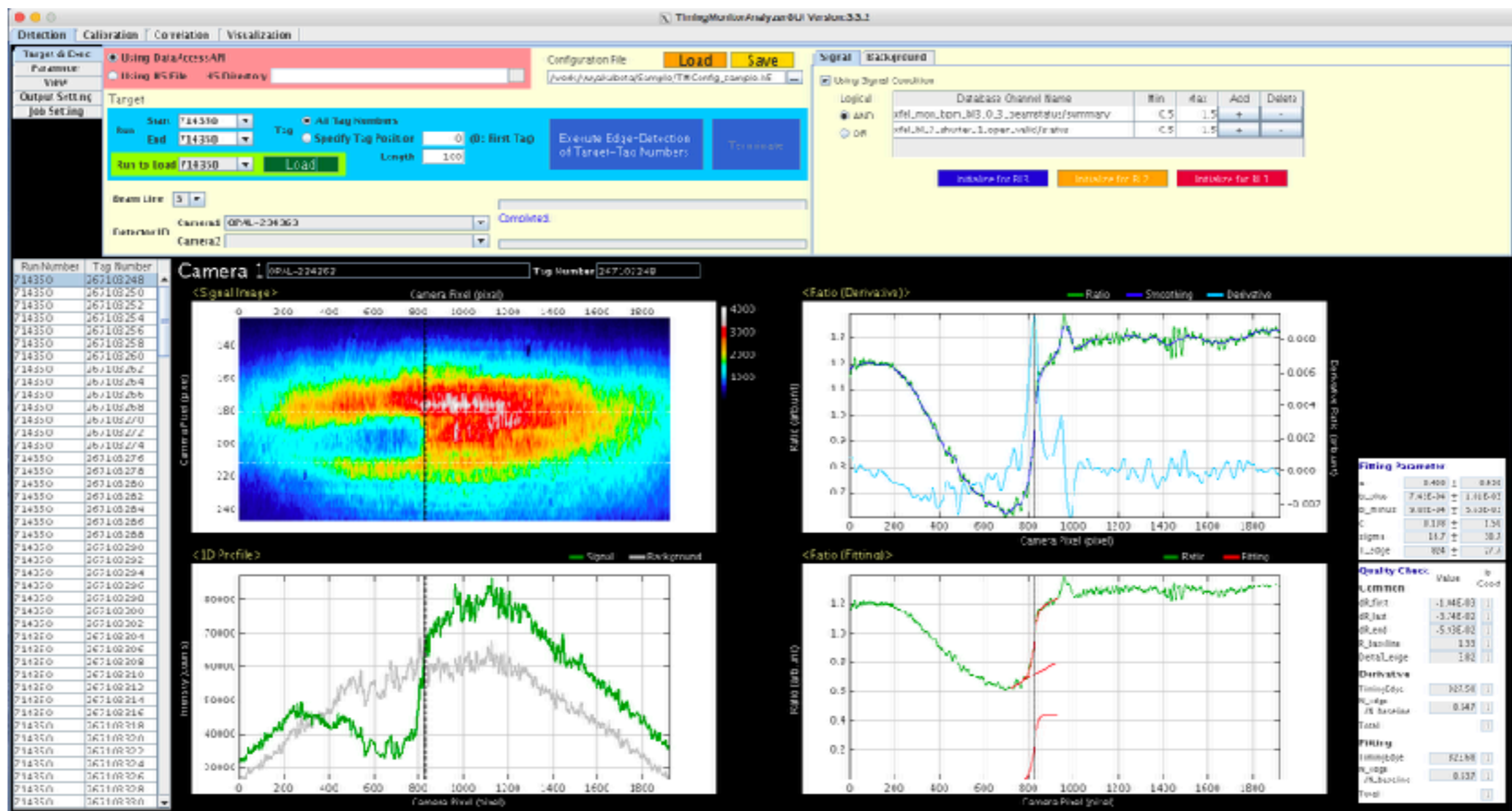
Please analyze the data in HDF files



4. Jitter correction with Timing Monitor

1. Analysis of timing jitter using TimingMonitorAnalyzer

1. \$TimingMonitorAnalyzerGUI
2. Open GUI window



4. Jitter correction with Timing Monitor (TM)

1. Analysis of timing jitter using TimingMonitorAnalyzer

Please refer to

http://xhpcfep.hpc.spring8.or.jp/assets/docs/TimingMonitorAnalyzerGUI_UsersManual_en.pdf

Please use a configure file

/work/yuyakubota/Sample/TMconfig_sample.h5

Examples of Result files for Run# 714350

/work/yuyakubota/Sample/714350.tma.h5 and 714350.csv and 714350.png

4. Jitter correction with Timing Monitor (TM)

Sample of HDF file (714350.tma.h5) for Run# 714350

quality check

results

jitter position

C	
0	1
1	1
2	1
3	1
4	1
5	1
6	1
7	1
8	1
9	1
10	1
11	1
12	1
13	1
14	1
15	1
16	0
17	1
18	1
19	1
20	1
21	1
22	1
23	1
24	1
25	1
26	1
27	0
28	1
29	1
30	1
31	1
32	0
33	1
34	0
35	1
36	1

C	
0	827.5
1	776.5
2	854.5
3	710.5
4	776.5
5	815.5
6	859.5
7	794.5
8	497.5
9	740.5
10	869.5
11	761.5
12	890.5
13	828.5
14	776.5
15	813.5
16	860.5
17	765.5
18	707.5
19	739.5
20	465.5
21	878.5
22	789.5
23	711.5
24	907.5
25	880.5
26	467.5
27	867.5
28	710.5
29	774.5
30	739.5
31	712.5
32	861.5
33	775.5
34	852.5
35	496.5
36	466.5
37	738.5
38	758.5

value (340176, 4)
64-bit floating-point, 359
Number of attributes = 0

4. Jitter correction with Timing Monitor (TM)

1. Analysis of timing jitter using TimingMonitorAnalyzer

quality check: 1 = good, 0 = not good

Delay time (fs) = [delay stage position (pulse)]*6.671 (fs) - ([jitter position] (pixel) - [Average of jitter position] (pixel)) * 3 (fs)

5. Result of the scan with jitter correction

