

Test CrystFEL GUI version 0.10.2

MAX IV cluster April 2023

Check CrystFEL versions available and start CrystFEL GUI

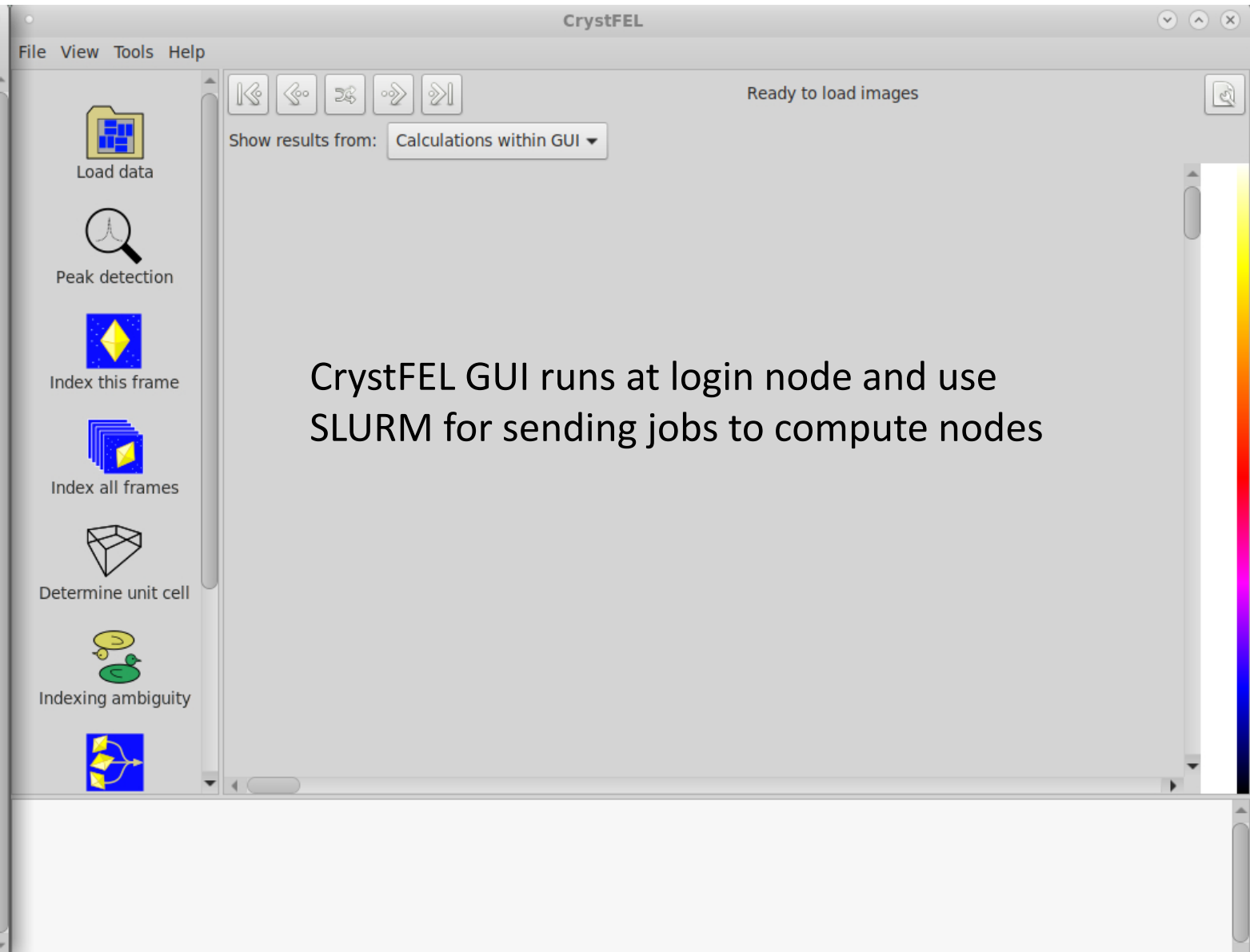
```
Mate Terminal
File Edit View Search Terminal Help
[marmoc2@offline-fe1 ~]$ module load gopresto
[marmoc2@offline-fe1 ~]$ module --ignore-cache avail CrystFEL

----- /sw/pkg/presto/modules/all -----
CrystFEL/0.8.0-1-PreSTO      CrystFEL/0.10.0-3-PreSTO
CrystFEL/0.8.0-2-PreSTO      CrystFEL/0.10.1-1-PreSTO
CrystFEL/0.8.0-3-PreSTO      CrystFEL/0.10.1-2-PreSTO
CrystFEL/0.8.0-4-PreSTO      CrystFEL/0.10.1-3-PreSTO
CrystFEL/0.9.1-2-PreSTO      CrystFEL/0.10.1-4-PreSTO
CrystFEL/0.9.1-3-PreSTO      CrystFEL/0.10.1-6-PreSTO
CrystFEL/0.9.1-6-PreSTO      CrystFEL/0.10.1-7-PreSTO (D)
CrystFEL/0.9.1-9-PreSTO      CrystFEL/0.10.2-PreSTO-8.0
CrystFEL/0.9.1-10-PreSTO

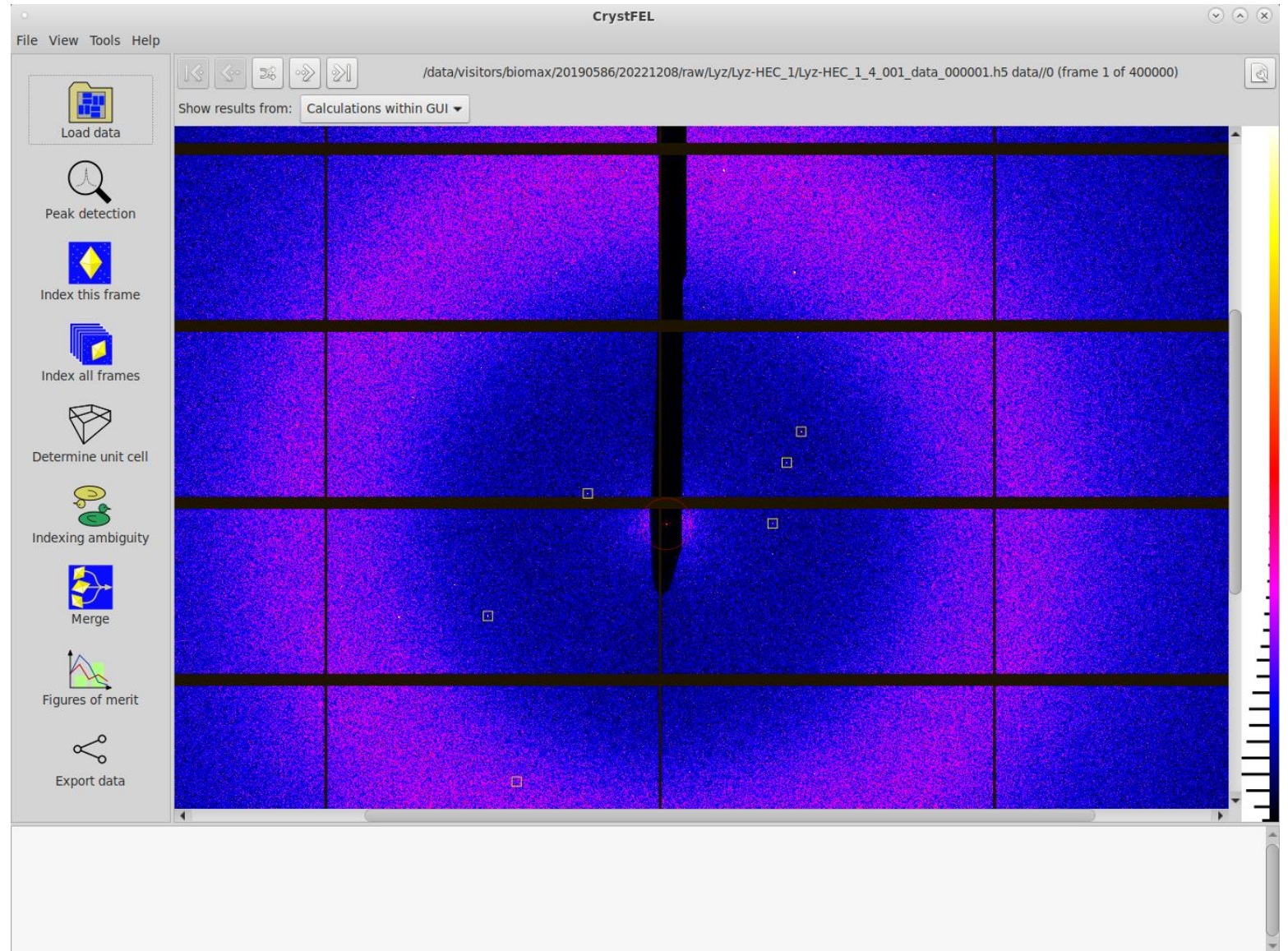
Where:
D: Default Module

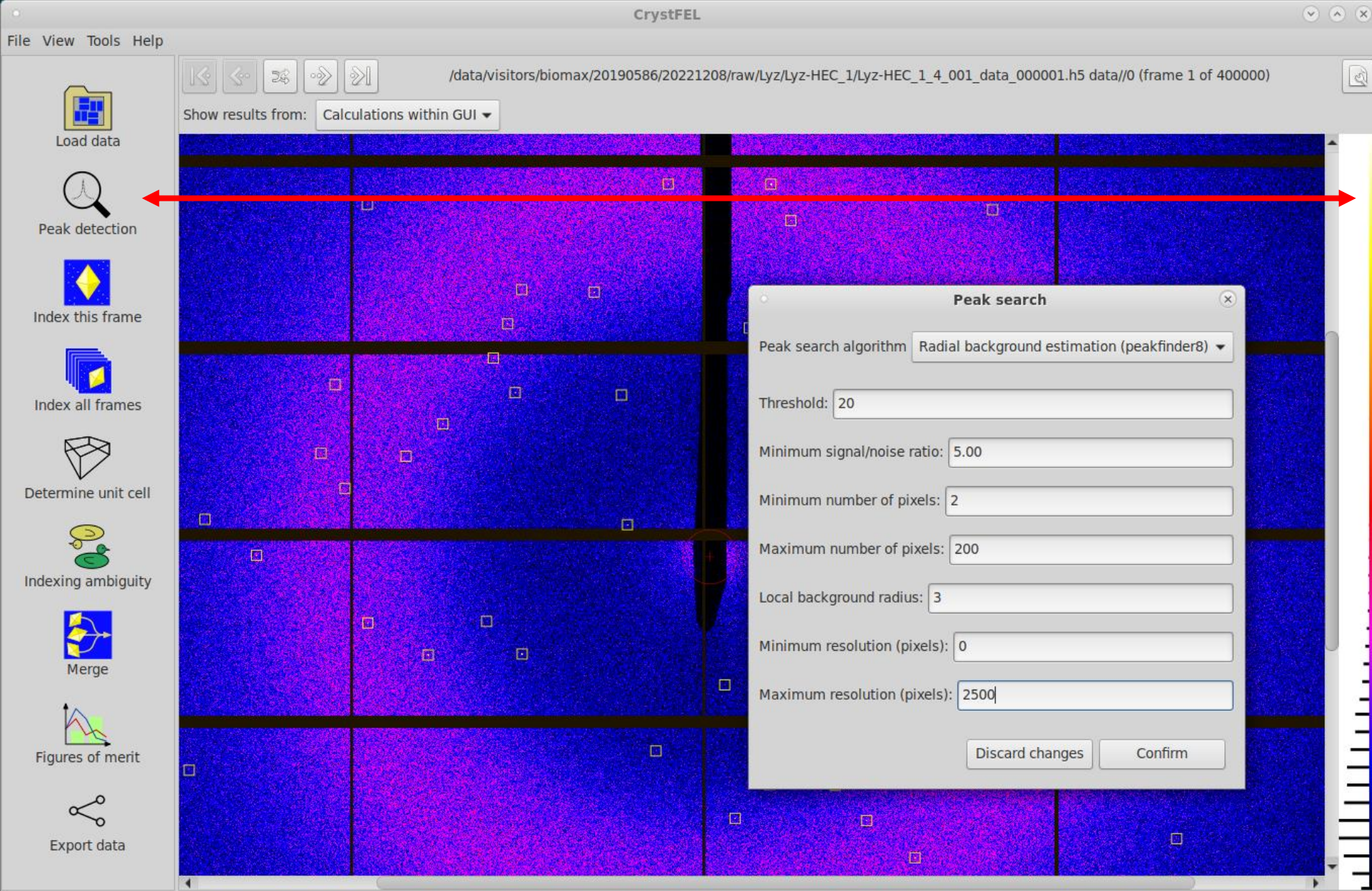
Use "module spider" to find all possible modules.
Use "module keyword key1 key2 ..." to search for all possible modules matching
any of the "keys".

[marmoc2@offline-fe1 ~]$ ml CrystFEL/0.10.2-PreSTO-8.0
[marmoc2@offline-fe1 ~]$ crystfel
```



Data is loaded,
takes a minute
or so...





Peak detection

Peak search parameters are dataset specific so these test data parameters are ok for this dataset

We now have more peaks on frame1, compared to previous slide

3. Set "Peak search" parameters, dataset specific

Index this frame

The screenshot shows the CrystFEL software interface. The main window displays a diffraction pattern with a grid overlay. A red arrow points from the text 'Index this frame' to the 'Index this frame' button in the left sidebar. Another red arrow points from the 'MOSFLM' option in the 'Index one frame' dialog box to the text 'MOSFLM option selected'.

CrystFEL

File View Tools Help

/data/visitors/biomax/20190586/20221208/raw/Lyz/Lyz-HEC_1/Lyz-HEC_1_4_001_data_000001.h5 data//0 (frame 1 of 400000)

Show results from: Calculations within GUI

Load data

Peak detection

Index this frame

Index all frames

Determine unit cell

Indexing ambiguity

Merge

Figures of merit

Export data

Index one frame

Unit cell file: (None)

Automatically choose the indexing methods

Select indexing methods and prior information

Method	Prior unit cell	Prior lattice type
<input type="checkbox"/> DirAx	<input type="checkbox"/>	<input type="checkbox"/>
<input checked="" type="checkbox"/> MOSFLM	<input type="checkbox"/>	<input type="checkbox"/>
<input type="checkbox"/> XDS	<input type="checkbox"/>	<input type="checkbox"/>
<input type="checkbox"/> XGANDALF	<input type="checkbox"/>	<input type="checkbox"/>
<input type="checkbox"/> PinkIndexer	<input type="checkbox"/>	<input type="checkbox"/>
<input type="checkbox"/> TakeTwo	<input type="checkbox"/>	<input type="checkbox"/>
<input type="checkbox"/> ASDF	<input type="checkbox"/>	<input type="checkbox"/>
<input type="checkbox"/> Felix	<input type="checkbox"/>	<input type="checkbox"/>

Attempt to find multiple lattices per frame

Refine the indexing solution

Retry indexing if unsuccessful

Check indexing solutions match peaks

Check indexing solutions against reference cell

Unit cell tolerances

Skip frames with fewer than 1 peaks

Cancel Run

MOSFLM option selected

Index this frame, frame1 (left) frame 400000 (right)

CrystFEL

/data/visitors/biomax/20190586/20221208/raw/Lyz/Lyz-HEC_1/Lyz-HEC_1_4_001_data_000001.h5 data//0 (frame 1 of 400000)

Show results from: Calculations within GUI

Refine indexing solutions: on
Multi-lattice indexing ("delete and retry"): off
Retry indexing: off
Number of crystals: 1
orthorhombic C, unique axis *, right handed.
a b c alpha beta gamma
152.86 158.44 79.37 A 90.04 90.00 90.00 deg

2 x Cell Parameters Lysozyme...

CrystFEL

/data/visitors/biomax/20190586/20221208/raw/Lyz/Lyz-HEC_1/Lyz-HEC_1_3_001_master.h5 data_000020//49 (frame 400000 of 400000)

Show results from: Calculations within GUI

Refine indexing solutions: on
Multi-lattice indexing ("delete and retry"): off
Retry indexing: off
Number of crystals: 1
tetragonal P, unique axis c, right handed.
a b c alpha beta gamma
79.16 79.29 38.18 A 90.01 89.97 89.99 deg

Correct Cell Parameters Lysozyme

Index all frames, indexing and cluster/batch SLURM settings at MAX IV

The screenshot shows the CrystFEL GUI with the 'Index all frames' dialog box open. The dialog box has the following settings:

- Job/output name: index1
- Indexing: Automatically choose the indexing methods
- Select indexing methods and prior information:

Method	Prior unit cell	Prior lattice type
<input type="checkbox"/> DirAx	<input type="checkbox"/>	<input type="checkbox"/>
<input checked="" type="checkbox"/> MOSFLM	<input type="checkbox"/>	<input type="checkbox"/>
<input type="checkbox"/> XDS	<input type="checkbox"/>	<input type="checkbox"/>
<input type="checkbox"/> XGANDALF	<input type="checkbox"/>	<input type="checkbox"/>
<input type="checkbox"/> PinkIndexer	<input type="checkbox"/>	<input type="checkbox"/>
<input type="checkbox"/> TakeTwo	<input type="checkbox"/>	<input type="checkbox"/>
<input type="checkbox"/> ASDF	<input type="checkbox"/>	<input type="checkbox"/>
<input type="checkbox"/> Felix	<input type="checkbox"/>	<input type="checkbox"/>
- Attempt to find multiple lattices per frame
- Refine the indexing solution
- Retry indexing if unsuccessful
- Check indexing solutions match peaks
- Check indexing solutions against reference cell
- Unit cell tolerances:
 - Skip frames with fewer than 1 peaks

Buttons: Cancel, Run

The screenshot shows the CrystFEL GUI with the 'Index all frames' dialog box open, showing SLURM settings. The dialog box has the following settings:

- Job/output name: index1
- Batch system: SLURM
- Submit job to partition: maxwell
- Send notifications to: myself@example.org
- Charge resource usage: SLURM account
- Required node features: SLURM constraint
- Job time limit (minutes): 120
- Split job into blocks of 10000 frames

Buttons: Cancel, Run

**400 000 frames in total
10 000 frames per block
120 min per block
40 blocks**

Index all frames - running

CrystFEL

/data/visitors/biomax/20190586/20221208/raw/Lyz-HEC_1/Lyz-HEC_1_3_001_master.h5 data_000020/49 (frame 400000 of 400000)

Show results from: Calculations within GUI

Index all frames

Job/output name: index1

Indexing

Integration

Advanced indexing

Stream contents

Cluster/batch system

Notes

Batch system: SLURM

Submit job to partition: maxwell

Send notifications to: myself@example.org

Charge resource use to: SLURM account

Required node features: SLURM constraint

Job time limit (minutes): 120

Split job into blocks of 10000 frames

Cancel Run

Refine indexing solutions: on
Multi-lattice indexing ("delete and retry"): off
Retry indexing: off

Number of crystals: 1
tetragonal P, unique axis c, right handed.
a b c alpha beta gamma
79.16 79.29 38.18 Å 90.01 89.97 89.99 deg

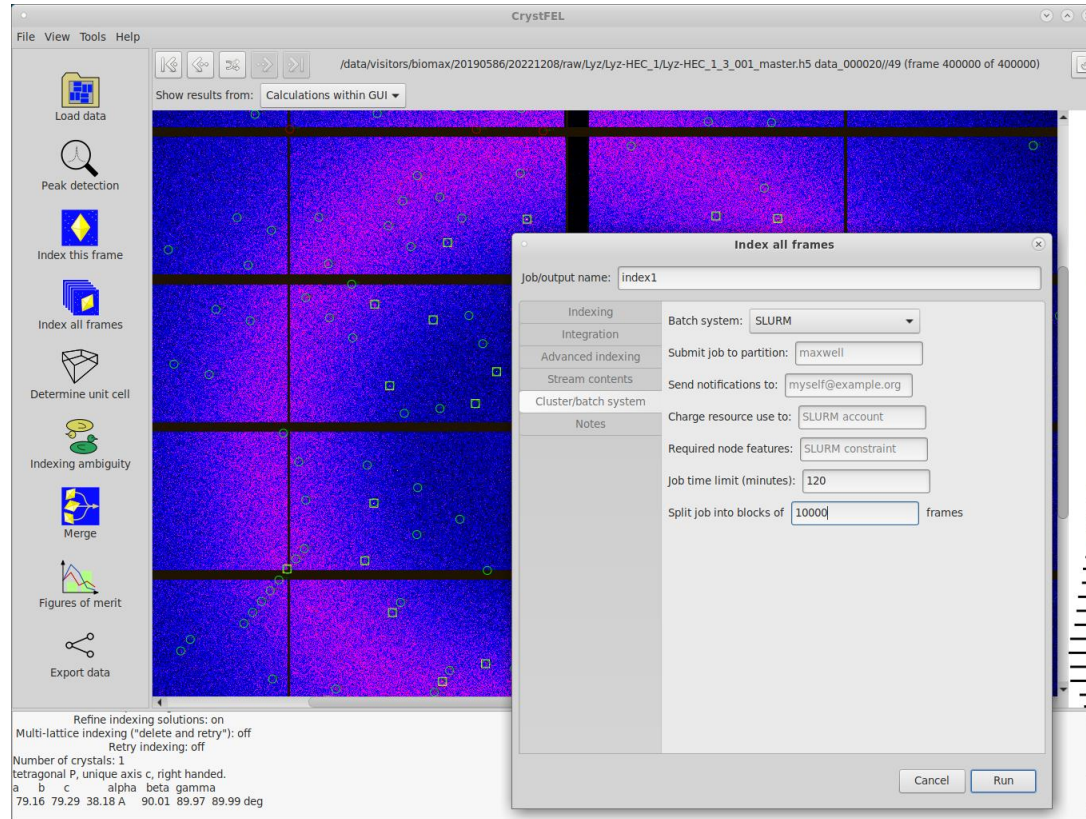
400 000 frames in total
10 000 frames per block
120 min per block
40 blocks => 40 CPUs

```
[marmoc2@offline-fe1 demo]$ squeue -u marmoc2
```

JOBID	PARTITION	NAME	USER	ST	TIME	NODES	NODELIST(REASON)
237626_0	all	index1	marmoc2	R	0:43	1	offline-cn11
237626_1	all	index1	marmoc2	R	0:43	1	offline-cn11
237626_2	all	index1	marmoc2	R	0:43	1	offline-cn11
237626_3	all	index1	marmoc2	R	0:43	1	offline-cn11
237626_4	all	index1	marmoc2	R	0:43	1	offline-cn11
237626_5	all	index1	marmoc2	R	0:43	1	offline-cn11
237626_6	all	index1	marmoc2	R	0:43	1	offline-cn11
237626_7	all	index1	marmoc2	R	0:43	1	offline-cn11
237626_8	all	index1	marmoc2	R	0:43	1	offline-cn11
237626_9	all	index1	marmoc2	R	0:43	1	offline-cn11
237626_10	all	index1	marmoc2	R	0:43	1	offline-cn11
237626_11	all	index1	marmoc2	R	0:43	1	offline-cn11
237626_12	all	index1	marmoc2	R	0:43	1	offline-cn8
237626_13	all	index1	marmoc2	R	0:43	1	offline-cn8
237626_14	all	index1	marmoc2	R	0:43	1	offline-cn8
237626_15	all	index1	marmoc2	R	0:43	1	offline-cn8
237626_16	all	index1	marmoc2	R	0:43	1	offline-cn8
237626_17	all	index1	marmoc2	R	0:43	1	offline-cn8
237626_18	all	index1	marmoc2	R	0:43	1	offline-cn8
237626_19	all	index1	marmoc2	R	0:43	1	offline-cn8
237626_20	all	index1	marmoc2	R	0:43	1	offline-cn8
237626_21	all	index1	marmoc2	R	0:43	1	offline-cn8
237626_22	all	index1	marmoc2	R	0:43	1	offline-cn8
237626_23	all	index1	marmoc2	R	0:43	1	offline-cn8
237626_24	all	index1	marmoc2	R	0:43	1	offline-cn8
237626_25	all	index1	marmoc2	R	0:43	1	offline-cn5
237626_26	all	index1	marmoc2	R	0:43	1	offline-cn2
237626_27	all	index1	marmoc2	R	0:43	1	offline-cn2
237626_28	all	index1	marmoc2	R	0:43	1	offline-cn2
237626_29	all	index1	marmoc2	R	0:43	1	offline-cn2
237626_30	all	index1	marmoc2	R	0:43	1	offline-cn2
237626_31	all	index1	marmoc2	R	0:43	1	offline-cn2
237626_32	all	index1	marmoc2	R	0:43	1	offline-cn2
237626_33	all	index1	marmoc2	R	0:43	1	offline-cn2
237626_34	all	index1	marmoc2	R	0:43	1	offline-cn2
237626_35	all	index1	marmoc2	R	0:43	1	offline-cn2
237626_36	all	index1	marmoc2	R	0:43	1	offline-cn2
237626_37	all	index1	marmoc2	R	0:43	1	offline-cn2
237626_38	all	index1	marmoc2	R	0:43	1	offline-cn2
237626_39	all	index1	marmoc2	R	0:43	1	offline-cn2

```
[marmoc2@offline-fe1 demo]$
```

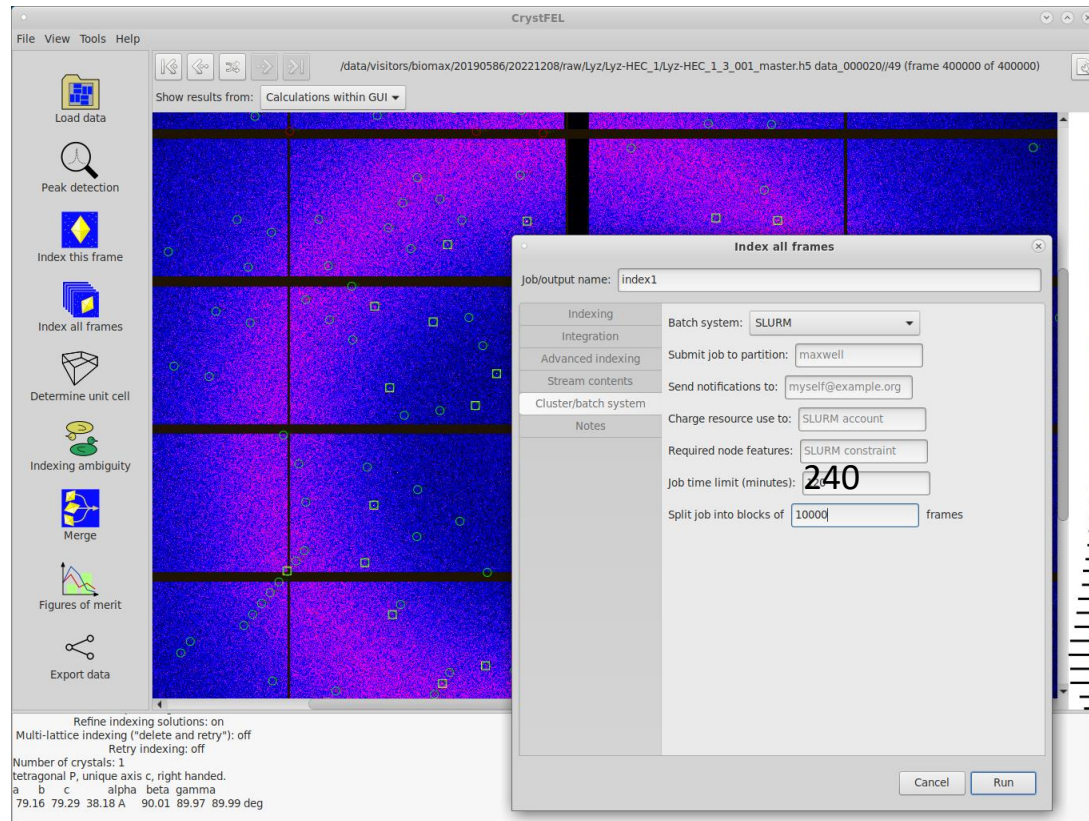
Index all frames did not finish – index1



```
[marmoc2@offline-fe1 index1]$ pwd
/home/marmoc2/demo/crystfel-lyz5/index1
[marmoc2@offline-fe1 index1]$ tail -10 stderr-10.log
5090 images processed, 5090 hits (100.0%), 2659 indexable (52.2% of hits, 52.2% overall), 2659 crystals, 0.6 images/sec.
WARNING: 1 implausibly negative reflection in /data/visitors/biomax/20190586/20221208/raw/Lyz/Lyz-HEC_1/Lyz-HEC_1_9_001_data_000011.h5 data//91
5094 images processed, 5094 hits (100.0%), 2663 indexable (52.3% of hits, 52.3% overall), 2663 crystals, 0.8 images/sec.
5098 images processed, 5098 hits (100.0%), 2664 indexable (52.3% of hits, 52.3% overall), 2664 crystals, 0.7 images/sec.
5101 images processed, 5101 hits (100.0%), 2666 indexable (52.3% of hits, 52.3% overall), 2666 crystals, 0.6 images/sec.
5105 images processed, 5105 hits (100.0%), 2668 indexable (52.3% of hits, 52.3% overall), 2668 crystals, 0.7 images/sec.
5110 images processed, 5110 hits (100.0%), 2672 indexable (52.3% of hits, 52.3% overall), 2672 crystals, 0.7 images/sec.
5113 images processed, 5113 hits (100.0%), 2673 indexable (52.3% of hits, 52.3% overall), 2673 crystals, 0.6 images/sec.
5117 images processed, 5117 hits (100.0%), 2674 indexable (52.3% of hits, 52.3% overall), 2674 crystals, 0.8 images/sec.
slurmstepd: error: *** JOB 237637 ON offline-cn11 CANCELLED AT 2023-04-28T13:55:44 DUE TO TIME LIMIT ***
[marmoc2@offline-fe1 index1]$
```

Index1 failed!
- Job time 120 min too short

Index2 did not finish, but it was close...



```
[marmoc2@offline-fe1 index2]$ pwd
/home/marmoc2/demo/crystfel-lyz5/index2
[marmoc2@offline-fe1 index2]$ tail -10 stderr-22.log
9969 images processed, 9969 hits (100.0%), 4765 indexable (47.8% of hits, 47.8% overall), 4765 crystals, 0.8 images/sec.
9974 images processed, 9974 hits (100.0%), 4769 indexable (47.8% of hits, 47.8% overall), 4769 crystals, 0.9 images/sec.
9978 images processed, 9978 hits (100.0%), 4773 indexable (47.8% of hits, 47.8% overall), 4773 crystals, 0.8 images/sec.
9981 images processed, 9981 hits (100.0%), 4775 indexable (47.8% of hits, 47.8% overall), 4775 crystals, 0.6 images/sec.
9985 images processed, 9985 hits (100.0%), 4776 indexable (47.8% of hits, 47.8% overall), 4776 crystals, 0.8 images/sec.
9989 images processed, 9989 hits (100.0%), 4776 indexable (47.8% of hits, 47.8% overall), 4776 crystals, 0.8 images/sec.
9993 images processed, 9993 hits (100.0%), 4776 indexable (47.8% of hits, 47.8% overall), 4776 crystals, 0.8 images/sec.
9996 images processed, 9996 hits (100.0%), 4776 indexable (47.8% of hits, 47.8% overall), 4776 crystals, 0.6 images/sec.
Waiting for the last patterns to be processed...
slurmstepd: error: *** JOB 237829 ON offline-cn2 CANCELLED AT 2023-04-28T18:00:16 DUE TO TIME LIMIT ***
[marmoc2@offline-fe1 index2]$
```

Index2 failed!

- 240 min slightly too short
- 9 996 of 10 000 images processed!

Index3 finished but what happen then?

The screenshot shows the CrystFEL GUI interface. The main window displays a diffraction pattern with a color scale on the right. A dialog box titled "Index all frames" is open, showing configuration options for indexing. The dialog includes fields for "job/output name" (index3), "Batch system" (SLURM), "Submit job to partition" (maxwell), "Send notifications to" (myself@example.org), "Charge resource use to" (SLURM account), "Required node features" (SLURM constraint), "job time limit (minutes)" (480), and "Split job into blocks of" (10000) frames. The "Run" button is highlighted.

```
[marmoc2@offline-fe1 index3]$ pwd
/home/marmoc2/demo/crystfel-lyz5/index3
[marmoc2@offline-fe1 index3]$ grep Final *.log
stderr-0.log:Final: 10000 images processed, 10000 hits (100.0%), 4930 indexable (49.3% of hits, 49.3% overall), 4930 crystals.
stderr-10.log:Final: 10000 images processed, 10000 hits (100.0%), 5026 indexable (50.3% of hits, 50.3% overall), 5026 crystals.
stderr-11.log:Final: 10000 images processed, 10000 hits (100.0%), 4847 indexable (48.5% of hits, 48.5% overall), 4847 crystals.
stderr-12.log:Final: 10000 images processed, 10000 hits (100.0%), 4966 indexable (49.7% of hits, 49.7% overall), 4966 crystals.
stderr-13.log:Final: 10000 images processed, 10000 hits (100.0%), 5092 indexable (50.9% of hits, 50.9% overall), 5092 crystals.
stderr-14.log:Final: 10000 images processed, 10000 hits (100.0%), 4949 indexable (49.5% of hits, 49.5% overall), 4949 crystals.
stderr-15.log:Final: 10000 images processed, 10000 hits (100.0%), 4383 indexable (43.8% of hits, 43.8% overall), 4383 crystals.
stderr-16.log:Final: 10000 images processed, 10000 hits (100.0%), 4973 indexable (49.7% of hits, 49.7% overall), 4973 crystals.
stderr-17.log:Final: 10000 images processed, 10000 hits (100.0%), 5026 indexable (50.3% of hits, 50.3% overall), 5026 crystals.
```

Index3 completed but what went wrong..?

The screenshot shows the CrystFEL GUI interface. The main window displays a progress bar for "Indexing all frames (Index3)". Below the progress bar, there is a log window showing the following messages:

```
Scanning index1/crystfel-36.stream
Scanning index1/crystfel-37.stream
Scanning index1/crystfel-38.stream
Scanning index1/crystfel-39.stream
Failed to load chunk from stream. Just displaying the image.
Splitting job into 40 blocks of max 10000 frames
Submitted batch job ID 237806
Splitting job into 40 blocks of max 10000 frames
Submitted batch job ID 237862
```

Index1 failure disturb subsequent jobs?
Restart CrystFEL GUI
Right-click to save logfile...

crystfel.project

- Check crystfel.project saved from GUI
- Very many lines in crystfel.project– problem?
- All ExitCodes are 0 for index3

```
[marmoc2@offline-fe1 crystfel-lyz5]$ pwd
/home/marmoc2/demo/crystfel-lyz5
[marmoc2@offline-fe1 crystfel-lyz5]$ more crystfel.project
geom /home/marmoc2/demo/crystfel-lyz5/MAXIV.geom
data_folder /data/visitors/biomax/20190586/20221208/raw/Lyz/Lyz-HEC_1
search_pattern everything
peak_search_params.method peakfinder8
peak_search_params.threshold 20.000000
peak_search_params.min_sq_gradient 100000.000000
peak_search_params.min_snr 5.000000
peak_search_params.min_pix_count 2
peak_search_params.max_pix_count 200
peak_search_params.local_bg_radius 3
```

```
[marmoc2@offline-fe1 crystfel-lyz5]$ cat crystfel.project | wc -l
400217
[marmoc2@offline-fe1 crystfel-lyz5]$
```

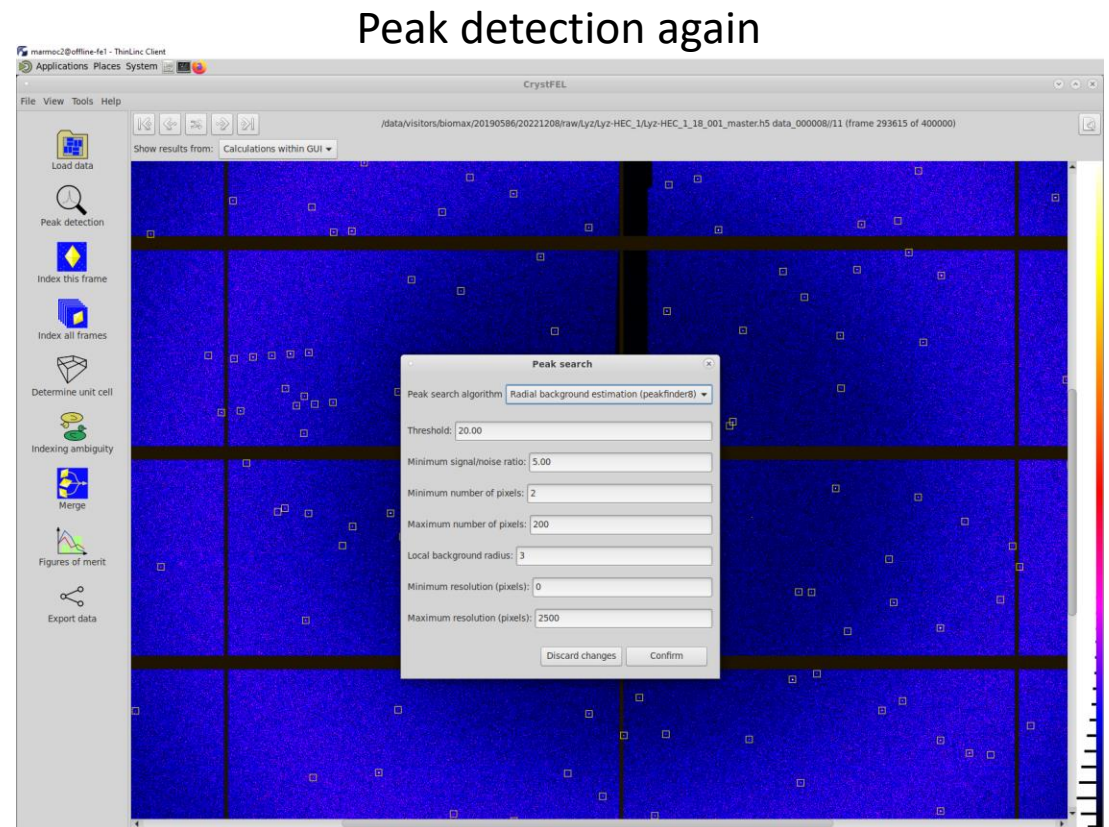
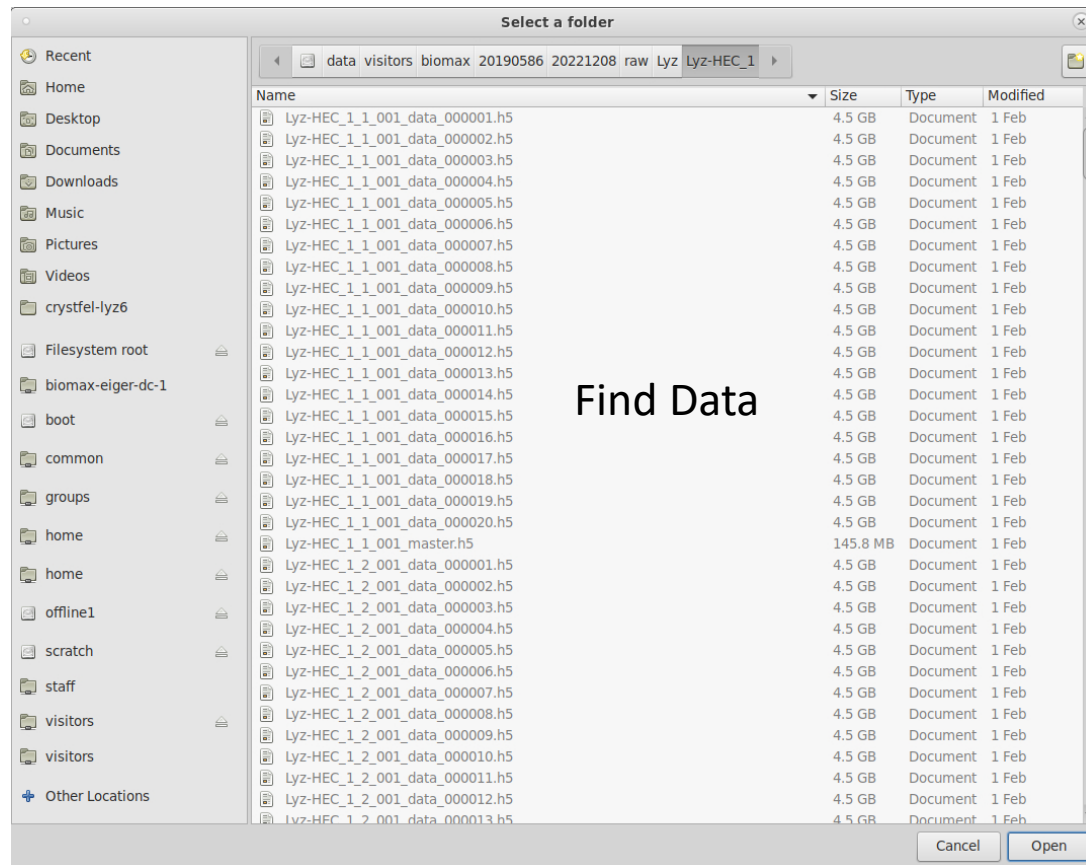
```
[marmoc2@offline-fe1 crystfel-lyz5]$ sacct -j 237862 --format=JobID,JobName,Start,End,MaxRSS,MaxVMSize,ExitCode
JobID      JobName      Start      End      MaxRSS      MaxVMSize      ExitCode
-----
237862_0   index3      2023-05-02T15:26:38 2023-05-02T18:22:34      0:0
237862_0.ba+  batch      2023-05-02T15:26:38 2023-05-02T18:22:34      832524K      3374368K      0:0
237862_0.ex+  extern      2023-05-02T15:26:38 2023-05-02T18:22:34      1028K      143604K      0:0
237862_1   index3      2023-05-02T15:26:38 2023-05-02T18:20:42      0:0
237862_1.ba+  batch      2023-05-02T15:26:38 2023-05-02T18:20:42      816668K      3357600K      0:0
237862_1.ex+  extern      2023-05-02T15:26:38 2023-05-02T18:20:42      1048K      143604K      0:0
237862_2   index3      2023-05-02T15:26:38 2023-05-02T18:49:20      0:0
```

For index1, exit codes is 15
15 means terminated by SIGTERM
237626 – index1
237862 – index3

```
[marmoc2@offline-fe1 crystfel-lyz5]$ sacct -j 237626 --format=JobID,JobName,Start,End,MaxRSS,MaxVMSize,ExitCode
JobID      JobName      Start      End      MaxRSS      MaxVMSize      ExitCode
-----
237626_0   index1      2023-04-28T11:55:36 2023-04-28T13:55:44      0:0
237626_0.ba+  batch      2023-04-28T11:55:36 2023-04-28T13:55:46      811612K      3360420K      0:15
237626_0.ex+  extern      2023-04-28T11:55:36 2023-04-28T13:55:44      352K      108056K      0:0
237626_1   index1      2023-04-28T11:55:36 2023-04-28T13:55:44      0:0
237626_1.ba+  batch      2023-04-28T11:55:36 2023-04-28T13:55:45      995628K      3378456K      0:15
237626_1.ex+  extern      2023-04-28T11:55:36 2023-04-28T13:55:44      1044K      143604K      0:0
237626_2   index1      2023-04-28T11:55:36 2023-04-28T13:55:44      0:0
237626_2.ba+  batch      2023-04-28T11:55:36 2023-04-28T13:55:46      833688K      3378072K      0:15
```

Restart crystfel from scratch in new directory

/home/marmoc2/demo/crystfel-lyz6



Index one frame (left) and all frames (right)

The screenshot shows the CrystFEL GUI with the 'Index one frame' dialog box open. The dialog box has the following settings:

- Unit cell file: (None)
- Automatically choose the indexing methods:
- Select indexing methods and prior information:
- Attempt to find multiple lattices per frame:
- Refine the indexing solution:
- Retry indexing if unsuccessful:
- Check indexing solutions match peaks:
- Check indexing solutions against reference cell:
- Unit cell tolerances:
- Skip frames with fewer than 1 peaks:

At the bottom of the window, the status bar shows: Refine indexing solutions: on; Multi-lattice indexing ("delete and retry"): off; Retry indexing: off; Number of crystals: 1; tetragonal P, unique axis c, right handed; a b c alpha beta gamma; 79.26 79.22 38.18 A 89.98 89.96 90.08 deg.

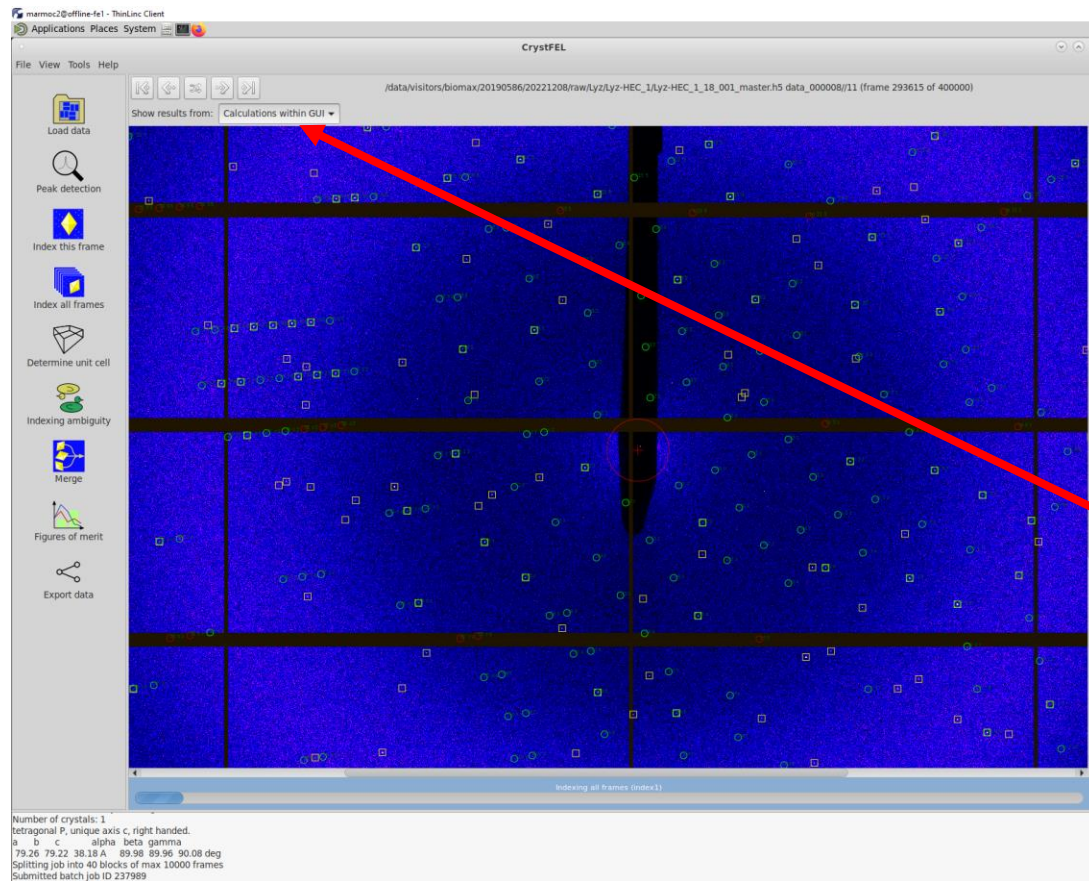
The screenshot shows the CrystFEL GUI with the 'Index all frames' dialog box open. The dialog box has the following settings:

- Job/output name: index1
- Batch system: SLURM
- Submit job to partition: maxwell
- Stream contents: myself@example.org
- Charge resource use to: SLURM account
- Required node features: SLURM constraint
- Job time limit (minutes): 480
- Split job into blocks of 10000 frames

At the bottom of the window, the status bar shows: Refine indexing solutions: on; Multi-lattice indexing ("delete and retry"): off; Retry indexing: off; Number of crystals: 1; tetragonal P, unique axis c, right handed; a b c alpha beta gamma; 79.26 79.22 38.18 A 89.98 89.96 90.08 deg.

Job time 480 min - so that job will finish...

Wake up CrystFEL after Index1



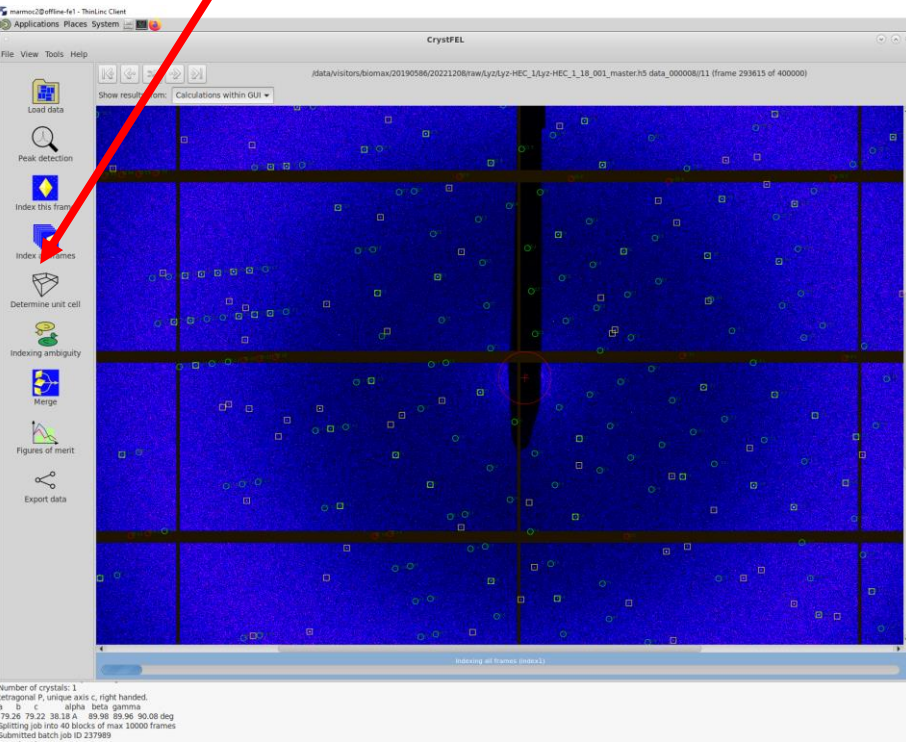
```
Mate Terminal
File Edit View Search Terminal Tabs Help
Mate Terminal
top - 15:26:02 up 294 days, 5:23, 49 users, load average: 1.62, 1.24, 1.02
Tasks: 1290 total, 3 running, 1286 sleeping, 0 stopped, 1 zombie
%Cpu(s): 3.3 us, 1.3 sy, 0.0 ni, 95.3 id, 0.1 wa, 0.0 hi, 0.1 si, 0.0 st
KiB Mem : 19647008+total, 3403868 free, 96400464 used, 96665752 buff/cache
KiB Swap: 4194300 total, 0 free, 4194300 used. 91502656 avail Mem

  PID USER      PR  NI  VIRT  RES  SHR S %CPU %MEM    TIME+  COMMAND
142938 marmoc2  20   0 5288784 694084 160584 R  97.7  0.4   5:51.38  crystfel
100347 marmoc2  20   0 1385960 246372 46156 S   2.0  0.1  10:45.62  Xvnc
 32778 marmoc2  20   0 162864  3632  1592 R   1.0  0.0   0:02.21  top
29532  marmoc2  20   0 163168  4976  1112 S   0.3  0.0   0:02.43  sshd
89761  marmoc2  20   0 116220  3292  1648 S   0.0  0.0   0:00.08  bash
99764  marmoc2  20   0 4051176 451156 114704 S   0.0  0.2   3:55.82  firefox
99861  marmoc2  20   0  538468  4436  3636 S   0.0  0.0   0:00.02  xdg-desktop-por
99867  marmoc2  20   0  588688  3008  2496 S   0.0  0.0   0:00.00  xdg-document-po
99871  marmoc2  20   0  364712  2644  2172 S   0.0  0.0   0:00.00  xdg-permission-
99909  marmoc2  20   0  372660  28604 20688 S   0.0  0.0   0:00.14  Socket Process
99937  marmoc2  20   0 2722812 103264 52968 S   0.0  0.1   0:02.63  Privileged Cont
100022 marmoc2  20   0 2706244  64472 42804 S   0.0  0.0   0:00.80  WebExtensions
```

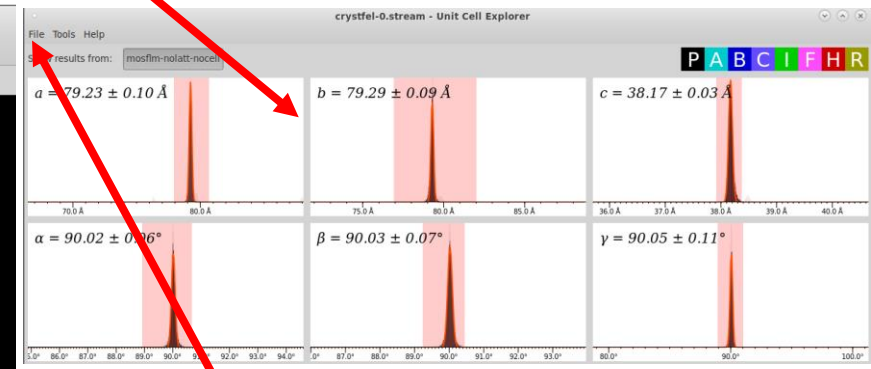
By clicking in the GUI I could wake-up CrystFEL

”Determine unit cell”
opens cell explorer
and triggers reading
of streams

- Cell Explorer commands:
 - Move in diagram by mouse
 - ”+” sets binning
 - Select peak by shift-mouse drag
 - Zoom by scroll wheel



```
Mate Terminal
File Edit View Search Terminal Tabs Help
Mate Terminal
[marmoc2@offline-fe1 ~]$ module load gopresto
[marmoc2@offline-fe1 ~]$ ml CrystFEL/0.10.2-PreSTO-8.0
[marmoc2@offline-fe1 ~]$ cd /home/marmoc2/demo/crystfel-ly26
[marmoc2@offline-fe1 ~]$ crystfel
Invalid integer 'q'
index1/crystfel-0.stream: Loaded 4930 cells from 10000 chunks
index1/crystfel-1.stream: Loaded 4816 cells from 10000 chunks
index1/crystfel-2.stream: Loaded 5629 cells from 10000 chunks
index1/crystfel-3.stream: Loaded 5896 cells from 10000 chunks
index1/crystfel-4.stream: Loaded 5632 cells from 10000 chunks
index1/crystfel-5.stream: Loaded 5898 cells from 10000 chunks
index1/crystfel-6.stream: Loaded 5289 cells from 10000 chunks
index1/crystfel-7.stream: Loaded 5728 cells from 10000 chunks
index1/crystfel-8.stream: Loaded 5316 cells from 10000 chunks
index1/crystfel-9.stream: Loaded 5322 cells from 10000 chunks
index1/crystfel-10.stream: Loaded 5026 cells from 10000 chunks
index1/crystfel-11.stream: Loaded 4847 cells from 10000 chunks
index1/crystfel-12.stream: Loaded 4966 cells from 10000 chunks
index1/crystfel-13.stream: Loaded 5092 cells from 10000 chunks
index1/crystfel-14.stream: Loaded 4949 cells from 10000 chunks
index1/crystfel-15.stream: Loaded 4383 cells from 10000 chunks
index1/crystfel-16.stream: Loaded 4973 cells from 10000 chunks
index1/crystfel-17.stream: Loaded 5026 cells from 10000 chunks
index1/crystfel-18.stream: Loaded 2359 cells from 5000 chunks
```



File - Save unit cell as cell1.cell

Reading streams takes 1-2 min

Save unit cell
and merge
data

CrystFEL

File View Tools Help

Job/output name: merge1 Input: index1

Merging Batch system: Local (run on this computer)

Cluster/batch system

Notes

Number of threads: 4

Partialator uses one core?

Mate Terminal

File Edit View Search Terminal Tabs Help

Mate Terminal

```
top - 16:01:44 up 294 days, 5:59, 49 users, load average: 0.52, 0.44, 0.61
Tasks: 1282 total, 2 running, 1279 sleeping, 0 stopped, 1 zombie
%Cpu(s): 3.1 us, 0.4 sy, 0.0 ni, 96.4 id, 0.0 wa, 0.0 hi, 0.0 si, 0.0 st
KiB Mem : 19647008+total, 17409848 free, 97513648 used, 81546592 buff/cache
KiB Swap: 4194300 total, 4 free, 4194296 used, 90347184 avail Mem
```

PID	USER	PR	NI	VIRT	RES	SHR	S	%CPU	%MEM	TIME+	COMMAND
44510	marmoc2	20	0	873320	838664	3612	R	99.7	0.4	0:14.00	partialator
100347	marmoc2	20	0	1385448	246372	46156	S	3.3	0.1	11:48.53	Xvnc
32778	marmoc2	20	0	162864	3636	1596	R	1.6	0.0	0:37.89	top
29532	marmoc2	20	0	163168	4976	1112	S	0.3	0.0	0:05.85	sshd
101035	marmoc2	20	0	567432	15220	10908	S	0.3	0.0	0:04.22	wnck-applet
161235	marmoc2	20	0	727548	34464	16100	S	0.3	0.0	0:54.18	mate-terminal

Save Unit Cell File

Name: cell1.cell

Home Desktop Documents Downloads Music Pictures Videos crystfel-lyz6

Filesystem root

biomax-eiger-dc-1 boot common groups home home offline1 scratch staff

visitors

Enforce lattice type: Tetragonal, unique axis c

Unit cell: tetragonal P, unique axis c, a=79.26 Å, b=79.26 Å, c=38.17 Å, alpha=90.00° beta=90.00° gamma=90.00°

CrystFEL

File View Tools Help

Job/output name: merge1 Input: index1

Merging Model: No partialities (unity)

Cluster/batch system

Notes

Symmetry: 4mmm

Intensities Debye-Waller scaling Post-refinement

Number of scaling/post-refinement cycles: 3

Polarisation: Horizontal e-field (most synchrotrons and FELs)

Reject bad patterns according to ACCV

Detector saturation cutoff: inf

Minimum number of measurements per merged reflection: 2

Split datasets after merging (None)

Write partiality model diagnostics

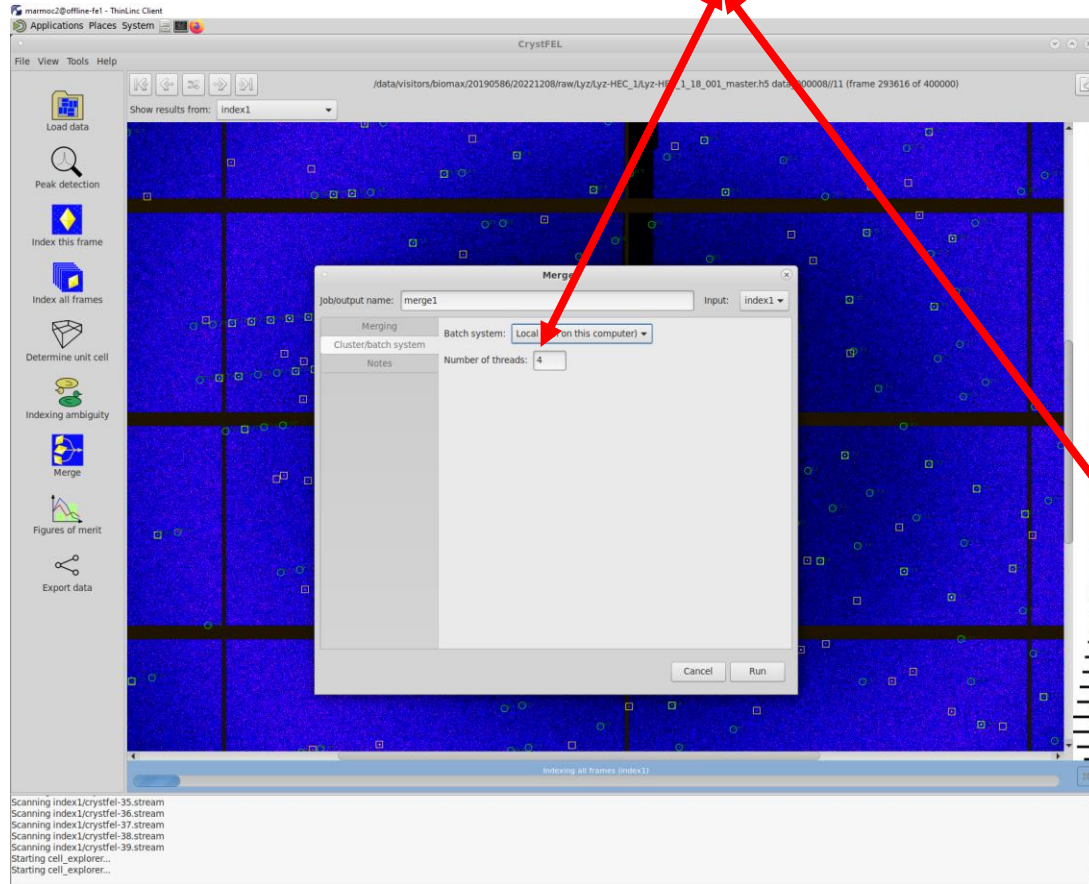
Require minimum estimated pattern resolution inf Å

Exclude measurements more than inf nm⁻¹ above resolution limit

Refine indexing assignments click to choose

Scanning index1/crystfel-35 stream
Scanning index1/crystfel-36 stream
Scanning index1/crystfel-37 stream
Scanning index1/crystfel-38 stream
Scanning index1/crystfel-39 stream
Starting cell_explorer...
Starting cell_explorer...

merge1 - I ask for 4 threads but did I get it?



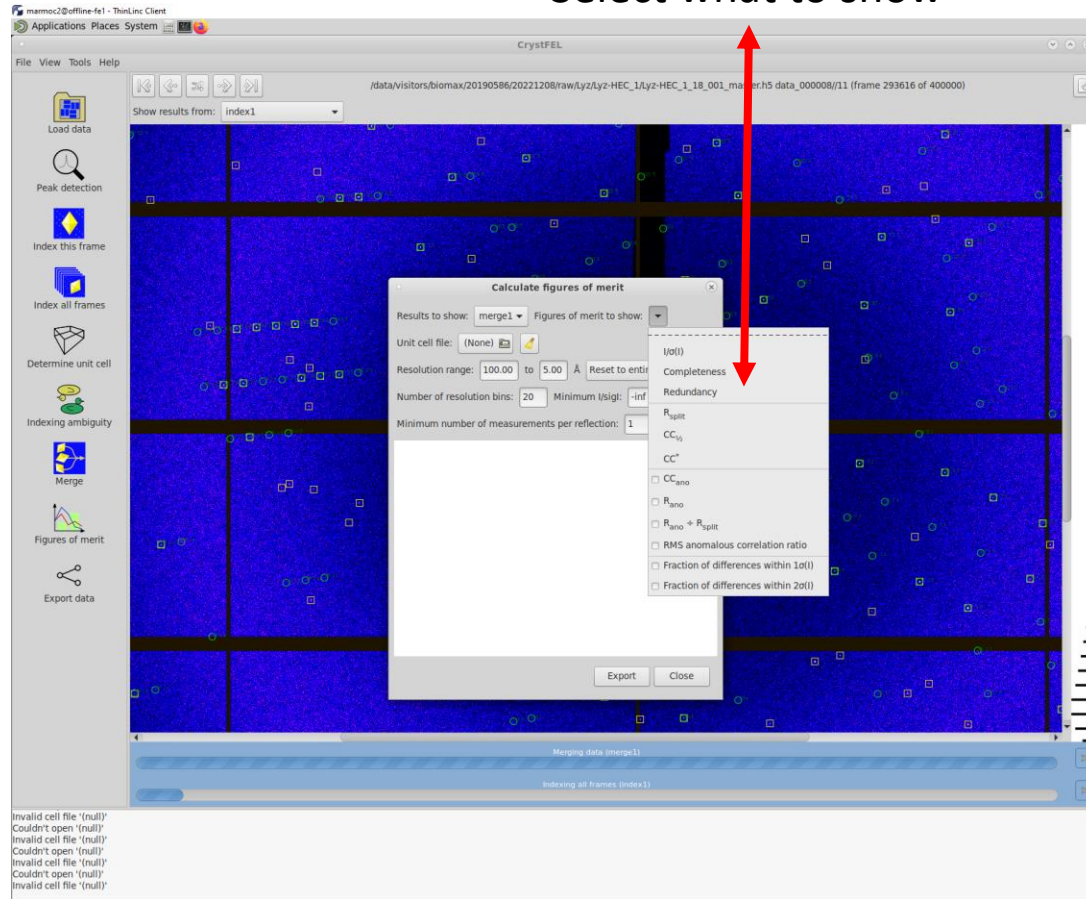
```
[marmoc2@offline-fel1 crystfel-lyz6]$ more merge1/run_merge.sh
#!/bin/sh
partialator \
"index1/crystfel-0.stream" \
"index1/crystfel-1.stream" \
"index1/crystfel-2.stream" \
"index1/crystfel-3.stream" \
"index1/crystfel-4.stream" \
"index1/crystfel-5.stream" \
"index1/crystfel-6.stream" \
"index1/crystfel-7.stream" \
"index1/crystfel-8.stream" \
"index1/crystfel-9.stream" \
"index1/crystfel-10.stream" \
"index1/crystfel-11.stream" \
"index1/crystfel-12.stream" \
"index1/crystfel-13.stream" \
"index1/crystfel-14.stream" \
"index1/crystfel-15.stream" \
"index1/crystfel-16.stream" \
"index1/crystfel-17.stream" \
"index1/crystfel-18.stream" \
"index1/crystfel-19.stream" \
"index1/crystfel-20.stream" \
"index1/crystfel-21.stream" \
"index1/crystfel-22.stream" \
"index1/crystfel-23.stream" \
"index1/crystfel-24.stream" \
"index1/crystfel-25.stream" \
"index1/crystfel-26.stream" \
"index1/crystfel-27.stream" \
"index1/crystfel-28.stream" \
"index1/crystfel-29.stream" \
"index1/crystfel-30.stream" \
"index1/crystfel-31.stream" \
"index1/crystfel-32.stream" \
"index1/crystfel-33.stream" \
"index1/crystfel-34.stream" \
"index1/crystfel-35.stream" \
"index1/crystfel-36.stream" \
"index1/crystfel-37.stream" \
"index1/crystfel-38.stream" \
"index1/crystfel-39.stream" \
--model=unity -j 4 -o "merge1/crystfel.hkl" -y 4/mmm --polarisation=horiz --min-measurements=2 --max-adu=inf
--min-res=inf --push-res=inf --iterations=3 --harvest-file=merge1/parameters.json --log-folder=merge1/pr-logs
>merge1/stdout.log 2>merge1/stderr.log
[marmoc2@offline-fel1 crystfel-lyz6]$
```

```
1 [|||||] 53.4%] 11 [|||||] 0.6%] 21 [|||||] 0.0%] 31 [|||||] 0.0%]
2 [|||||] 74.1%] 12 [|||||] 33.9%] 22 [|||||] 0.0%] 32 [|||||] 0.0%]
3 [|||||] 64.6%] 13 [|||||] 0.0%] 23 [|||||] 1.2%] 33 [|||||] 0.0%]
4 [|||||] 2.4%] 14 [|||||] 0.0%] 24 [|||||] 0.0%] 34 [|||||] 0.0%]
5 [|||||] 1.8%] 15 [|||||] 1.8%] 25 [|||||] 1.2%] 35 [|||||] 0.0%]
6 [|||||] 0.0%] 16 [|||||] 90.1%] 26 [|||||] 19.4%] 36 [|||||] 0.0%]
7 [|||||] 0.6%] 17 [|||||] 0.6%] 27 [|||||] 0.0%] 37 [|||||] 0.0%]
8 [|||||] 0.0%] 18 [|||||] 25.1%] 28 [|||||] 0.0%] 38 [|||||] 2.4%]
9 [|||||] 0.6%] 19 [|||||] 18.1%] 29 [|||||] 1.8%] 39 [|||||] 0.0%]
10 [|||||] 0.0%] 20 [|||||] 17.5%] 30 [|||||] 0.0%] 40 [|||||] 0.0%]
Mem [|||||] Tasks: 828, 5259 thr; 6 running
Swp [|||||] Load average: 2.50 1.91 1.45
Uptime: 294 days(!), 06:24:45
```

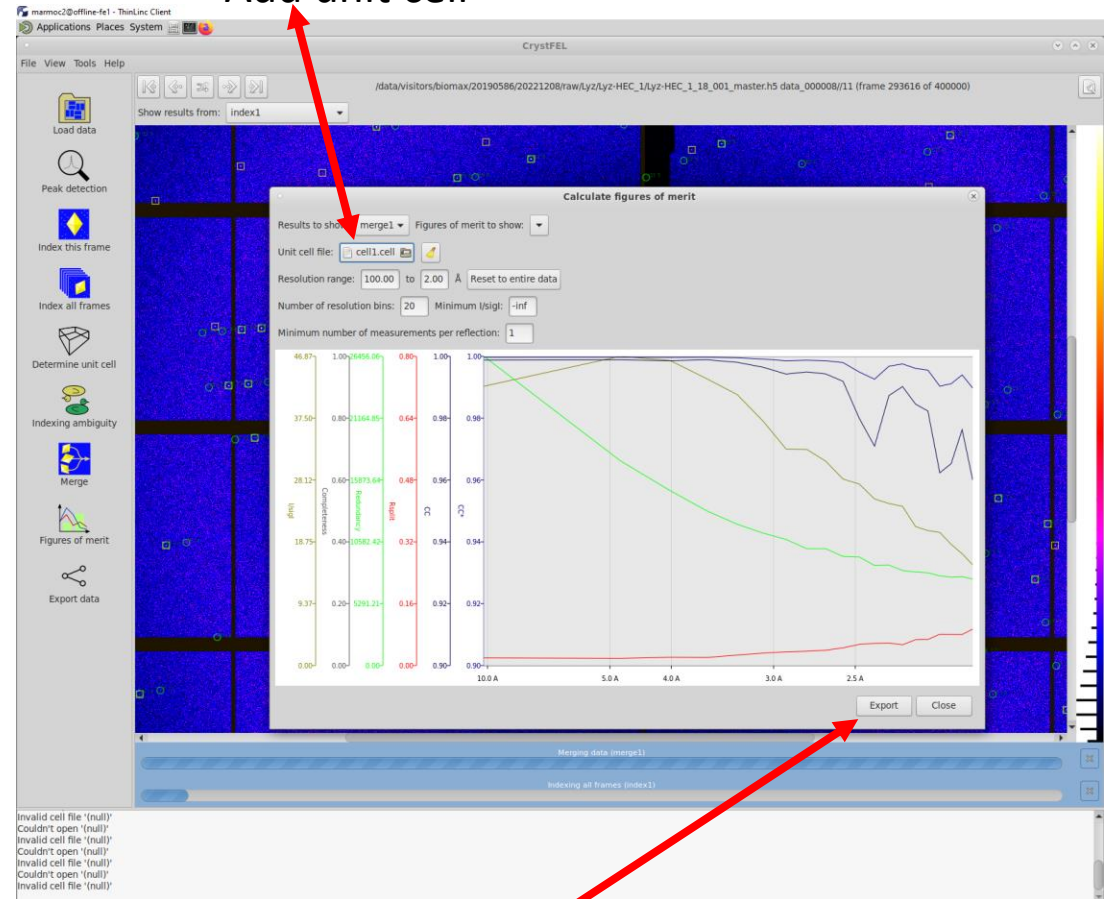
PID	USER	PR	NI	VIRT	RES	SHR	S	CPU%	MEM%	TIME+	Command
44510	marmoc2	20	0	44.1G	43.9G	3916	S	354	23.4	36:43.86	partialator index1/crystfel-0.stream index1/crystfel-1.stream index1/crystfel-2.stream index1/crystfel-3.stream index1/crystfel-4.stream index1/crystfel-5.stream index1/crystfel-6.stream index1/crystfel-7.stream index1/crystfel-8.strea
76033	marmoc2	20	0	44.1G	43.9G	3916	R	90.3	23.4	1:47.80	partialator index1/crystfel-0.stream index1/crystfel-1.stream index1/crystfel-2.stream index1/crystfel-3.stream index1/crystfel-4.stream index1/crystfel-5.stream index1/crystfel-6.stream index1/crystfel-7.stream index1/crystfel-8.strea
76034	marmoc2	20	0	44.1G	43.9G	3916	R	89.7	23.4	1:47.77	partialator index1/crystfel-0.stream index1/crystfel-1.stream index1/crystfel-2.stream index1/crystfel-3.stream index1/crystfel-4.stream index1/crystfel-5.stream index1/crystfel-6.stream index1/crystfel-7.stream index1/crystfel-8.strea
76035	marmoc2	20	0	44.1G	43.9G	3916	R	87.2	23.4	1:46.44	partialator index1/crystfel-0.stream index1/crystfel-1.stream index1/crystfel-2.stream index1/crystfel-3.stream index1/crystfel-4.stream index1/crystfel-5.stream index1/crystfel-6.stream index1/crystfel-7.stream index1/crystfel-8.strea
76036	marmoc2	20	0	44.1G	43.9G	3916	R	87.2	23.4	1:45.62	partialator index1/crystfel-0.stream index1/crystfel-1.stream index1/crystfel-2.stream index1/crystfel-3.stream index1/crystfel-4.stream index1/crystfel-5.stream index1/crystfel-6.stream index1/crystfel-7.stream index1/crystfel-8.strea
100347	marmoc2	20	0	1376M	263M	46428	R	19.3	0.1	12:56.46	/opt/thinlinc/libexec/Xvnc :25 -depth 24 -geometry 1024x768 -fp catalogue:/etc/X11/fontpath.d,/usr/share/fonts/default/Type1 -auth /var/opt/thinlinc/sessions/marmoc2/25/Xauthority -rfbport 5925 -rfbauth /var/opt/thinlinc/sessions/marmoc2
76077	marmoc2	20	0	125M	8204	1472	R	9.6	0.0	0:11.57	htop -u marmoc2

Figure of Merit – merge1

Select what to show

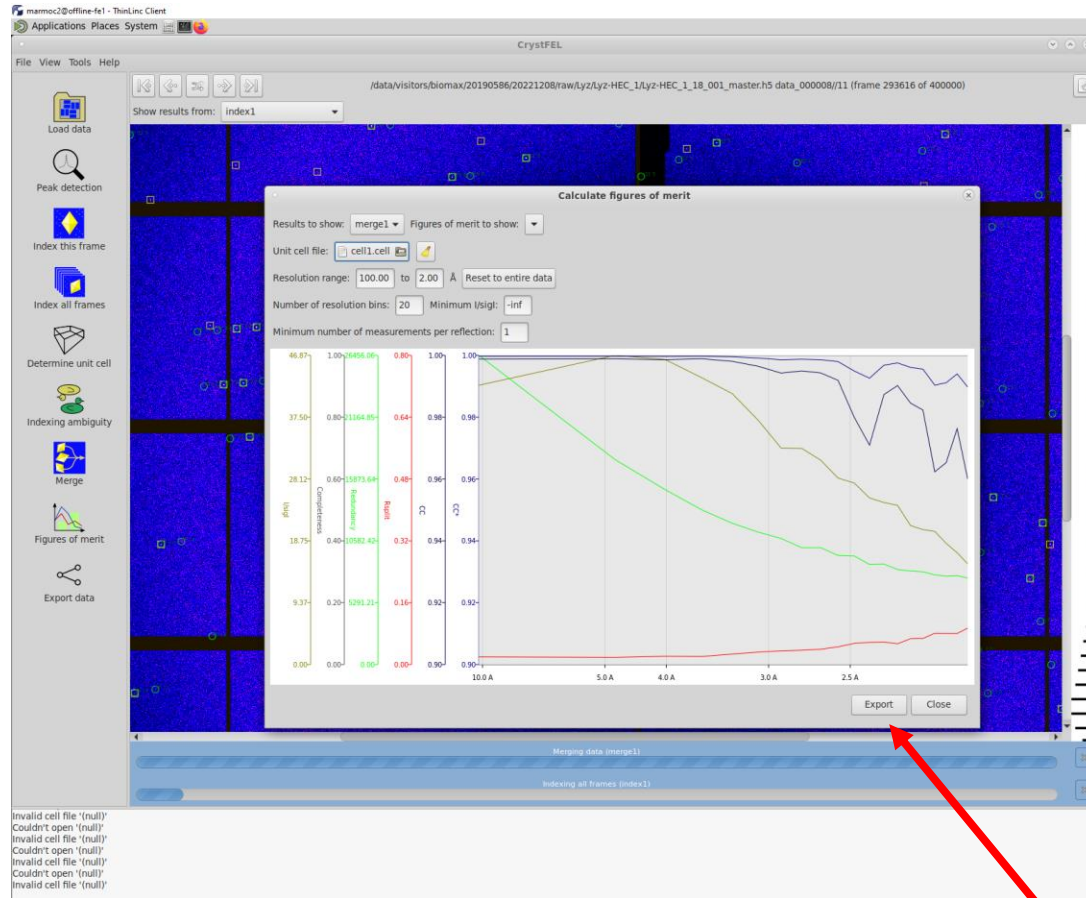


Add unit cell



All Figure of Merit data be exported as .csv file open as text in Excel

Figure of Merit – exported and open in Excel



Column1	Column2	Column3	Column4	Column5	Column6	Column7	Column8	Column9	Column10
1/d min/nm^-1	1/d center/nm^-1	1/d max/nm^-1	d center/Å	I/sig	Completeness	Redundancy	Rsplit	CC	CC*
0.100000	0.971055	1.842109	10.298083	42.338833	1.000000	26456.058939	0.019759	0.998754	0.999688
1.842109	2.081480	2.320850	4.804275	46.874815	1.000000	17535.471861	0.018577	0.998845	0.999711
2.320850	2.488768	2.656687	4.018052	46.249221	1.000000	14971.283146	0.021392	0.998578	0.999644
2.656687	2.790368	2.924049	3.583757	43.464106	1.000000	13228.145414	0.020859	0.998879	0.999720
2.924049	3.036938	3.149828	3.292790	41.072450	1.000000	12089.225287	0.027077	0.998056	0.999513
3.149828	3.248507	3.347186	3.078338	37.039449	1.000000	11328.454955	0.032144	0.996469	0.999115
3.347186	3.435426	3.523667	2.910847	32.829795	1.000000	10792.112172	0.035448	0.994253	0.998558
3.523667	3.603857	3.684046	2.774805	32.765791	1.000000	9998.498845	0.036988	0.994959	0.998736
3.684046	3.757803	3.831560	2.661129	30.990952	1.000000	10000.315789	0.039517	0.994320	0.998575
3.831560	3.900036	3.968513	2.564079	28.267618	1.000000	9332.297424	0.045820	0.991911	0.997968
3.968513	4.032564	4.096615	2.479812	27.513376	1.000000	9288.851064	0.054732	0.979936	0.994920
4.096615	4.156893	4.217171	2.405643	25.256782	1.000000	8560.410256	0.057493	0.970950	0.992603
4.217171	4.274186	4.331202	2.339627	24.560982	1.000000	8595.807339	0.058264	0.987298	0.996799
4.331202	4.385363	4.439525	2.280313	24.135915	1.000000	8130.034568	0.053711	0.990227	0.997542
4.439525	4.491165	4.542806	2.226594	21.067670	1.000000	8005.702381	0.066899	0.984550	0.996100
4.542806	4.592199	4.641592	2.177606	20.459280	1.000000	7934.765957	0.067444	0.982314	0.995529
4.641592	4.688968	4.736343	2.132666	20.182927	1.000000	7676.112412	0.080958	0.962323	0.990353
4.736343	4.781896	4.827448	2.091221	18.372252	1.000000	7556.358974	0.080636	0.965293	0.991131
4.827448	4.871343	4.915239	2.052822	16.949527	1.000000	7607.825980	0.080370	0.976286	0.993982
4.915239	4.957619	5.000000	2.017097	15.262258	1.000000	7396.436019	0.094177	0.959971	0.989736

Overall I/sig = 30.115224

Overall Completeness = 1.000000

Overall Redundancy = 11030.316705

Overall Rsplit = 0.033657

Overall CC = 0.998197

Overall CC* = 0.999549

Note: R-factors are given as decimal numbers (usually <1) not as percentages

Save as filename.csv and open in Excel

$2\text{\AA} = 0.2\text{nm}$, $1/0.2 = 5$
Data better than 2\AA !

Export as mtz - preliminary space group reminder

CrystFEL

File View Tools Help

Load data

Peak detection

Index this frame

Index all frames

Determine unit cell

Indexing ambiguity

Merge

Figures of merit

Export data

Export data

Name: data_from_crystfel.mtz

Home

Desktop

Documents

Downloads

Music

Pictures

Videos

crystfel-lyz6

Filesystem root

biomax-eiger-dc-1

boot

common

groups

home

home

offline1

scratch

staff

Name

Size

Type

Modified

Name	Size	Type	Modified
FOM1			09:13
cell1.cell	174 bytes	Text	Thu
crystfel.project	40.0 MB	Text	Thu
index1		Text	Thu
merge1		Text	Thu

Results to export: merge1 Format: MTZ Unit cell file: cell1.cell

Restrict resolution range: inf to 0.00 Å

Cancel Save

Couldn't open '(null)'
Invalid cell file '(null)'
Couldn't open '(null)'
Invalid cell file '(null)'
Couldn't open '(null)'
Invalid cell file '(null)'
Couldn't open '(null)'
Invalid cell file '(null)'
Saving to /home/marmoc2/demo/crystfel-lyz6/FOM1/fom1.txt

CrystFEL

File View Tools Help

Load data

Peak detection

Index this frame

Index all frames

Determine unit cell

Indexing ambiguity

Merge

Figures of merit

Export data

Export data

Name: data_from_crystfel.mtz

Home

Desktop

Documents

Downloads

Music

Pictures

Videos

crystfel-lyz6

Filesystem root

biomax-eiger-dc-1

boot

common

groups

home

home

offline1

scratch

staff

Name

Size

Type

Modified

Name	Size	Type	Modified
FOM1			09:13
cell1.cell	174 bytes	Text	Thu
crystfel.project	40.0 MB	Text	Thu
data_from_crystfel.mtz	11.6 MB	unknown	09:38
index1		Text	Thu
merge1		Text	Thu

Results to export: merge1 Format: MTZ Unit cell file: cell1.cell

Restrict resolution range: inf to 0.00 Å

Reminder

CrystFEL does not know the space group of your structure.

The space group written into the MTZ header is just a representation of the processing done within CrystFEL.

You may need to change the space group in the MTZ header, to allow structure solution programs to find the correct space group.

[Click here for some background information](#)

OK

Couldn't open '(null)'
Couldn't open '(null)'
Invalid cell file '(null)'
Invalid cell file '(null)'
Couldn't open '(null)'
Invalid cell file '(null)'
Couldn't open '(null)'
Invalid cell file '(null)'
Saving to /home/marmoc2/demo/crystfel-lyz6/FOM1/fom1.txt
Exporting dataset merge1 to /home/marmoc2/demo/crystfel-lyz6/data_from_crystfel.mtz, in format mtz, using unit cell /home/marmoc2/demo/crystfel-lyz6/cell1.cell, 0.000000 to inf m^-1