

# Test CrystFEL 0.11.0-PReSTO-sebth

Data in: /proj/xray/users/x\_marmo/2021a/data/Lyz

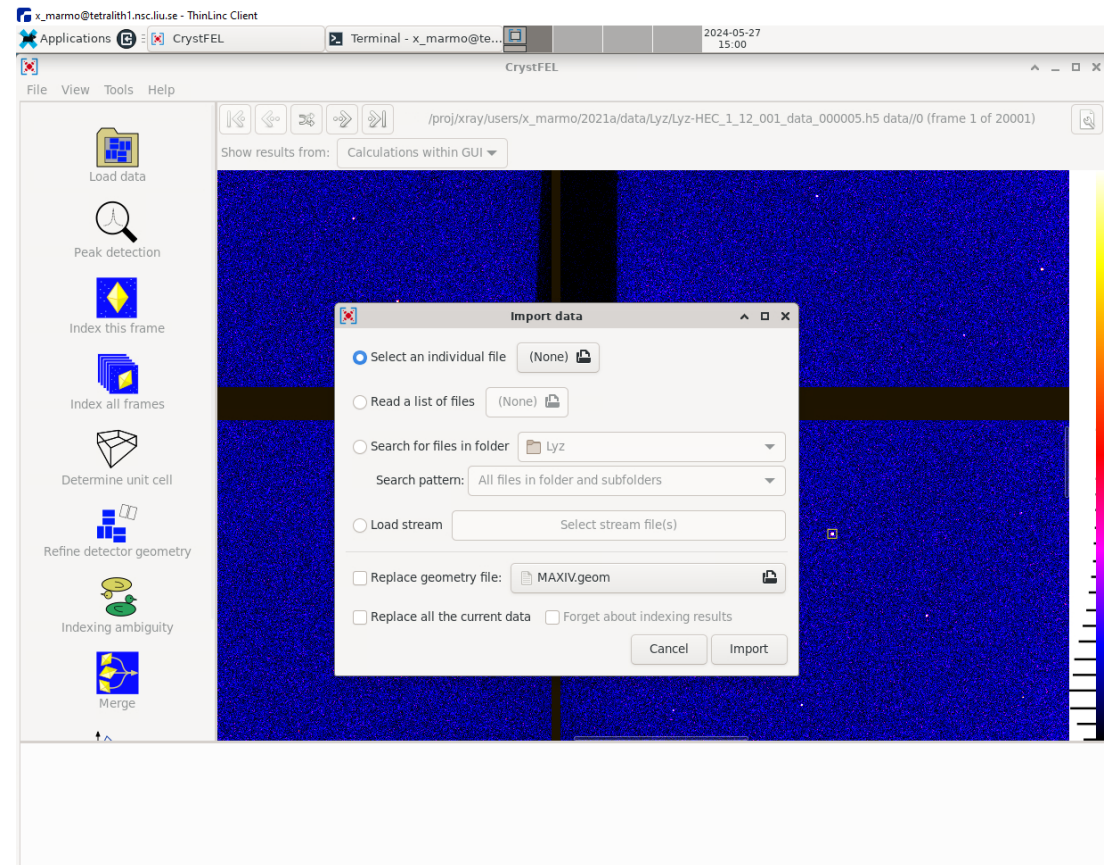
Run1 in: /proj/xray/users/x\_marmo/2021a/crystfel/0.11.0-PReSTO-sebth

Some crash happen so:

Run2 in: /proj/xray/users/x\_marmo/2021a/crystfel/0.11.0-PReSTO-sebth\_2

# Load data

- Use "Search for files in folder" option
- MAXIV.geom in same directory as started the software being: /proj/xray/users/x\_marmo/2021a/crystfel/0.11.0-PReSTO-sebth



x\_marmo@tetralith2.nslc.liu.se - ThinLinc Client

Applications CrystFEL Test CrystFEL GUI - Test... Terminal - x\_marmo@te... 2024-05-29 10:14

CrystFEL

File View Tools Help

/proj/xray/users/x\_marmo/2021a/data/Lyz/Lyz-HEC\_1\_12\_001\_data\_000005.h5 data//0 (frame 1 of 20001)

Show results from: Calculations within GUI

Load data

Peak detection

Index this frame

Index all frames

Determine unit cell

Refine detector geometry

Indexing ambiguity

Merge

Figures of merit

Export data

Index all frames

Job/output name: index1\_all

Indexing Batch system: SLURM

Integration Submit job to partition: maxwell

Advanced indexing Send notifications to: myself@example.org

Stream contents Charge resource use to: SLURM account

Cluster/batch system Required node features: SLURM constraint

Notes Job time limit (minutes): 20

Reservation: SLURM reservation

Quality of service: SLURM QoS

Split job into blocks of 5000 frames

Cancel Run

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

Number of crystals: 1  
monoclinic P, unique axis b, right handed.  
a b c alpha beta gamma  
79.05 38.16 79.17 Å 90.01 90.19 90.02 deg

Use SLURM to index all 20 000 frames  
- Select 30 min and 5000 frames per job, 4 jobs

```
[x_marmo@tetralith2 0.11.0-PreSTO-sebth_run2]$ squeue -u x_marmo
JOBID PARTITION NAME USER ST TIME NODES NODELIST(REASON)
35186060 [1-4] tetralith index1_a x_marmo PD 0:00 1 (Resources)
35186060_0 tetralith index1_a x_marmo R 0:13 1 n27
[x_marmo@tetralith2 0.11.0-PreSTO-sebth_run2]$ squeue -u x_marmo
JOBID PARTITION NAME USER ST TIME NODES NODELIST(REASON)
35186060 [2-4] tetralith index1_a x_marmo PD 0:00 1 (Resources)
35186060_1 tetralith index1_a x_marmo R 0:09 1 n457
35186060_0 tetralith index1_a x_marmo R 0:34 1 n27
[x_marmo@tetralith2 0.11.0-PreSTO-sebth_run2]$ squeue -u x_marmo
JOBID PARTITION NAME USER ST TIME NODES NODELIST(REASON)
35186060 [3-4] tetralith index1_a x_marmo PD 0:00 1 (Priority)
35186060_2 tetralith index1_a x_marmo R 0:24 1 n1559
35186060_1 tetralith index1_a x_marmo R 0:54 1 n457
35186060_0 tetralith index1_a x_marmo R 1:19 1 n27
[x_marmo@tetralith2 0.11.0-PreSTO-sebth_run2]$ squeue -u x_marmo
JOBID PARTITION NAME USER ST TIME NODES NODELIST(REASON)
35186060_3 tetralith index1_a x_marmo R 3:23 1 n1762
35186060_2 tetralith index1_a x_marmo R 4:01 1 n1559
35186060_1 tetralith index1_a x_marmo R 4:31 1 n457
35186060_0 tetralith index1_a x_marmo R 4:56 1 n27
[x_marmo@tetralith2 0.11.0-PreSTO-sebth_run2]$
```



# Review computing at n1762

```
[x_marmo@tetralith2 0.11.0-PreSTO-sebth_run2]$ squeue -u x_marmo
  JOBID PARTITION   NAME     USER ST       TIME  NODES NODELIST(REASON)
  35186060 [1-4] tetralith indexl_a x_marmo PD      0:00      1 (Resources)
  35186060 0 tetralith indexl_a x_marmo R      0:13      1 n27
[x_marmo@tetralith2 0.11.0-PreSTO-sebth_run2]$ squeue -u x_marmo
  JOBID PARTITION   NAME     USER ST       TIME  NODES NODELIST(REASON)
  35186060 [2-4] tetralith indexl_a x_marmo PD      0:00      1 (Resources)
  35186060 1 tetralith indexl_a x_marmo R      0:09      1 n457
  35186060 0 tetralith indexl_a x_marmo R      0:34      1 n27
[x_marmo@tetralith2 0.11.0-PreSTO-sebth_run2]$ squeue -u x_marmo
  JOBID PARTITION   NAME     USER ST       TIME  NODES NODELIST(REASON)
  35186060 [3-4] tetralith indexl_a x_marmo PD      0:00      1 (Priority)
  35186060 2 tetralith indexl_a x_marmo R      0:24      1 n1559
  35186060 1 tetralith indexl_a x_marmo R      0:54      1 n457
  35186060 0 tetralith indexl_a x_marmo R      1:19      1 n27
[x_marmo@tetralith2 0.11.0-PreSTO-sebth_run2]$ squeue -u x_marmo
  JOBID PARTITION   NAME     USER ST       TIME  NODES NODELIST(REASON)
  35186060 3 tetralith indexl_a x_marmo R      3:23      1 n1762
  35186060 2 tetralith indexl_a x_marmo R      4:01      1 n1559
  35186060 1 tetralith indexl_a x_marmo R      4:31      1 n457
  35186060 0 tetralith indexl_a x_marmo R      4:56      1 n27
[x_marmo@tetralith2 0.11.0-PreSTO-sebth_run2]$
```

```
$ jobsh n1762
$ top -u x_marmo
```

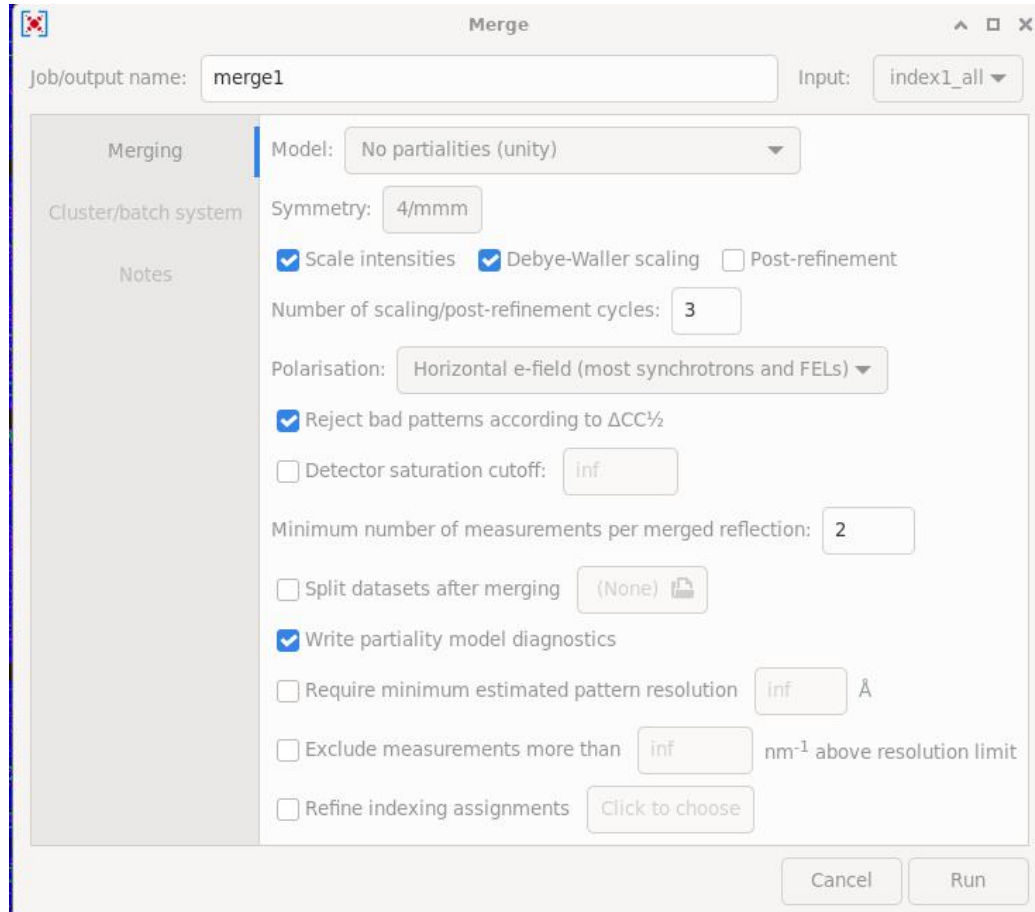
```
Terminal - x_marmo@n1762:~
File Edit View Terminal Tabs Help

x_marmo@tetralith2:proj/xray/users/x_marmo/2021a/crystfel/0.11.0-PreSTO-sebth_run2 x x_marmo@n1762:~

top - 10:25:10 up 32 days, 14:24, 0 users, load average: 76.81, 65.74, 34.27
Tasks: 697 total, 30 running, 666 sleeping, 0 stopped, 1 zombie
%Cpu(s): 95.3 us, 2.6 sy, 0.0 ni, 1.3 id, 0.0 wa, 0.6 hi, 0.1 si, 0.0 st
MiB Mem : 95350.9 total, 83948.6 free, 11741.7 used, 275.0 buff/cache
MiB Swap: 1953.0 total, 1953.0 free, 0.0 used, 83609.2 avail Mem

  PID USER      PR  NI   VIRT   RES   SHR  S  %CPU  %MEM    TIME+  COMMAND
  955467 x_marmo   20   0 2464324 338868 7472 S 197.7  0.3   5:20.00 indexamajig
  955488 x_marmo   20   0 2443352 325264 7500 R 139.1  0.3   4:48.60 indexamajig
  955475 x_marmo   20   0 2401964 281180 7480 S 104.3  0.3   3:42.46 indexamajig
  955470 x_marmo   20   0 2358848 242312 7472 S  87.7  0.2   4:41.62 indexamajig
  963861 x_marmo   20   0 1117436  44820 1856 R  85.8  0.0   0:02.62 mosflm
  963799 x_marmo   20   0 1117660  45128 1860 R  82.8  0.0   0:06.07 mosflm
  963859 x_marmo   20   0 1117304  38460 1676 R  78.1  0.0   0:02.43 mosflm
  963864 x_marmo   20   0 1117304  44828 1860 R  77.2  0.0   0:02.33 mosflm
  955492 x_marmo   20   0 2407912 286424 7500 S  68.9  0.3   3:53.83 indexamajig
  955465 x_marmo   20   0 2414136 292100 7468 D  68.2  0.3   5:44.96 indexamajig
  963872 x_marmo   20   0 1117304  38452 1680 R  61.6  0.0   0:01.86 mosflm
  955491 x_marmo   20   0 2387256 270960 7500 S  56.0  0.3   3:13.57 indexamajig
  955464 x_marmo   20   0 2354236 237944 7468 S  55.6  0.2   6:07.97 indexamajig
  955471 x_marmo   20   0 2363828 247408 7476 S  55.6  0.3   4:15.47 indexamajig
  955483 x_marmo   20   0 2476424 357376 7500 S  52.3  0.4   3:08.26 indexamajig
  955476 x_marmo   20   0 2407868 290804 7480 S  51.3  0.3   6:02.77 indexamajig
  955478 x_marmo   20   0 2464356 338900 7480 S  51.3  0.3   3:29.67 indexamajig
  955481 x_marmo   20   0 2350772 234524 7500 S  51.3  0.2   3:57.76 indexamajig
  955490 x_marmo   20   0 2478720 362192 7500 R  51.0  0.4   4:46.04 indexamajig
  955468 x_marmo   20   0 2470304 345076 7472 S  50.3  0.4   4:24.71 indexamajig
  955473 x_marmo   20   0 2407908 286188 7476 S  49.0  0.3   4:35.02 indexamajig
  955466 x_marmo   20   0 2476308 357340 7468 S  46.0  0.4   4:51.76 indexamajig
  955472 x_marmo   20   0 2470288 345064 7476 S  40.7  0.4   3:57.89 indexamajig
  955495 x_marmo   20   0 2402020 285444 7500 R  26.5  0.3   4:11.13 indexamajig
  963894 x_marmo   20   0 1117208  44660 1768 R  23.2  0.0   0:00.70 mosflm
  963887 x_marmo   20   0 1117204  44644 1772 R  20.9  0.0   0:00.63 mosflm
  955494 x_marmo   20   0 2369516 253052 7500 D  19.9  0.3   3:11.38 indexamajig
  955480 x_marmo   20   0 2464364 338916 7484 S  17.9  0.3   4:01.17 indexamajig
  963891 x_marmo   20   0 1117192  38264 1628 R  17.9  0.0   0:00.54 mosflm
  955477 x_marmo   20   0 2358444 241624 7484 S  17.5  0.2   4:08.18 indexamajig
  963893 x_marmo   20   0 1117196  38268 1628 R  16.9  0.0   0:00.51 mosflm
  955474 x_marmo   20   0 2404956 265288 7476 R  16.2  0.3   3:45.45 indexamajig
  963898 x_marmo   20   0 1117192  38252 1628 R  16.2  0.0   0:00.49 mosflm
  963896 x_marmo   20   0 1117192  38272 1628 R  15.2  0.0   0:00.46 mosflm
  963899 x_marmo   20   0 1117196  38256 1628 R  14.6  0.0   0:00.44 mosflm
  963895 x_marmo   20   0 1117192  38256 1628 R  13.9  0.0   0:00.42 mosflm
  963892 x_marmo   20   0 1117192  38264 1628 R  13.6  0.0   0:00.41 mosflm
  963901 x_marmo   20   0 1117192  38256 1628 R  12.6  0.0   0:00.38 mosflm
  963897 x_marmo   20   0 1117192  38260 1628 R  12.3  0.0   0:00.37 mosflm
  955462 x_marmo   20   0 100292  77532 5284 S  10.3  0.1   0:36.41 indexamajig
  963900 x_marmo   20   0 1117196  38256 1628 R   8.9  0.0   0:00.27 mosflm
  963902 x_marmo   20   0 1117196  38268 1628 R   5.6  0.0   0:00.17 mosflm
  955487 x_marmo   20   0 2358404 242264 7500 R   5.0  0.2   4:35.66 indexamajig
  955493 x_marmo   20   0 2346352 229648 7500 R   4.6  0.2   4:18.28 indexamajig
  955479 x_marmo   20   0 2407912 291228 7476 R   4.0  0.3   4:20.98 indexamajig
  955482 x_marmo   20   0 2545172 417576 7500 S   3.3  0.4   4:56.20 indexamajig
  955486 x_marmo   20   0 2350796 234264 7500 S   3.0  0.2   6:13.23 indexamajig
  955485 x_marmo   20   0 2470304 351236 7500 R   2.3  0.4   3:03.32 indexamajig
```

# Merge settings 1 (2)



Job/output name:  Input:

Merging

Cluster/batch system

Notes

Model:

Symmetry:

Scale intensities  Debye-Waller scaling  Post-refinement


Number of scaling/post-refinement cycles:

Polarisation:

Reject bad patterns according to  $\Delta CC\frac{1}{2}$

Detector saturation cutoff:

Minimum number of measurements per merged reflection:

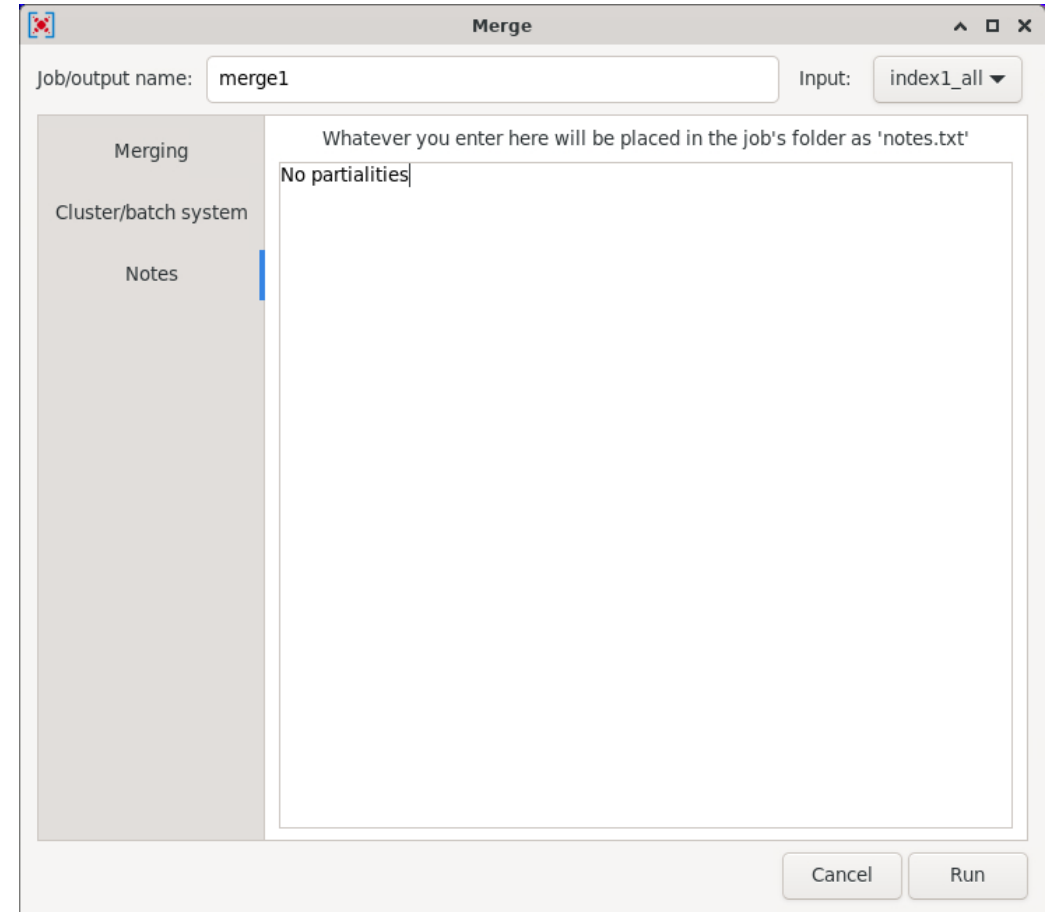
Split datasets after merging  

Write partiality model diagnostics

Require minimum estimated pattern resolution  Å

Exclude measurements more than  nm<sup>-1</sup> above resolution limit

Refine indexing assignments



Job/output name:  Input:

Merging

Cluster/batch system

Notes

Whatever you enter here will be placed in the job's folder as 'notes.txt'

# Merge at login node - 2 (2)

Job/output name:  Input:

Merging

Batch system:

Cluster/batch system

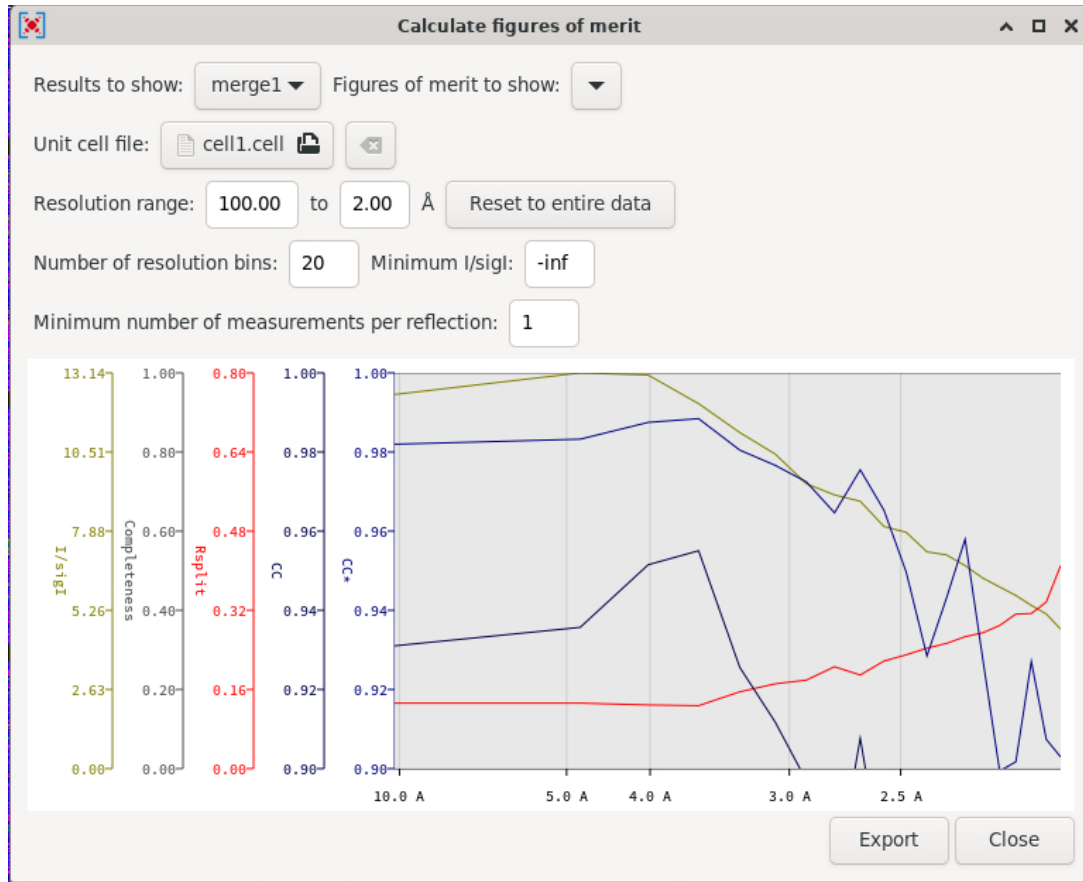
Number of threads:

Notes

```
Terminal - x_marmo@tetralith2:/proj/xray/users/x_marmo/2021a/crystfel/0.11.0-PreSTO-sebth_run2
File Edit View Terminal Tabs Help
x_marmo@tetralith2:/proj/xray/users/x_marmo/2021a/crystfel/0.11.0-PreSTO-sebth_run2 x_marmo@tetralith2:/proj/xray/users/x_marmo/2021a/
top - 10:45:16 up 37 days, 24 min, 128 users, load average: 37.75, 21.67, 17.08
Tasks: 7542 total, 6 running, 7297 sleeping, 233 stopped, 6 zombie
%Cpu(s): 26.2 us, 6.8 sy, 0.0 ni, 65.5 id, 0.0 wa, 0.5 hi, 0.9 si, 0.0 st
MiB Mem : 385141.1 total, 65307.6 free, 311599.7 used, 16408.4 buff/cache
MiB Swap: 4096.0 total, 0.3 free, 4095.7 used, 73541.4 avail Mem

  PID USER      PR  NI   VIRT   RES   SHR  S  %CPU  %MEM    TIME+  COMMAND
2115756 x_marmo  20   0 1785668 1.7g  4780 R  99.1  0.4  0:29.50 partialator
2116185 x_marmo  20   0 234464 12828 3604 R   7.4  0.0  0:01.76 top
2021161 x_marmo  20   0 1358276 173816 36952 S   1.2  0.0  2:44.77 Xvnc
2021894 x_marmo  20   0 20056 8200 5308 S   0.6  0.0  0:08.47 sshd
2028397 x_marmo  20   0 4686412 493068 234788 S   0.6  0.1  4:05.07 crystfel
2031130 x_marmo  20   0 4357008 494544 225176 S   0.6  0.1  1:43.73 firefox
2023576 x_marmo  20   0 681016 44780 33156 S   0.3  0.0  0:02.79 xfce4-terminal
269938 x_marmo  20   0 8608 216 0 S   0.0  0.0  0:00.00 ssh-agent
1301561 x_marmo  20   0 8608 204 0 S   0.0  0.0  0:00.00 ssh-agent
2021099 x_marmo  20   0 4144 2516 2344 S   0.0  0.0  0:00.00 tl-xinit
2021257 x_marmo  20   0 223168 4164 3272 S   0.0  0.0  0:00.06 xsession
2021506 x_marmo  20   0 161852 7100 6498 S   0.0  0.0  0:00.41 xt-epi2 register
```

# FOM & mtzdump



```

Terminal - x_marmo@tetralith2:/proj/xray/users/x_marmo/2021a/crystfel/0.11.0-PreSTO-sebth_run2
File Edit View Terminal Tabs Help

x_marmo@tetralith2:/proj/xray/users/x_marmo/2021a/crystfel/0.11.0-PreSTO-sebth_run2 x_marmo@tetralith2:/proj/xray/users/x_marmo

#####
#####
#####
## CCP4 8.0.017: MTZDUMP version 1.1 : ##
#####
User: x_marmo Run date: 29/ 5/2024 Run time: 13:19:05

Please reference: Collaborative Computational Project, Number 4, 2011.
"Overview of the CCP4 suite and current developments". Acta Cryst. D67, 235-242.
as well as any specific reference in the program write-up.

<!--SUMMARY_END--></FONT></B>

Optional input follows.

Keywords: RESO STATS LRESO HEAD NREF START SKIP SYMM
          BATCH FORMAT RUN/GO/END
RESO max min - resolution limits for listing (default all)
STATS [NBIN num] [RESO max min] - no. of reso. bins and limits for stats.
LRESO - S is given for each listed reflection
HEAD - print MTZ file header only
NREF num - number of reflections listed (default 10)
START H0 K0 L0 - first reflection listed (default first)
SKIP nskip - no. of refls. skipped before listing (default 0)
SYMMETRY - list symmetry info
VALM num - missing data set to this value
BATCH - list batch orientation blocks

FORMAT fmt - format of listed refls. .e.g. '(3i4,10f8.2)'
RUN/GO/END - to start dump

go

OPENED INPUT MTZ FILE
Logical Name: HKLIN Filename: data_from_crystfel.mtz

* Title:

Data exported via CrystFEL version 0.11.0

* Base dataset:

0 HKL_base
HKL_base
HKL_base

* Number of Datasets = 1

* Dataset ID, project/crystal/dataset names, cell dimensions, wavelength:

1 0.11.0-PreSTO-sebth_run2
index1_all
merge1
79.2700 79.2700 38.1700 90.0000 90.0000 90.0000
0.00000

* Number of Columns = 5
* Number of Reflections = 468443
* Missing value set to NaN in input mtz file
* HISTORY for current MTZ file :

* Column Labels :
H K L I SIGI

* Column Types :
H H H J Q

* Associated datasets :
0 0 0 1 1

* Cell Dimensions : (obsolete - refer to dataset cell dimensions above)
79.2700 79.2700 38.1700 90.0000 90.0000 90.0000
  
```