Test CrystFEL 0.11.0-PReSTO-sebth

Data in: /proj/xray/users/x_marmo/2021a/data/Lyz

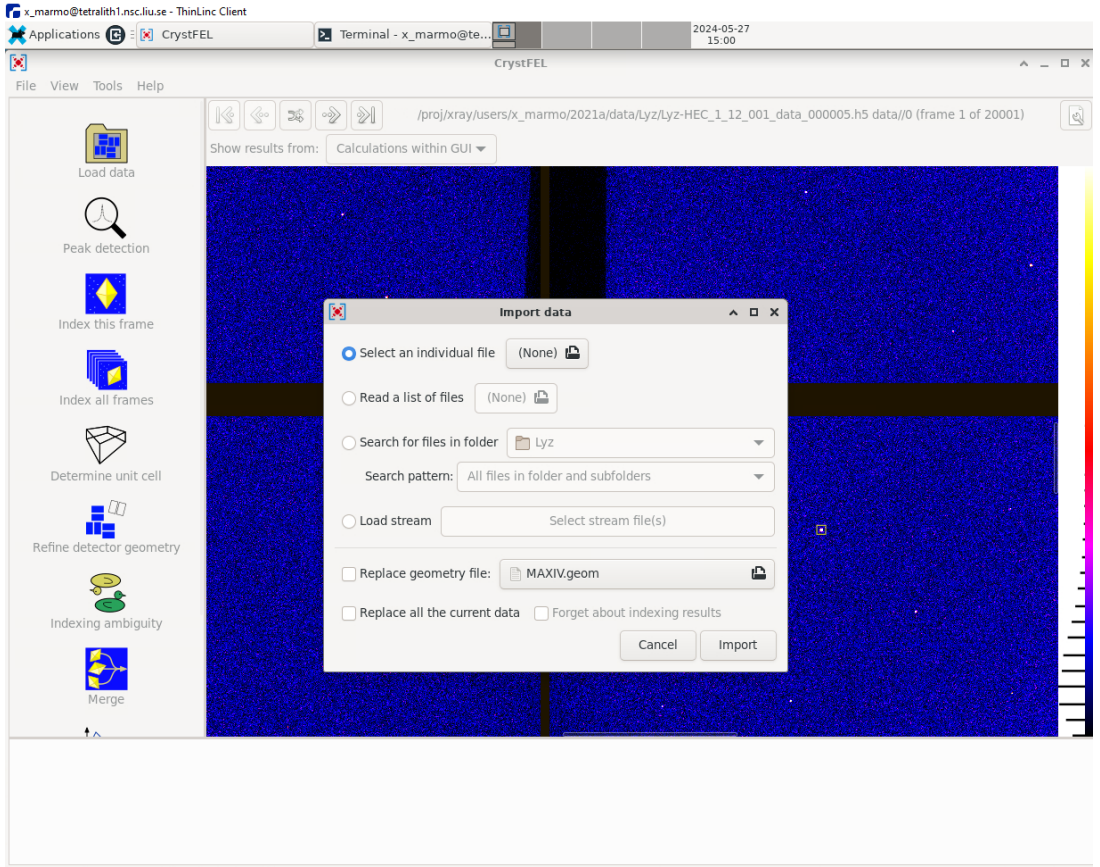
Run1 in: /proj/xray/users/x_marmo/2021a/crystfel/0.11.0-PReSTO-sebth

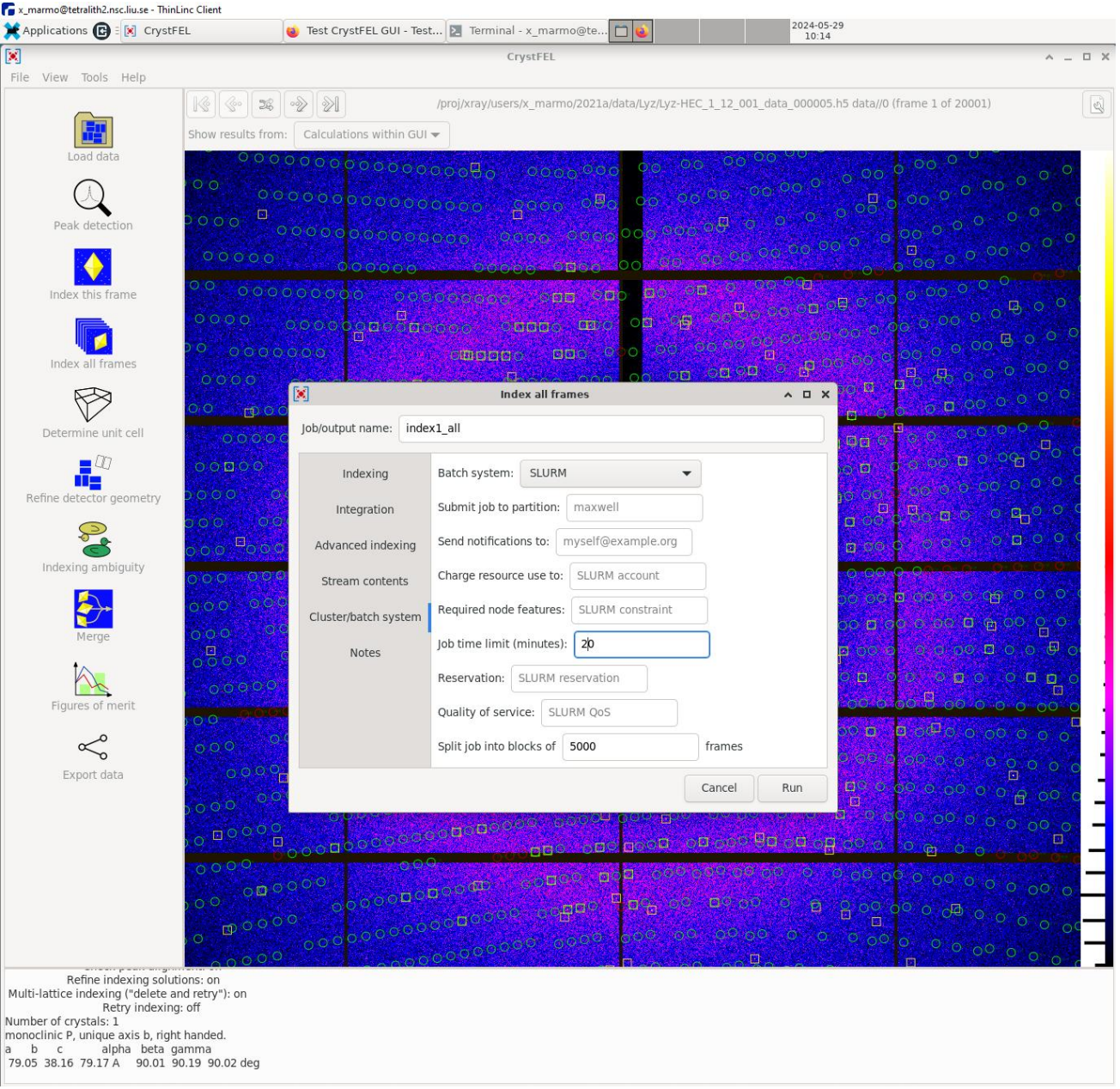
Some crash happen so:

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





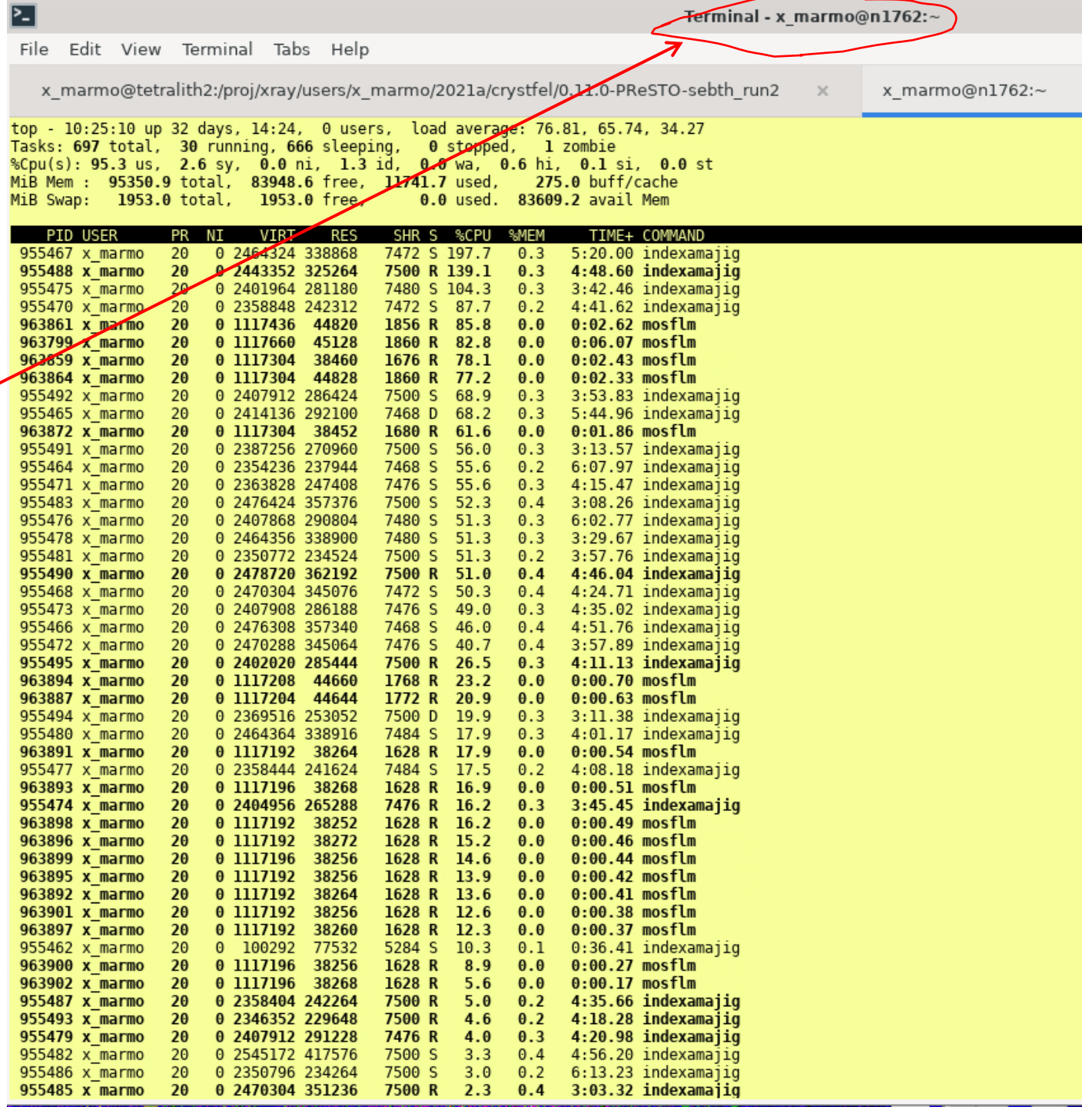
Use SLURM to index all 20 000 frames
- Select 30 min and 5000 frames per job, 4 jobs

```
[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]$
```

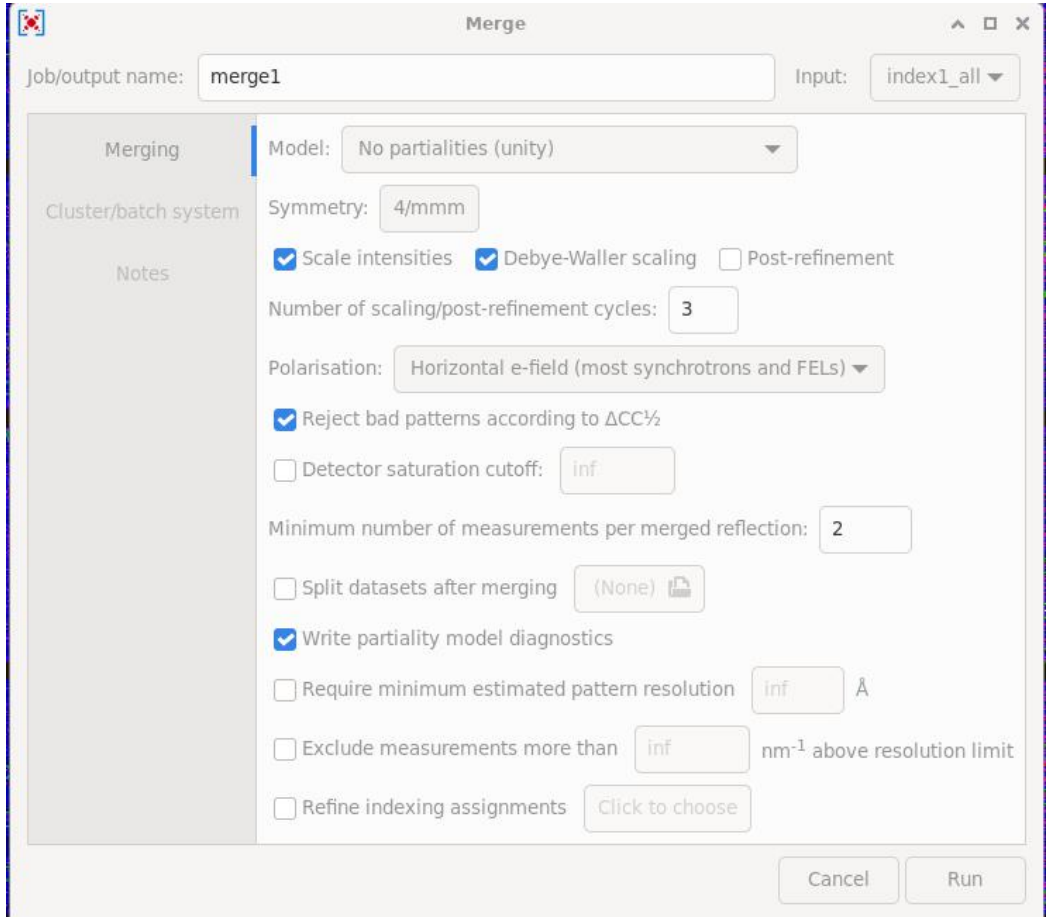
Review computing at n1762

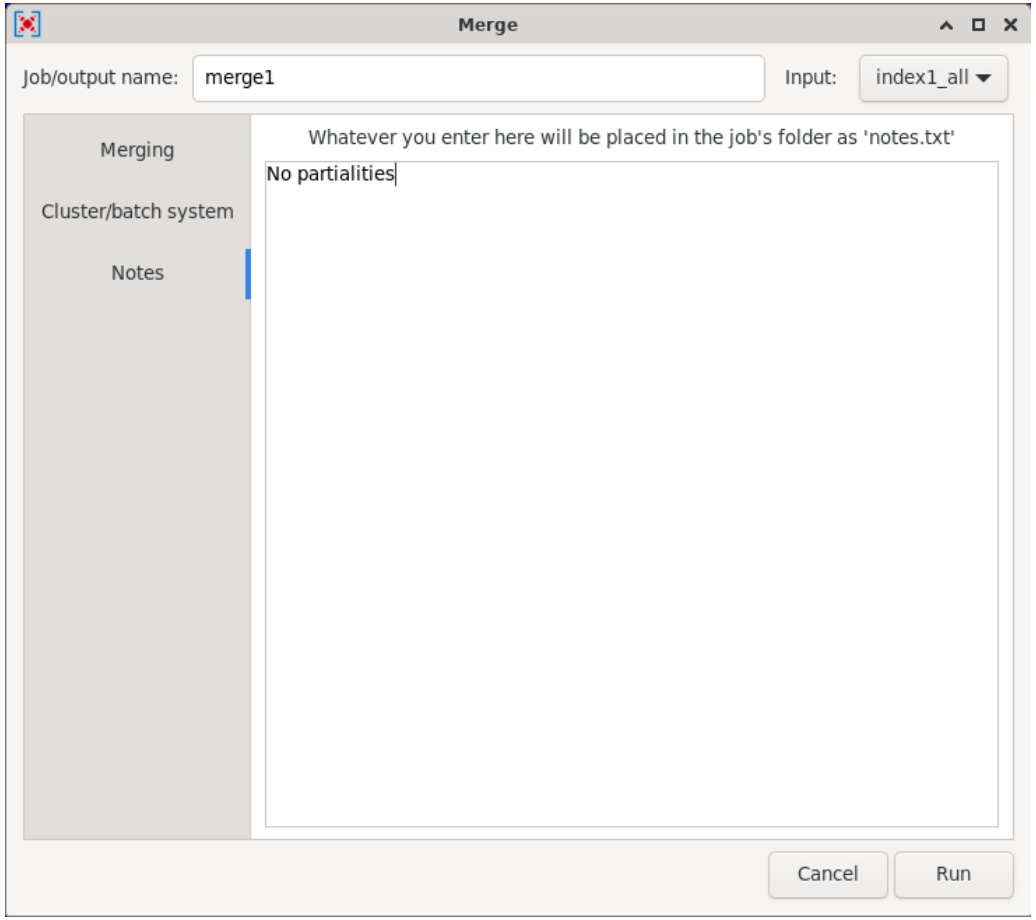
```
[x_marmo@tetralith2 0.11.0-PReSTO-sebth_run2]$ squeue -u x_marmo
             JOBID PARTITION     NAME     USER ST       TIME  NODES NODELIST(REASON)
    35186060_[1-4] tetralith index1_a  x_marmo PD       0:00      1 (Resources)
        35186060_0 tetralith index1_a  x_marmo  R       0:13      1 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]$
```

$ jobsh n1762
$ top –u x_marmo

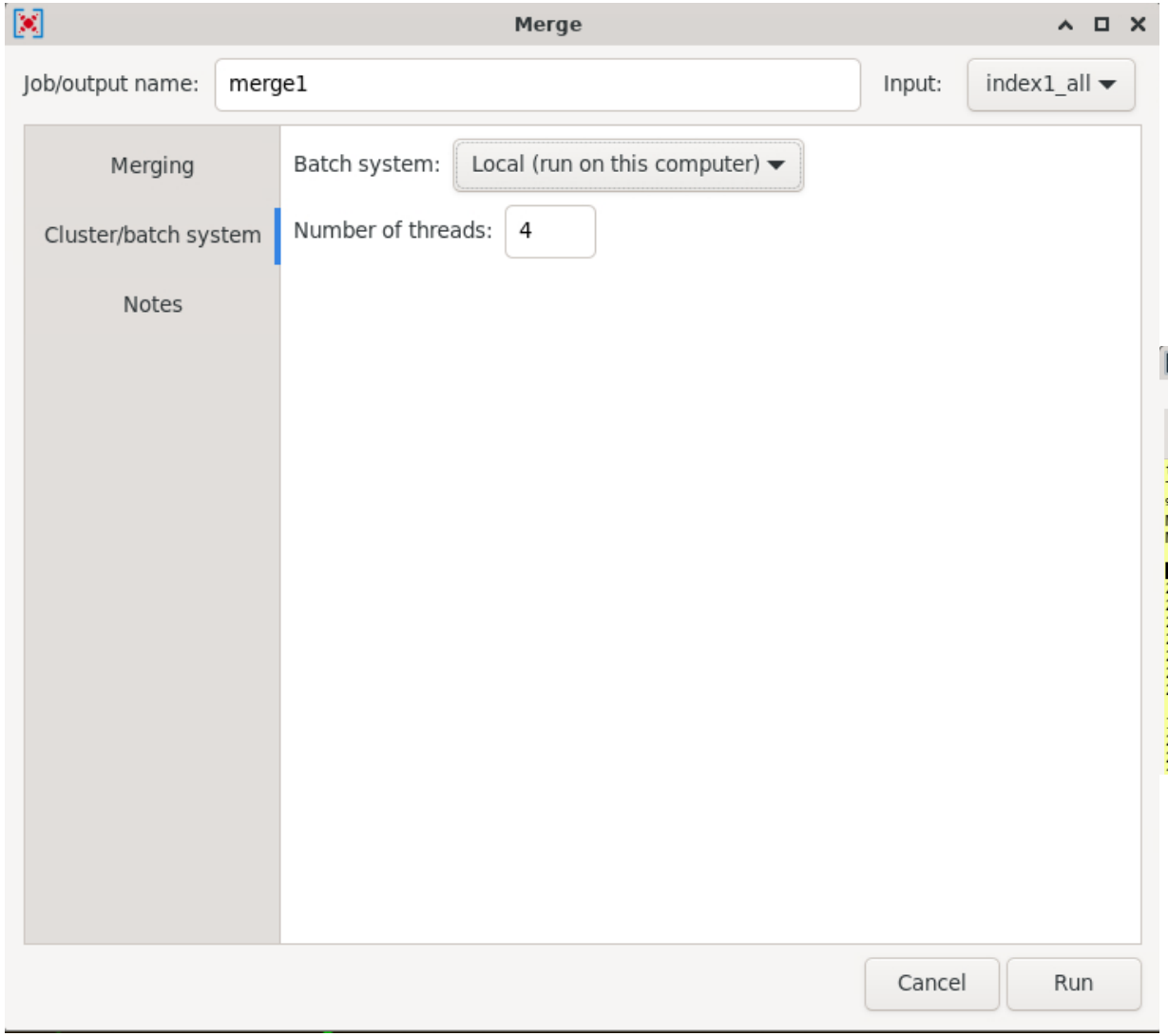


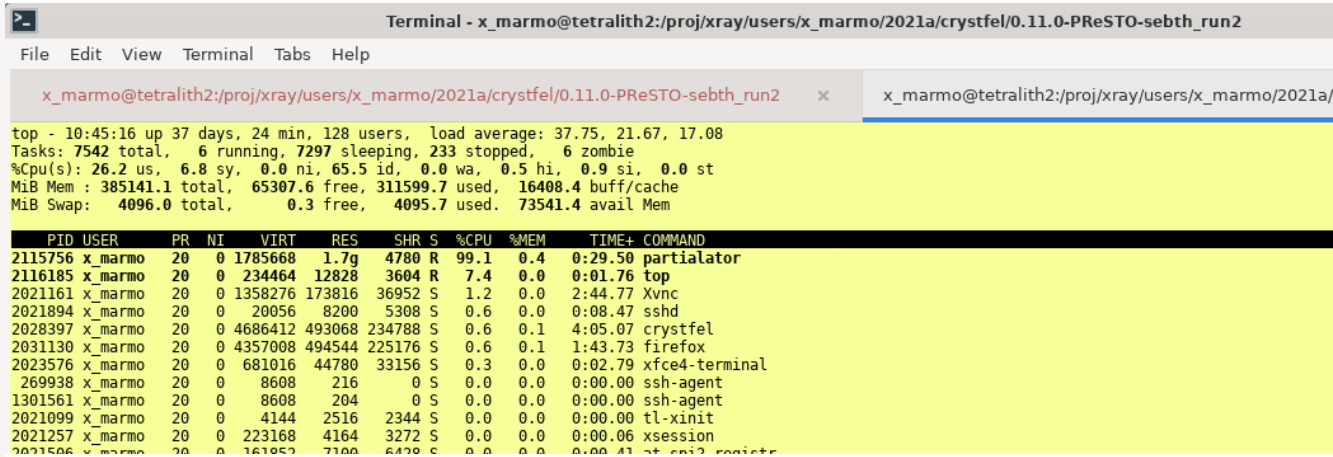
Merge settings 1 (2)



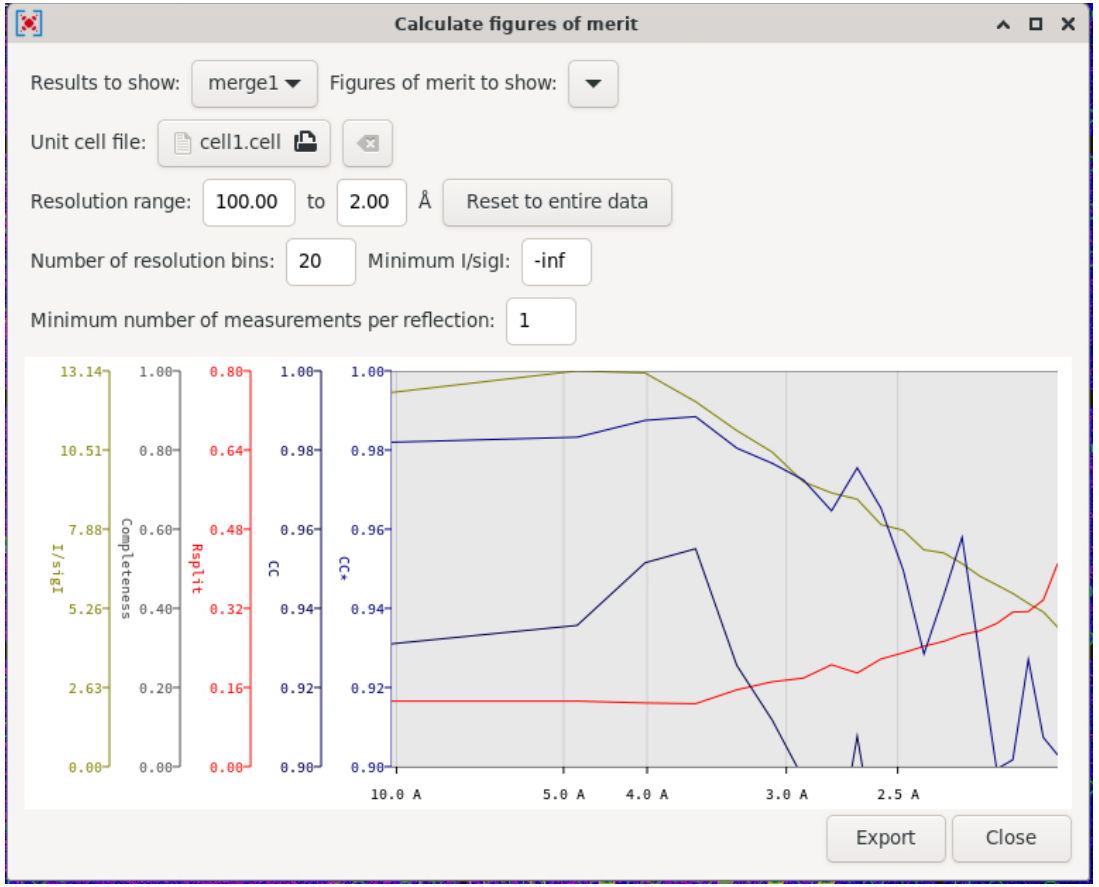


Merge at login node - 2 (2)





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
```