

## Some issues on PC4 – Crystallography workflow

### For the Stage 1 and 2.

- What are the parameters to execute mosflm to visualize the images? We used the following (on windows it did not return any image):

```
TITLE f9u test data
IMAGE f9u-2_MS_2_001.img
BEAM 94.60 92.89
SCANNER ADSC
WAVE 0.979
DISTANCE 180
RESOLUTION 1.8 (if known)
MOSAIC (if known)
SYMM p422 (if known)
CELL 79.388 79.388 37.831 90 90 90 (if known)
GO
```

- How include the matrix.mat file in the command line?
- For the crystallographer, how to obtain, visualize or determine the quality of the images, it is only visual? How we can decide that the second interaction is better than the first one? Or we could obtain some outputs to analyze quantitatively?
- Is this first loop non interactive? How could we stop at this point (if we would want to run into a script)

### For the Stage 3.

- In the table it is said: Using CCP4 To Produce Unmerged Reflection File. But is mosflm or ccp4? and what are the parameters to execute it (or them)?

### For the Stage 4.

- The execution of SORT and TRUNCATE was OK (with the examples).
- But, SCALA returned the following error messages: (We use ccp4 6.1.1.3, tried to install other version, run with other parameters, but SCALA did not execute correctly)

```
kernel32.dll 7C87655C Unknown Unknown Unknown
kernel32.dll 7C80B729 Unknown Unknown Unknown
Run(s): 1
forrtl: severe (8): internal consistency check failure, file for_exit_handler.c,
line 354

C:\Documents and Settings\kary\Meus documentos\Downloads>scala HKLIN mosflm1-sor
ted.mtz HKLOUT mosflm1_scala.mtz >EOF-scala
Last system error message: No such file or directory
scala: Cannot find input file

C:\Documents and Settings\kary\Meus documentos\Downloads>scala HKLIN mosflm1-sor
ted.mtz HKLOUT mosflm1_scala.mtz >EOF-scala
run 1 batches 1 to 180
cycles 100 converge 0.03
reject 6 smaller
exclude sdmin 3
intensities pr_part
intensities partials check
scales batch bfactor on brotation spacing 20
resolution low 100 high 1.7
anomalous off
EOF-scala
Scala: ***** Error in input *****
```

- For FREE the error was the following:

freerflag unrecognized keyword

### **For the Stage 5.**

- Is the program Phenix? What are the parameters?
- (We are going to test it on Linux, which was recommended by the author :)

```
Hi Kary, only a subset of Phenix runs on Windows. These are only
command-line tools. The Phenix Graphical User Interface is not
available. If you are just getting started with Phenix, I highly
recommend you use a Linux or Macintosh system.
We don't have documentation specific to Windows. The documentation
for
the Phenix commands available under Windows is platform independent.
Ralf
```

### **For the Stage 6.**

- What are the Coot parameters? And what would be the considerations of this point decision that need to be taken? This point can be non interactive?

### **For the Stage 7.**

- Is the program Phenix? What are the parameters?