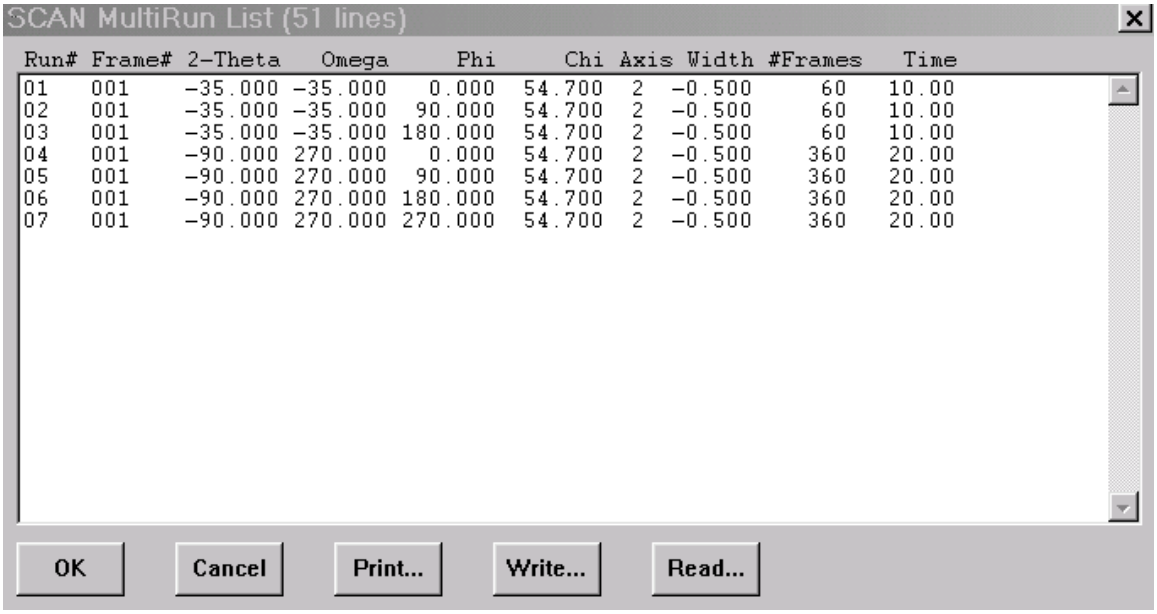
Data Collection FRAMO/GADDS Advanced

Instructors : Joseph Reibenspies, Ph.D.
Nattamai Bhuvanesh, Ph.D.

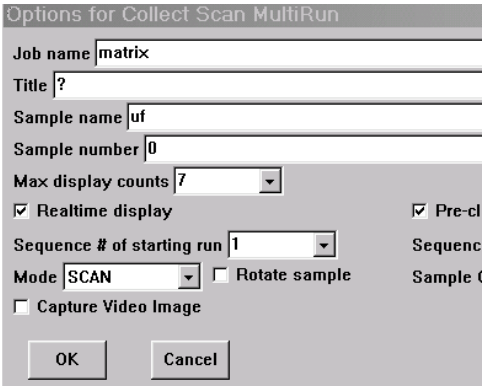
Version 1.0.0

Data Collection on the GADDS system with FRAMBO or GADDS software.

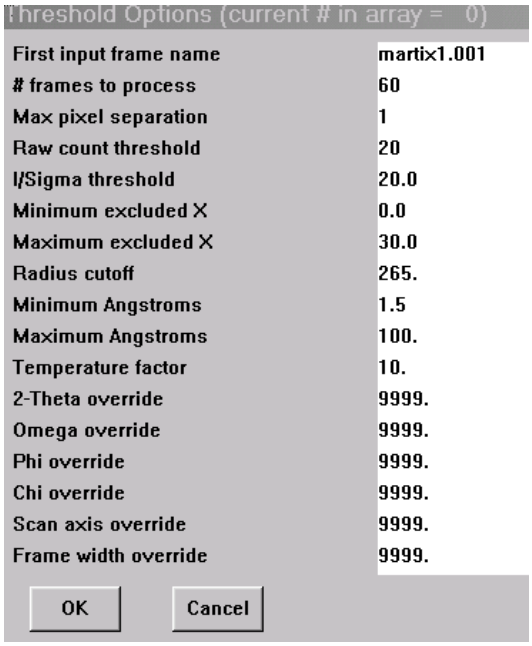
start VIDEO
start FRAMBO (or GADDS).
Point to Collect/Goiniometer/Optical
Point to OK
Use the 1,2,3 and 4 keys on the remote keypad (same as A,B,C and D on the SMART remote keypad) to align xtal.
For a short matrix point to Collect/Scan/Editruns.



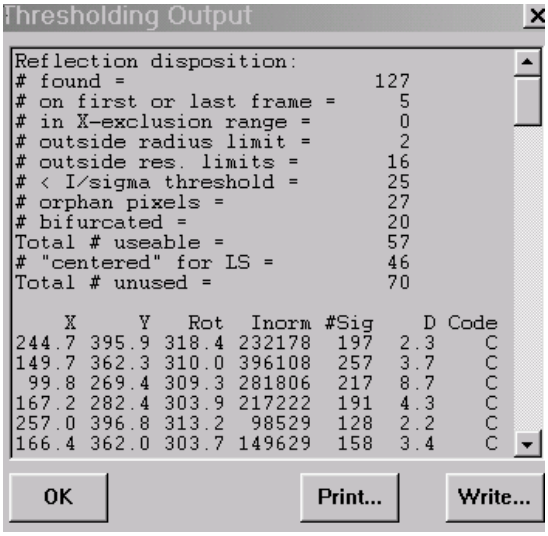
For the first 3 "runs" set the # frames to 60.



Collect a short data set. Point to Collect/Scan/Multirun. For the Job name input matrix. Make sure that the Rotate sample box (next to the Mode box) is not checked. Point to OK

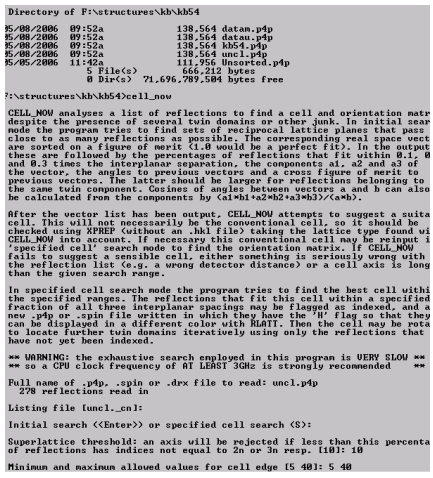


This will take about 30 mins. Stop after the third run.
Point to Peaks/Refl.array/Clear and OK.
Point to Peaks/Refl.array/Threshold.
The First Input Frame Name is matrix1.001. There are 60 frames. Leave the raw count and I/Sigma threshold at 20. Point to OK. You should see around 10 to 100 usable reflections. If not you may need to collect more frames. Point to OK.



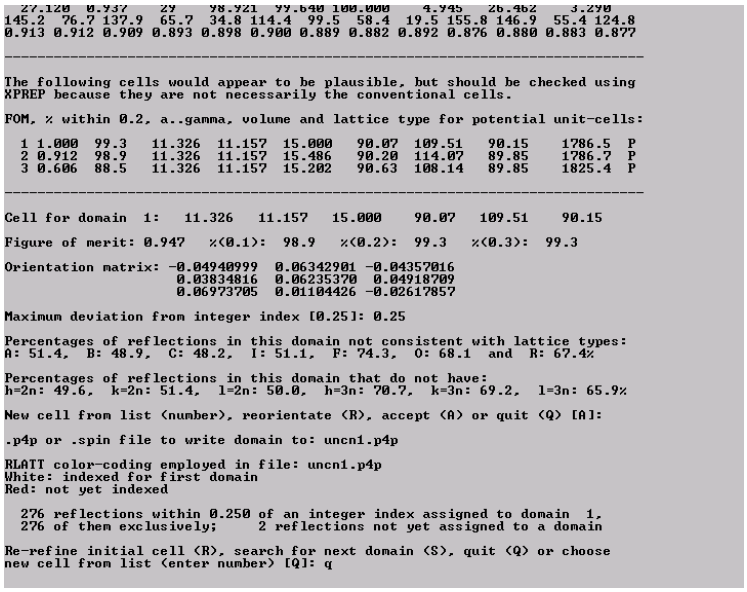
Repeat for martix2.001, matrix3.001 etc.
You need to save the reflections to a file. Point to Peaks/Refl.array/LeastSQ. Near the bottom of the window you will see. Change the output file name to fit your needs. Always add the p4p extension. Point to Cancel (not OK). Now point to Point to Peaks/Refl.array/Save and the save the file to disk. Start a command prompt (point START/RUN 

and type cmd). Navigate to your data directory and type cell_now. Input the P4P file (here it is uncl.p4p) and use the defaults for Initial Search, Threshold 10 and cell edge 5 ,40. If you think you may have a larger cell then change the cell edge setting to 3, 80. Remember this will slow the program down!

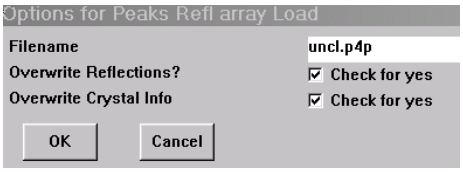


Let the program think. It may take a while depending on your computer etc.

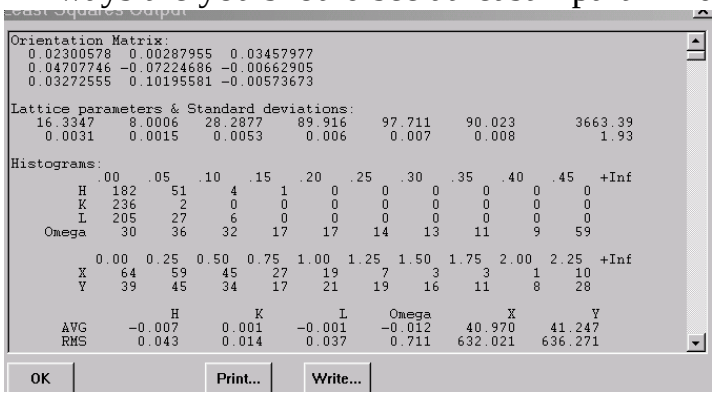
Cell_now found three solutions. All are very similar. Solution number 1 is the best with 99.3 % coverage and a Figure of Merit of one.



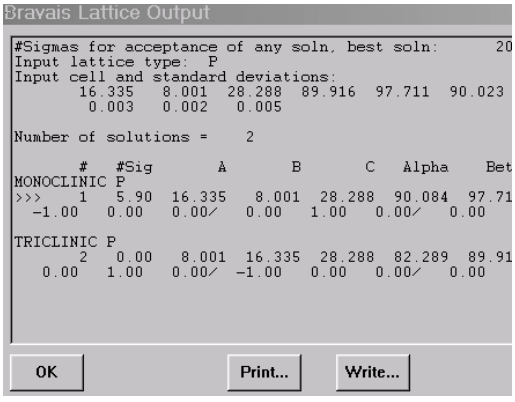
Accept this solution (A) and write a new P4P file in this case uncn1.p4p. Notice that of the 278 reflections the cell "fits" 276.
Return to FRAMBO and read in the new file. Point to Peaks/Refl.array/Load. Find the new file and



load it. Point to Peaks/Refl.array/LeastSQ and OK. You will see the cell parameters. As Always the you should see at least 1 part in 1000



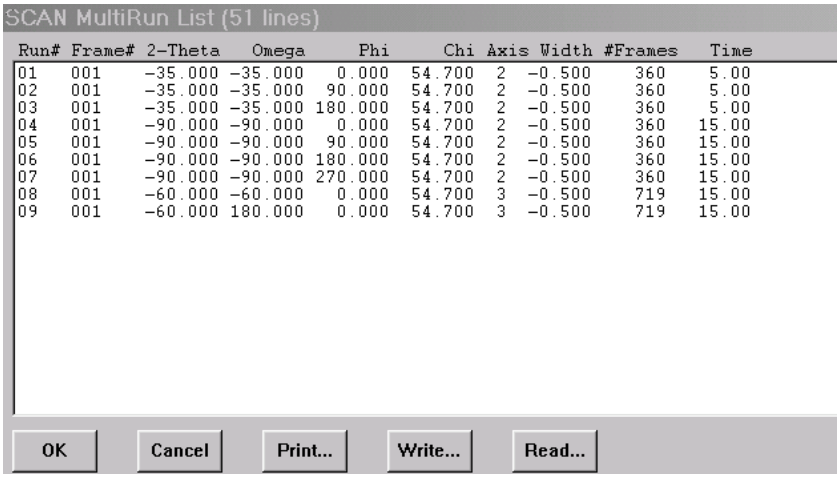
for the e.s.d. of the Volume for an acceptable cell. Point to Peaks/Refl.array/Bravais and do the reduction. In this case the program predicts a



monoclinic cell. Finally save the cell with the Peaks/Refl.array/Save or Peaks/Refl.array/LeastSQ command.

Now you are ready to collect data.

Start a generic data collection. Point to Collect/Scan/Editruns and edit the data collection runs. Change the 60 back to 360. Change the time as necessary. A good rule of thumb is to collect the first run slow enough so that you will see some reflections near the left hand edge of the detector. For SMART sized crystals this will take only 3 to 10 secs. For very small crystals this may take 60 secs. Do not exceed 60 secs / frame, more time will only result in more air scatter. If you do need to collect the frames much longer see the manager for a special beam stop apparatus that will reduce air scatter.



Now Point to Collect/Scan/Multirun. Give the data collection a job name. I prefer data and point to OK.

You may want to run COSMO to refine your data collection strategy. See the corresponding handout for details on how to run COSMO for GADDS.

Reduce the data as you would with the SMART data sets.