

Advanced Data Reduction

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Version 1.0.0

SAINT OUTPUT

Program SIFT (J. Reibenspies programmer).

Start a command prompt (point START/RUN  and type cmd). Navigate to your data directory and type

sift proj_name where the proj_name is the name of the *_ls file from saint

e.g.

sift data01

will output

```
C:\Documents and Settings\jhr6675\Desktop\class\twin\work>sift data01
Sift (1.0.0) :: PROJ :: data01
Summary
% observed/predicted      :   62.05%
Average Intensity        : 21140.00
Average I/Sigma(I)      :   49.03
% Very Strong Reflections:   60.90%
% Very Weak Reflections  :   14.88%
% Spot width > 1 frame   :   94.64%
Avg. x,y,z, position error :    0.03    -0.33    -0.06
% x,y,z > 0.5 pixel      : 17.82    42.91    2.08
% x,y,z > 1.0 pixel      :  3.29    13.67    0.35
Angstrms   #Obs Theory %Compl Redund  Rsym Pairs
to 2.674    37    62  59.68  1.00  0.000  0
to 2.141    75   108 69.44  1.00  0.000  0
to 1.876   112  167 67.07  1.00  0.000  0
to 1.707   136  214 63.55  1.00  0.000  0
to 1.587   166  264 62.88  1.00  0.000  0
to 1.494   191  325 58.77  1.00  0.000  0
to 1.420   213  371 57.41  1.00  0.000  0
to 1.358   236  413 57.14  1.00  0.000  0
to 1.306   251  460 54.57  1.00  0.000  0
to 1.262   255  519 49.13  1.00  0.000  0
...
% COMPLETE =    59.96
Redundancy =    1.00
Rsym       =    0.00
```

This is a summary of the file data01_ls

In this case 62% of the data is observed (which is good)

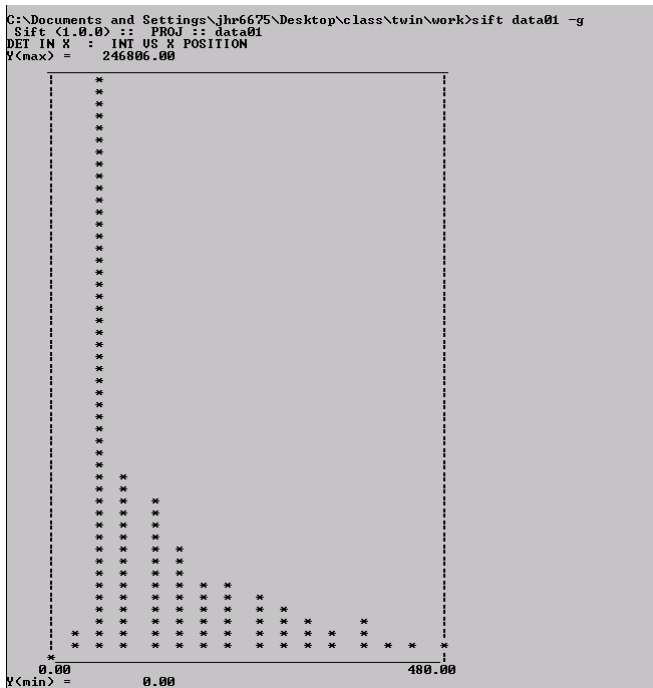
95% of the reflections covered more than one frame. If below 50 one may need to use narrower frames.

The average error in x, y and z are all below 1.0 which is good.

The y direction is shifting the most, but the shift is ok

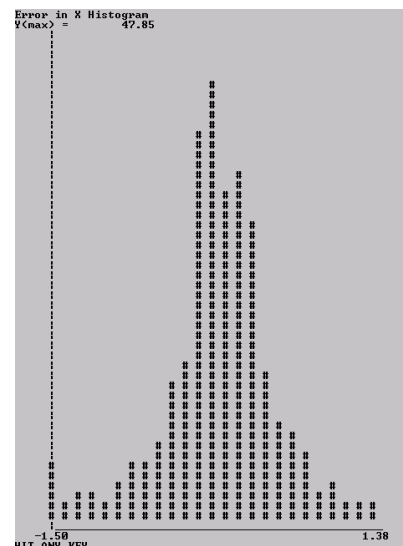
Other information can be extracted with sift.

- 1 ' Sift (1.0.0) ',
- 2 ' usage : sift proj_name -commands',
- 2 ' commands : -t = write excel table',
- 3 ' : -p = print spot shapes',
- 4 ' : -g = print histograms'



print a histogram of the data errors with -g. The first is the intensity vs X direction. Note: the steady fall off which is expected for the detector in the negative two-theta region. A few other intensity histograms will follow. They should be more or less

flat. A few spikes are acceptable. The error histograms should all be bell shaped like the one to the right. Finally the R(sym) should be clustered near zero.



```

Input X,Y,Z spot spread (deg): 1.200 1.200 0.600
Final Averaged Profile
+++++++
+ + + + +
+ + + + +
+ + + + +
+ X + + ### + + ### +
+ + + + ### + + #..# +
+ + + + ### + + #X.# +
+ + + + + + + +
+ + + + + + + +
+++++++
+ ### + + ### + + ### +
+ #..# + + #..# + + #..# +
+ #..# + + #..# + + #..# +
+ #X.# + + #X.# + + #X.# +
+ #..# + + #..# + + #..# +
+ ### + + #..# + + #..# +
+ + + + + + + +
+++++++
+ + + + + + + +
+ + + + + + + +
+ #..# + + ## + + + +
+ #X.# + + #X.# + + X +
+ #..# + + #..# + + + +
+ #..# + + # + + + +
+ ### + + + + + +
+++++++
TYPE ANY KEY

```

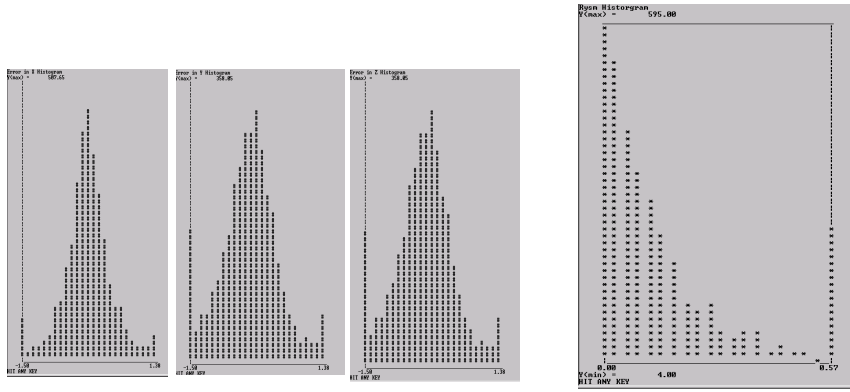
Spot shapes are of interest. The final averaged spot shape should look something like the one to the left. The spot should be fully contained in the box.

Use sift to examine the final *m._ls file.

Angstrms	#Obs	Theory	%Compl	Redund	Rsym	Pairs
to 1.870	141	168	83.93	3.89	0.056	131
to 1.489	285	325	87.69	4.03	0.065	260
to 1.302	426	462	92.21	4.14	0.074	387
to 1.184	570	634	89.91	3.81	0.076	504
to 1.099	688	758	90.77	3.54	0.078	583
to 1.034	808	908	88.99	3.36	0.079	671
to 0.983	910	1079	84.34	3.15	0.079	701
to 0.940	1023	1200	85.25	2.96	0.079	732
to 0.904	1113	1325	84.00	2.84	0.079	756
to 0.873	1201	1514	79.33	2.73	0.079	776

The Rsym should be less than 0.2 and the redundancy greater than 2.

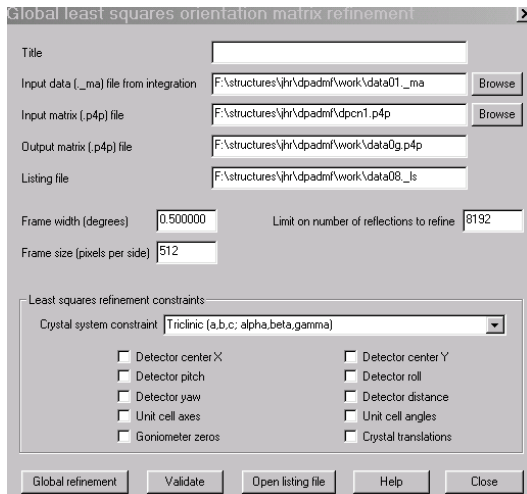
The error plots will be bell shapes and the Rsym histogram should falloff smoothly.



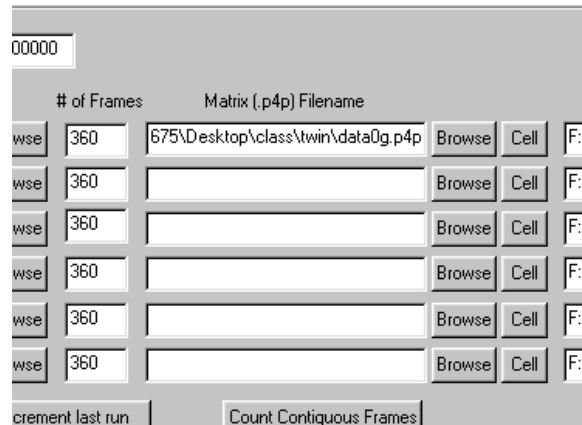
What to "tweak" if the data reduction fails.

If the R(sym) is poor or the output shows clear signs of data problems try these measures.

After your first data reduction, point to Global and generate

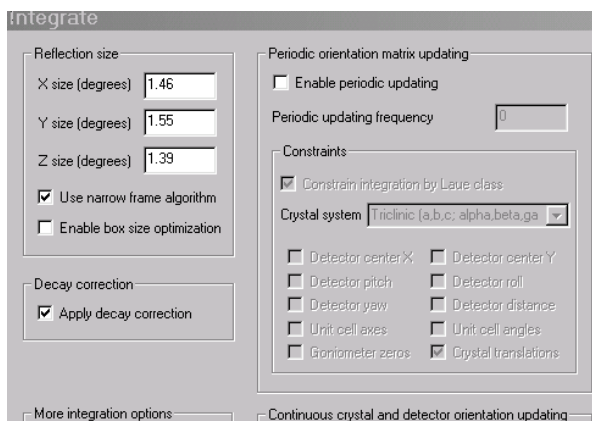


a good *.p4p file. Leave the title blank and point to Global refinement. The file generated will be *g.p4p and will be found in the work file. Return to the main menu and input the *g.p4p file. Point to



Cell to check the data. Now point to open listing file and open the *1._ls file. Scroll down a bit and find a reasonable spot box size.

All 108 .109 1 0.39 0.20 0.05 0.39 0.20 0.05 707.67 5 0 0.74 7 1.47 1.55 1.39 1.000



In this case 1.46, 1.55 and 1.39. Input the box size in SAINT and uncheck the enable box size optimization and enable periodic updating boxes

Point to advanced integration. Lower the values for the

Model profiles

	I/sigma lower limit for reflections used to update model profiles	5
	Fraction of model profile maximum used to generate simple sum limits	0.050000
	I/sigma threshold for least squares fit (below) vs. simple sum (above)	4
	Resolution lower limit (Å) above which simple sum is always used	9999.0000

Blend 9 profiles

model profile from 10 and 8 to 5 and 4. Change instrument error from 0.005 to 0 and increase the active frame queue half-width from 7 to 9. Point to Integrate+Sort+Global and reduce the data. If necessary repeat the global refinement until a reasonable unit cell is seen and then reduce data on that cell.

Corrections to intensity esd's

Instrument error (fraction of intensity)	0
Factor multiplying intensity esd's	1.000000

Frames stored to monitor reflection overlap

Active frame queue half-width	9
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Crystal

Starting exposure time (hours)	0.000000		
Batch #	1	Crystal #	1