Simulated-1g1c

From XDSwiki

This is an exercise, devised by James Holton, which deals with merging of datasets that were obtained in the presence of strong radiation damage.

The datasets were actually simulated using his program MLFSOM. There are 100 of them, and they are in random orientations wrt each other. Each dataset consists of 15 frames of 1 degree rotation.

The goal of data processing is to obtain a good and complete dataset. In this case, it is tempting to think about the possibility of only using the first frame of each dataset. This has three advantages:

1. radiation damage does not lower the resolution
2. the completeness should be adequate if the symmetry is at least orthorhombic
3. a successful procedure could also serve for processing data from a X-ray Free Electron Laser (see the recent Nature paper at [1] (http://www.nature.com/nature/journal/v470/n7332 /abs/nature09750.html))

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Preparation

From visual inspection (using adxv) we realize that the first frame of each dataset looks good (diffraction to 2 A), the last bad (10 A), and there is an obvious degradation from each frame to the next.

We have to get some idea about possible spacegroups first. This means processing some of the datasets. Let's choose "xtal100", the last one.

```
generate_XDS.INP "../../Illuin/microfocus/xtal100_1_0??.img"
```

To maximize the number of reflections that should be used for spacegroup determination, the only changes to XDS.INP are:

```
TEST_RESOLUTION_RANGE= 50 0 ! default is 10 4 ; we want all reflections instead
DATA_RANGE= 1 1             ! R-factors involving more than 1 frame are meaningless
                            ! with such strong radiation damage
```

We run "xds" and, after a few seconds, can inspect IDXREF.LP and CORRECT.LP. It turns out that the primitve cell is 38.3, 79.2, 79.2, 90, 90, 90 which is compatible with tetragonal spacegroups, or those with lower symmetry:

```
 LATTICE-  BRAVAIS-   QUALITY  UNIT CELL CONSTANTS (ANGSTROEM & DEGREES)    REINDEXING TRANSFORMA
CHARACTER  LATTICE     OF FIT      a      b      c   alpha  beta gamma

*  31        aP          0.0      38.3   79.2   79.2  90.0  90.0  90.0    1  0  0  0  0  1  0  0
*  44        aP          0.1      38.3   79.2   79.2  90.0  90.0  90.0   -1  0  0  0  0 -1  0  0
*  35        mP          0.4      79.2   38.3   79.2  90.0  90.0  90.0    0  1  0  0  1  0  0  0
*  33        mP          0.9      38.3   79.2   79.2  90.0  90.0  90.0   -1  0  0  0  0 -1  0  0
*  34        mP          1.1      38.3   79.2   79.2  90.0  90.0  90.0    1  0  0  0  0  0 -1  0
*  32        oP          1.2      38.3   79.2   79.2  90.0  90.0  90.0   -1  0  0  0  0 -1  0  0
*  20        mC          1.2     112.0  111.9   38.3  90.0  90.0  90.0    0  1  1  0  0  1 -1  0
*  23        oC          1.4     111.9  112.0   38.3  90.0  90.0  90.0    0 -1  1  0  0  1  1  0
*  25        mC          1.4     111.9  112.0   38.3  90.0  90.0  90.0    0 -1  1  0  0  1  1  0
*  21        tP          2.2      79.2   79.2   38.3  90.0  90.0  90.0    0 -1  0  0  0  0  1  0
   37        mC        249.8     162.9   38.3   79.2  90.0  90.0  76.4   -1  0  2  0 -1  0  0  0
```

This table exists in both IDXREF.LP and CORRECT.LP. The next table in CORRECT.LP tells us the Rmeas of the starred (*) lattices:

```
SPACE-GROUP         UNIT CELL CONSTANTS            UNIQUE   Rmeas  COMPARED  LATTICE-
  NUMBER      a      b      c   alpha beta gamma                             CHARACTER

     5     112.0  111.9   38.3  90.0  90.0  90.0     973     0.0         0    20 mC
    75      79.2   79.2   38.3  90.0  90.0  90.0     961    93.5        12    21 tP
    89      79.2   79.2   38.3  90.0  90.0  90.0     946    30.9        27    21 tP
    21     111.9  112.0   38.3  90.0  90.0  90.0     965    31.6         8    23 oC
     5     111.9  112.0   38.3  90.0  90.0  90.0     970    77.9         3    25 mC
     1      38.3   79.2   79.2  90.0  90.0  90.0     973     0.0         0    31 aP
    16      38.3   79.2   79.2  90.0  90.0  90.0     954     6.8        19    32 oP
     3      79.2   38.3   79.2  90.0  90.0  90.0     968     5.4         5    35 mP
     3      38.3   79.2   79.2  90.0  90.0  90.0     966     5.2         7    33 mP
     3      38.3   79.2   79.2  90.0  90.0  90.0     966    10.7         7    34 mP
     1      38.3   79.2   79.2  90.0  90.0  90.0     973     0.0         0    44 aP
```

Obviously the tetragonal lattices seem unfavourable, whereas orthorhombic is good. We repeat this procedure with a few other datasets, and observe that the "orthorhombic hypothesis" is confirmed. E.g. with xtal001 we obtain:

```
SPACE-GROUP         UNIT CELL CONSTANTS            UNIQUE   Rmeas  COMPARED  LATTICE-
  NUMBER      a      b      c   alpha beta gamma                              CHARACTER

     5     111.9  111.9   38.3  90.0  90.0  90.0     939   119.8         5    20 mC
    75      79.1   79.1   38.3  90.0  90.0  90.0     939    47.0         5    21 tP
    89      79.1   79.1   38.3  90.0  90.0  90.0     865    21.6        79    21 tP
    21     111.9  111.9   38.3  90.0  90.0  90.0     939   119.8         5    23 oC
     5     111.9  111.9   38.3  90.0  90.0  90.0     939   119.8         5    25 mC
     1      38.3   79.1   79.1  90.0  90.0  90.0     944     0.0         0    31 aP
    16      38.3   79.1   79.1  90.0  90.0  90.0     875     6.3        69    32 oP
     3      79.1   38.3   79.1  90.0  90.0  90.0     944     0.0         0    35 mP
     3      38.3   79.1   79.1  90.0  90.0  90.0     875     6.3        69    33 mP
     3      38.3   79.1   79.1  90.0  90.0  90.0     944     0.0         0    34 mP
     1      38.3   79.1   79.1  90.0  90.0  90.0     944     0.0         0    44 aP
```

devising a bootstrap procedure

We have to realize that, since the b and c axes are equal, we can index each dataset in two non-equivalent ways. This is the same situation as occurs e.g. for spacegroups P3(x) and P4(x), and means that we'll have to use a REFERENCE_DATA_SET to get the right setting for each of the 100 datasets.

However, we cannot expect that all of the datasets have enough reflections in common with a given dataset. Thus, we have to update and enlarge the REFERENCE_DATA_SET after the first round, using those datasets that have reflections in common with the old REFERENCE_DATA_SET. Then in a second round, we can hopefully identify the correct setting for all datasets. After that, we can scale everything together.

first round of bootstrap

We choose xtal100 as the first reference, and move its XDS_ASCII.HKL to bootstrap/reference.ahkl. A script that goes through all datasets, produces XDS.INP, and runs xds is the following (note that we only REFINE(IDXREF)= ORIENTATION BEAM , and the same for REFINE(INTEGRATE), since it may be useful to keep the b and c axis exactly the same):

```
#!/bin/csh -f
foreach f ( Illuin/microfocus/xtal*_1_001.img )
setenv x `echo $f | cut -c 19-25`
echo processing $x
rm -rf bootstrap/$x
mkdir bootstrap/$x
cd bootstrap/$x
cat>XDS.INP<<EOF
JOB= XYCORR INIT COLSPOT IDXREF DEFPIX INTEGRATE CORRECT
ORGX= 1511.2 ORGY= 1553.1 ! ORGX=1507 ORGY=1570 if BEAM is not refined
DETECTOR_DISTANCE= 250
OSCILLATION_RANGE= 1
X-RAY_WAVELENGTH= 0.979338
NAME_TEMPLATE_OF_DATA_FRAMES=../../Illuin/microfocus/${x}_1_0??.img
DATA_RANGE=1 1
SPOT_RANGE=1 1
REFERENCE_DATA_SET=../reference.ahkl
TEST_RESOLUTION_RANGE= 50.0 2.0 ! for correlating with reference
SPACE_GROUP_NUMBER=16                    ! 0 if unknown
UNIT_CELL_CONSTANTS= 38.3 79.1 79.1  90 90 90 ! mean of CORRECT outputs
INCLUDE_RESOLUTION_RANGE=60 1.8  ! after CORRECT, insert high resol limit; re-run CORRECT
TRUSTED_REGION=0.00 1.  ! partially use corners of detectors; 1.41421=full use
VALUE_RANGE_FOR_TRUSTED_DETECTOR_PIXELS=7000. 30000. ! often 8000 is ok
MINIMUM_ZETA=0.05        ! integrate close to the Lorentz zone; 0.15 is default
STRONG_PIXEL=5
MINIMUM_NUMBER_OF_PIXELS_IN_A_SPOT=3 ! default of 6 is sometimes too high
REFINE(INTEGRATE)=  ORIENTATION BEAM ! AXIS DISTANCE CELL
REFINE(IDXREF)= ORIENTATION BEAM ! AXIS DISTANCE CELL
! parameters specifically for this detector and beamline:
DETECTOR= ADSC MINIMUM_VALID_PIXEL_VALUE= 1 OVERLOAD= 65000
NX= 3072 NY= 3072  QX= 0.102539  QY= 0.102539 ! to make CORRECT happy if frames are unavailable
DIRECTION_OF_DETECTOR_X-AXIS=1 0 0
DIRECTION_OF_DETECTOR_Y-AXIS=0 1 0
INCIDENT_BEAM_DIRECTION=0 0 1 ! 0.00203 -0.0065 1.02107 ! mean of CORRECT outputs
ROTATION_AXIS=1 0 0    ! at e.g. SERCAT ID-22 this needs to be -1 0 0
FRACTION_OF_POLARIZATION=0.98   ! better value is provided by beamline staff!
POLARIZATION_PLANE_NORMAL=0 1 0
EOF
xds >& xds.log &
sleep 1
  cd ../..
end
```

Running this script takes 2 minutes. After this, it's a good idea to check whether the cell parameters are really what we assumed they are:

```
grep UNIT_CELL_CO xtal0[01]*/XDS_ASCII.HKL | cut -c24- > CELLPARM.INP
cellparm
cat CELLPARM.LP
```

and obtain:

```
     A         B         C       ALPHA     BETA      GAMMA     WEIGHT
  38.311    79.096    79.107    90.000    90.000    90.000       1.0
  38.292    79.081    79.078    90.000    90.000    90.000       1.0
  38.285    79.021    79.048    90.000    90.000    90.000       1.0
  38.308    79.106    79.099    90.000    90.000    90.000       1.0
  38.298    79.096    79.084    90.000    90.000    90.000       1.0
  38.310    79.117    79.109    90.000    90.000    90.000       1.0
  38.317    79.120    79.124    90.000    90.000    90.000       1.0
  38.302    79.102    79.097    90.000    90.000    90.000       1.0
  38.309    79.119    79.134    90.000    90.000    90.000       1.0
  38.288    79.098    79.128    90.000    90.000    90.000       1.0
  38.294    79.102    79.119    90.000    90.000    90.000       1.0
  38.299    79.104    79.100    90.000    90.000    90.000       1.0
  38.296    79.113    79.058    90.000    90.000    90.000       1.0
  38.322    79.091    79.120    90.000    90.000    90.000       1.0
  38.284    79.082    79.094    90.000    90.000    90.000       1.0
  38.284    79.103    79.098    90.000    90.000    90.000       1.0
  38.303    79.109    79.111    90.000    90.000    90.000       1.0
  38.293    79.084    79.083    90.000    90.000    90.000       1.0
  38.300    79.095    79.101    90.000    90.000    90.000       1.0
```

```
  38.300    79.097    79.100    90.000    90.000    90.000      19.0
```

Why not use all datasets? The reason is that cellparm has a limit of 20 datasets! But it seems to confirm that the cell axes are really 38.3, 79.1, 79.1.

Now we run xscale with the following XSCALE.INP :

```
OUTPUT_FILE=temp.ahkl

INPUT_FILE=../xtal001/XDS_ASCII.HKL
INPUT_FILE=../xtal002/XDS_ASCII.HKL
INPUT_FILE=../xtal003/XDS_ASCII.HKL
INPUT_FILE=../xtal004/XDS_ASCII.HKL
INPUT_FILE=../xtal005/XDS_ASCII.HKL
INPUT_FILE=../xtal006/XDS_ASCII.HKL
INPUT_FILE=../xtal007/XDS_ASCII.HKL
INPUT_FILE=../xtal008/XDS_ASCII.HKL
INPUT_FILE=../xtal009/XDS_ASCII.HKL
INPUT_FILE=../xtal010/XDS_ASCII.HKL
INPUT_FILE=../xtal011/XDS_ASCII.HKL
INPUT_FILE=../xtal012/XDS_ASCII.HKL
INPUT_FILE=../xtal013/XDS_ASCII.HKL
INPUT_FILE=../xtal014/XDS_ASCII.HKL
INPUT_FILE=../xtal015/XDS_ASCII.HKL
INPUT_FILE=../xtal016/XDS_ASCII.HKL
INPUT_FILE=../xtal017/XDS_ASCII.HKL
INPUT_FILE=../xtal018/XDS_ASCII.HKL
INPUT_FILE=../xtal019/XDS_ASCII.HKL
INPUT_FILE=../xtal020/XDS_ASCII.HKL
INPUT_FILE=../xtal021/XDS_ASCII.HKL
INPUT_FILE=../xtal022/XDS_ASCII.HKL
INPUT_FILE=../xtal023/XDS_ASCII.HKL
INPUT_FILE=../xtal024/XDS_ASCII.HKL
INPUT_FILE=../xtal025/XDS_ASCII.HKL
INPUT_FILE=../xtal026/XDS_ASCII.HKL
INPUT_FILE=../xtal027/XDS_ASCII.HKL
INPUT_FILE=../xtal028/XDS_ASCII.HKL
INPUT_FILE=../xtal029/XDS_ASCII.HKL
INPUT_FILE=../xtal030/XDS_ASCII.HKL
INPUT_FILE=../xtal031/XDS_ASCII.HKL
INPUT_FILE=../xtal032/XDS_ASCII.HKL
INPUT_FILE=../xtal033/XDS_ASCII.HKL
INPUT_FILE=../xtal034/XDS_ASCII.HKL
INPUT_FILE=../xtal035/XDS_ASCII.HKL
INPUT_FILE=../xtal036/XDS_ASCII.HKL
INPUT_FILE=../xtal037/XDS_ASCII.HKL
INPUT_FILE=../xtal038/XDS_ASCII.HKL
INPUT_FILE=../xtal039/XDS_ASCII.HKL
INPUT_FILE=../xtal040/XDS_ASCII.HKL
INPUT_FILE=../xtal041/XDS_ASCII.HKL
INPUT_FILE=../xtal042/XDS_ASCII.HKL
INPUT_FILE=../xtal043/XDS_ASCII.HKL
INPUT_FILE=../xtal044/XDS_ASCII.HKL
INPUT_FILE=../xtal045/XDS_ASCII.HKL
INPUT_FILE=../xtal046/XDS_ASCII.HKL
INPUT_FILE=../xtal047/XDS_ASCII.HKL
INPUT_FILE=../xtal048/XDS_ASCII.HKL
INPUT_FILE=../xtal049/XDS_ASCII.HKL
INPUT_FILE=../xtal050/XDS_ASCII.HKL
INPUT_FILE=../xtal051/XDS_ASCII.HKL
INPUT_FILE=../xtal052/XDS_ASCII.HKL
INPUT_FILE=../xtal053/XDS_ASCII.HKL
INPUT_FILE=../xtal054/XDS_ASCII.HKL
INPUT_FILE=../xtal055/XDS_ASCII.HKL
INPUT_FILE=../xtal056/XDS_ASCII.HKL
INPUT_FILE=../xtal057/XDS_ASCII.HKL
INPUT_FILE=../xtal058/XDS_ASCII.HKL
INPUT_FILE=../xtal059/XDS_ASCII.HKL
INPUT_FILE=../xtal060/XDS_ASCII.HKL
INPUT_FILE=../xtal061/XDS_ASCII.HKL
INPUT_FILE=../xtal062/XDS_ASCII.HKL
INPUT_FILE=../xtal063/XDS_ASCII.HKL
INPUT_FILE=../xtal064/XDS_ASCII.HKL
INPUT_FILE=../xtal065/XDS_ASCII.HKL
INPUT_FILE=../xtal066/XDS_ASCII.HKL
INPUT_FILE=../xtal067/XDS_ASCII.HKL
INPUT_FILE=../xtal068/XDS_ASCII.HKL
```

xscale writes XSCALE.LP which has the 5050 correlation coefficients of every dataset with every other dataset! The order of listing of the correlation coefficients is such that it turns out that is was a good choice to have xtal100 as the REFERENCE_DATA_SET, because we find this list:

```
    CORRELATIONS BETWEEN INPUT DATA SETS AFTER CORRECTIONS

DATA SETS  NUMBER OF COMMON  CORRELATION   RATIO OF COMMON   B-FACTOR
 #i   #j     REFLECTIONS     BETWEEN i,j  INTENSITIES (i/j)  BETWEEN i,j
```

with these final 99 lines:

1	100	12	0.601	0.8200	0.0085
2	100	24	0.998	0.9001	0.5637
3	100	16	0.990	0.9216	-0.2983
4	100	16	0.239	1.9141	-0.2253
5	100	31	0.996	0.9231	0.3755
6	100	22	0.997	0.9412	0.2726
7	100	11	0.976	0.8848	-0.1225
8	100	5	0.967	0.9166	0.0435
9	100	34	0.160	1.2885	0.0774
10	100	11	0.860	2.9740	-0.2614
11	100	8	0.997	0.8732	0.6032
12	100	8	0.998	1.0145	-0.4169
13	100	22	1.000	0.9313	0.1664
14	100	8	0.900	0.8040	0.2744
15	100	10	0.986	0.9510	0.1738
16	100	1	0.000	0.9685	0.0000
17	100	14	0.991	0.8700	0.3395
18	100	7	0.997	1.0546	-0.2113
19	100	23	1.000	1.0451	-0.0246
20	100	24	0.266	0.6392	0.1091
21	100	20	0.995	0.8529	0.6281
22	100	12	0.072	0.9376	-0.0406
23	100	19	0.999	0.9366	0.0670
24	100	14	0.998	1.0986	-0.7853
25	100	4	0.939	1.0483	-0.0886
26	100	26	0.993	0.9633	0.0813
27	100	30	0.990	0.9782	-0.0191
28	100	30	0.995	0.9124	-0.0781
29	100	13	0.488	2.1279	-0.2548
30	100	18	0.283	1.2442	0.0585
31	100	23	0.995	0.9249	0.4751
32	100	22	0.293	2.7799	-0.1715
33	100	7	1.000	1.0706	-0.2011
34	100	6	0.987	0.9888	-0.0007
35	100	8	0.989	0.9895	-0.1751
36	100	23	0.985	0.8494	0.3038
37	100	8	0.966	0.7378	-0.0108
38	100	7	1.000	1.1335	-0.0927
39	100	11	0.982	0.9994	-0.5811
40	100	16	0.994	0.7549	0.8741
41	100	12	0.986	0.9478	-0.4168
42	100	11	0.994	0.8285	0.7668
43	100	9	0.997	0.9595	-0.2219
44	100	15	1.000	0.8666	0.2884
45	100	13	0.517	1.6433	0.0034
46	100	13	0.296	1.4431	-0.0938
47	100	18	0.857	0.9734	0.3337
48	100	13	0.999	0.9627	0.2611
49	100	22	0.991	0.8798	0.2976
50	100	14	0.999	1.1206	-1.0748
51	100	10	0.999	0.9296	0.5194
52	100	8	0.899	1.3901	0.0190
53	100	24	0.998	1.0383	-0.3979
54	100	7	0.998	1.1332	-0.5519
55	100	8	0.993	0.9258	-0.0688
56	100	19	0.992	0.9138	0.0326
57	100	5	0.994	0.9209	-0.2679
58	100	22	0.996	0.8591	0.6813
59	100	7	0.650	1.5471	-0.0597
60	100	21	0.995	0.9013	0.0722
61	100	16	0.998	0.8689	0.4326
62	100	1	0.002	0.7717	0.0000
63	100	6	0.995	0.9921	0.0243
64	100	14	0.998	0.9398	-0.5243
65	100	12	0.515	1.7489	-0.0858
66	100	17	0.999	0.9457	0.0390
67	100	9	0.840	0.7706	0.5165
68	100	6	0.969	0.9477	0.0164
69	100	12	0.999	0.9503	-0.1039
70	100	10	0.949	0.8026	-0.1336

We note that there are many datasets with high correlation coefficients. We use some of those to generate the REFERENCE_DATA_SET for the second round - XSCALE.INP is now

```
OUTPUT_FILE=../reference.ahkl
INPUT_FILE=../xtal002/XDS_ASCII.HKL
INPUT_FILE=../xtal003/XDS_ASCII.HKL
INPUT_FILE=../xtal005/XDS_ASCII.HKL
INPUT_FILE=../xtal006/XDS_ASCII.HKL
INPUT_FILE=../xtal007/XDS_ASCII.HKL
INPUT_FILE=../xtal008/XDS_ASCII.HKL
INPUT_FILE=../xtal011/XDS_ASCII.HKL
INPUT_FILE=../xtal012/XDS_ASCII.HKL
INPUT_FILE=../xtal013/XDS_ASCII.HKL
INPUT_FILE=../xtal015/XDS_ASCII.HKL
INPUT_FILE=../xtal017/XDS_ASCII.HKL
INPUT_FILE=../xtal018/XDS_ASCII.HKL
INPUT_FILE=../xtal019/XDS_ASCII.HKL
INPUT_FILE=../xtal100/XDS_ASCII.HKL
```

we could have included more datasets but it's pretty clear that these 14 already provide a completeness of 34.5% :

```
SUBSET OF INTENSITY DATA WITH SIGNAL/NOISE >= -3.0 AS FUNCTION OF RESOLUTION
RESOLUTION     NUMBER OF REFLECTIONS    COMPLETENESS R-FACTOR  R-FACTOR COMPARED I/SIGMA   R-meas
  LIMIT     OBSERVED  UNIQUE  POSSIBLE     OF DATA   observed  expected                        
```

LIMIT	OBSERVED	UNIQUE	POSSIBLE	OF DATA	observed	expected			
8.05	111	92	304	30.3%	3.1%	4.2%	34	17.02	4.1%
5.69	198	161	515	31.3%	3.5%	3.4%	70	16.78	4.8%
4.65	289	230	639	36.0%	3.2%	3.5%	109	16.77	4.4%
4.03	354	267	753	35.5%	3.4%	3.6%	151	18.70	4.5%
3.60	367	287	840	34.2%	2.4%	3.6%	147	17.35	3.2%
3.29	408	326	919	35.5%	3.7%	3.6%	158	16.91	5.1%
3.04	422	324	987	32.8%	3.8%	3.9%	180	14.95	5.1%
2.85	498	387	1066	36.3%	5.2%	4.6%	212	12.72	7.1%
2.68	523	402	1124	35.8%	5.5%	5.4%	219	11.28	7.4%
2.55	512	399	1174	34.0%	5.8%	6.0%	210	9.98	7.9%
2.43	558	426	1263	33.7%	8.7%	8.6%	237	8.37	11.7%
2.32	589	446	1287	34.7%	8.1%	9.0%	261	8.05	11.0%
2.23	621	470	1350	34.8%	9.6%	10.4%	276	7.52	12.9%
2.15	653	487	1380	35.3%	8.0%	8.8%	298	7.70	10.8%
2.08	624	493	1459	33.8%	11.6%	11.6%	247	6.57	16.0%
2.01	660	510	1494	34.1%	11.3%	11.5%	271	6.16	15.0%
1.95	697	535	1546	34.6%	13.1%	13.8%	295	5.34	17.7%
1.90	765	576	1571	36.7%	15.9%	16.3%	351	5.12	21.7%
1.85	751	563	1635	34.4%	21.7%	22.0%	339	3.80	29.3%
1.80	697	531	1660	32.0%	24.5%	25.5%	298	3.51	33.1%
total	10297	7912	22966	34.5%	5.6%	5.9%	4363	9.17	7.6%

second round of bootstrap

Now we are ready to run our script "bootstrap.rc" a second time. Actually it would be enough to run the CORRECT step but since it only takes 2 minutes we don't bother to change the script. After this, we run xscale a third time, using the same XSCALE.INP (with all its 100 INPUT_FILE= lines) as the first time. The result is

```
SUBSET OF INTENSITY DATA WITH SIGNAL/NOISE >= -3.0 AS FUNCTION OF RESOLUTION
RESOLUTION     NUMBER OF REFLECTIONS    COMPLETENESS R-FACTOR  R-FACTOR COMPARED I/SIGMA   R-meas
  LIMIT     OBSERVED  UNIQUE  POSSIBLE     OF DATA   observed  expected

   8.05          794     270       304       88.8%       4.4%      4.2%      729   23.94     5.1%
   5.69         1495     478       515       92.8%       4.6%      4.5%     1404   23.48     5.4%
   4.65         1936     598       639       93.6%       5.4%      5.3%     1827   24.31     6.3%
   4.03         2381     714       752       94.9%       4.5%      4.8%     2266   24.56     5.3%
   3.60         2536     786       841       93.5%       5.5%      5.8%     2409   23.59     6.6%
   3.29         2832     875       918       95.3%       5.5%      5.7%     2693   23.10     6.5%
   3.04         3132     916       987       92.8%       5.7%      5.9%     3014   21.78     6.7%
   2.85         3383    1014      1067       95.0%       7.1%      7.1%     3234   18.61     8.3%
   2.68         3688    1079      1126       95.8%       8.3%      8.2%     3545   16.88     9.7%
   2.55         3709    1109      1171       94.7%       9.6%      9.8%     3530   14.93    11.3%
   2.43         4037    1194      1266       94.3%      10.8%     11.5%     3855   12.86    12.7%
   2.32         4160    1217      1281       95.0%      11.7%     12.4%     3979   12.14    13.6%
   2.23         4349    1286      1354       95.0%      12.1%     12.9%     4181   11.73    14.3%
   2.15         4599    1324      1378       96.1%      13.6%     14.3%     4416   11.26    15.9%
   2.08         4726    1379      1459       94.5%      15.5%     16.6%     4548    9.98    18.1%
   2.01         4729    1419      1500       94.6%      15.6%     16.5%     4521    9.46    18.3%
   1.95         4980    1480      1544       95.9%      20.3%     20.3%     4782    8.20    23.9%
   1.90         5217    1511      1575       95.9%      22.7%     23.7%     5016    7.51    26.5%
   1.85         5232    1555      1626       95.6%      29.8%     31.0%     5015    5.91    34.9%
   1.80         5024    1511      1669       90.5%      33.5%     34.6%     4790    5.25    39.4%
  total        72939   21715     22972       94.5%       8.2%      8.5%    69754   13.36     9.7%
```

so the data are practically complete, and actually quite good. The anomalous signal suggests that it may be possible to solve the structure from its anomalous signal.

We can find out the correct spacegroup (19 !) with "pointless xdsin temp.ahkl", and adjust our script accordingly.

Now we do another round, since the completeness is so good. We can then identify those few datasets which are still not indexed in the right setting, and fix those manually. It was only xtal085 which had a problem - it turned out that the indexing had not found the correct lattice, which was fixed with STRONG_PIXEL=6.

The final XSCALE.LP is then:

```
SUBSET OF INTENSITY DATA WITH SIGNAL/NOISE >= -3.0 AS FUNCTION OF RESOLUTION
RESOLUTION     NUMBER OF REFLECTIONS    COMPLETENESS R-FACTOR  R-FACTOR COMPARED I/SIGMA   R-meas
  LIMIT     OBSERVED  UNIQUE  POSSIBLE     OF DATA   observed  expected

    8.05          804     276       316       87.3%       4.4%      4.2%      733   23.80     5.1%
    5.69         1509     481       520       92.5%       4.5%      4.4%     1416   23.61     5.2%
    4.65         1951     601       644       93.3%       4.3%      4.4%     1842   24.49     5.1%
    4.03         2402     715       755       94.7%       4.1%      4.4%     2289   24.75     4.8%
    3.60         2555     788       843       93.5%       4.0%      4.5%     2427   23.81     4.7%
    3.29         2862     877       921       95.2%       4.2%      4.7%     2724   23.35     5.0%
    3.04         3146     916       989       92.6%       5.0%      5.1%     3030   22.00     5.8%
    2.85         3399    1016      1070       95.0%       5.9%      6.1%     3251   18.75     7.0%
    2.68         3717    1081      1128       95.8%       7.2%      7.2%     3579   17.01     8.4%
    2.55         3724    1110      1174       94.5%       8.3%      8.6%     3543   15.03     9.7%
    2.43         4058    1196      1266       94.5%       9.9%     10.6%     3877   12.96    11.5%
    2.32         4190    1220      1283       95.1%      11.1%     11.8%     4013   12.21    12.9%
    2.23         4371    1288      1357       94.9%      11.5%     12.4%     4207   11.79    13.6%
    2.15         4626    1324      1378       96.1%      13.2%     13.9%     4444   11.33    15.4%
    2.08         4756    1383      1461       94.7%      15.2%     16.2%     4577   10.02    17.8%
    2.01         4755    1423      1503       94.7%      15.4%     16.1%     4543    9.51    18.1%
    1.95         4995    1480      1544       95.9%      20.1%     19.9%     4794    8.24    23.6%
    1.90         5242    1512      1577       95.9%      22.3%     23.2%     5034    7.55    26.1%
    1.85         5261    1552      1626       95.4%      29.6%     30.6%     5054    5.95    34.6%
    1.80         5066    1514      1672       90.6%      33.4%     34.4%     4829    5.25    39.2%
   total        73389   21753     23027       94.5%       7.4%      7.7%    70206   13.45     8.6%
```

When inspecting the list of R-factors of each of the datasets it becomes clear that some of them are really good, but others are mediocre.

Optimizing the result

One method to improve XDS' knowledge of geometry would be to use all 15 frames for indexing, but still only to integrate frame 1. This is easily accomplished by changing in the script:

```
JOB=XYCORR INIT COLSPOT IDXREF DEFPIX
DATA_RANGE=1 15
SPOT_RANGE=1 15
```

and to use, instead of "xds >& xds.log &" the line "../../run_xds.rc &" with the following run_xds.rc :

```
#!/bin/csh -f
xds
egrep -v 'DATA_RANGE|JOB' XDS.INP >x
echo JOB=INTEGRATE CORRECT >XDS.INP
echo DATA_RANGE=1 1 >> XDS.INP
cat x >> XDS.INP
xds
```

Furthermore it seems good to change "sleep 1" to "sleep 5" because now each COLSPOT has to look at 15 frames, not one. Thus, this takes a little bit longer. Indeed the result is a bit better:

WITH SIGNAL/NOISE >= -3.0 AS FUNCTION OF RESOLUTION

```
RESOLUTION     NUMBER OF REFLECTIONS    COMPLETENESS R-FACTOR  R-FACTOR COMPARED I/SIGMA   R-meas
  LIMIT     OBSERVED  UNIQUE  POSSIBLE     OF DATA   observed  expected

    8.05          798     274       304       90.1%       4.4%      4.2%      726   23.88      5.2%
    5.69         1514     480       515       93.2%       4.5%      4.5%     1421   23.66      5.3%
    4.65         1951     599       639       93.7%       4.3%      4.4%     1845   24.57      5.0%
    4.03         2399     713       753       94.7%       4.1%      4.5%     2289   24.76      4.8%
    3.60         2546     786       840       93.6%       3.9%      4.5%     2417   23.78      4.6%
    3.29         2864     876       919       95.3%       4.2%      4.7%     2729   23.35      4.9%
    3.04         3154     918       987       93.0%       5.0%      5.2%     3037   21.98      5.8%
    2.85         3387    1015      1066       95.2%       5.9%      6.1%     3235   18.74      7.0%
    2.68         3724    1082      1126       96.1%       7.2%      7.2%     3583   17.03      8.4%
    2.55         3720    1111      1172       94.8%       8.3%      8.6%     3536   15.02      9.7%
    2.43         4079    1198      1267       94.6%       9.8%     10.6%     3898   12.96     11.5%
    2.32         4199    1221      1283       95.2%      11.1%     11.7%     4024   12.21     12.9%
    2.23         4365    1282      1350       95.0%      11.4%     12.2%     4205   11.87     13.4%
    2.15         4651    1332      1386       96.1%      13.3%     13.9%     4468   11.30     15.5%
    2.08         4745    1380      1455       94.8%      15.0%     16.0%     4569   10.04     17.6%
    2.01         4744    1418      1496       94.8%      15.4%     16.0%     4531    9.50     18.1%
    1.95         5019    1487      1550       95.9%      19.6%     19.7%     4813    8.27     23.0%
    1.90         5210    1504      1571       95.7%      21.9%     22.9%     5007    7.53     25.6%
    1.85         5272    1561      1633       95.6%      29.1%     30.1%     5054    5.98     34.1%
    1.80         5054    1505      1659       90.7%      33.2%     34.1%     4822    5.25     38.9%
   total        73395   21742     22971       94.6%       7.3%      7.7%    70209   13.46      8.6%
```

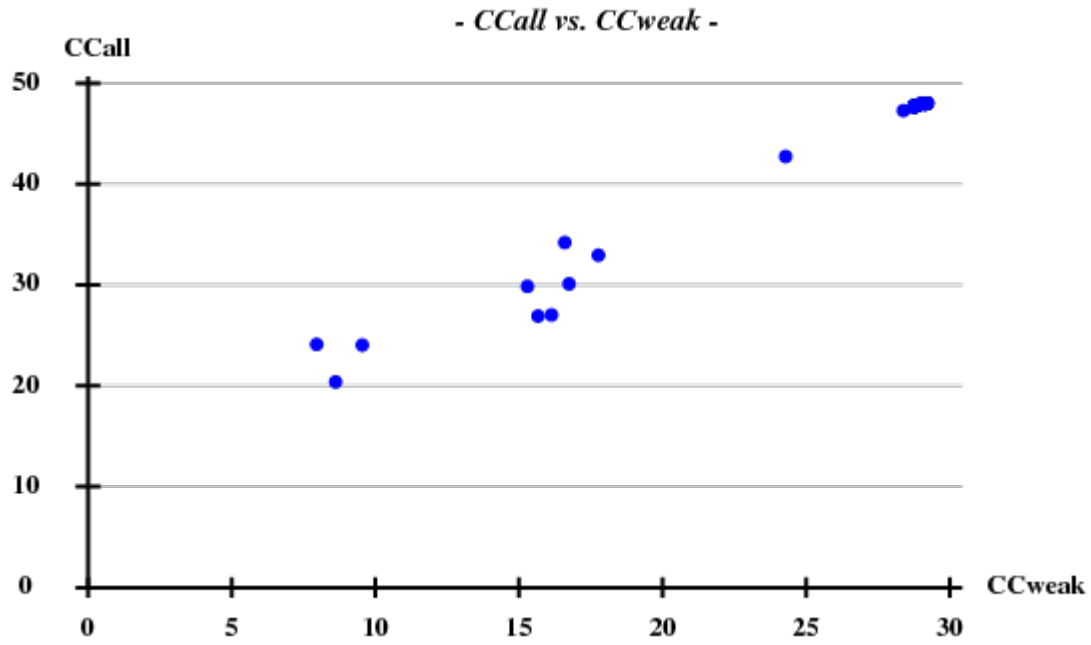
but there does not appear a "magic bullet" that would produce much better data than with the quick bootstrap approach.

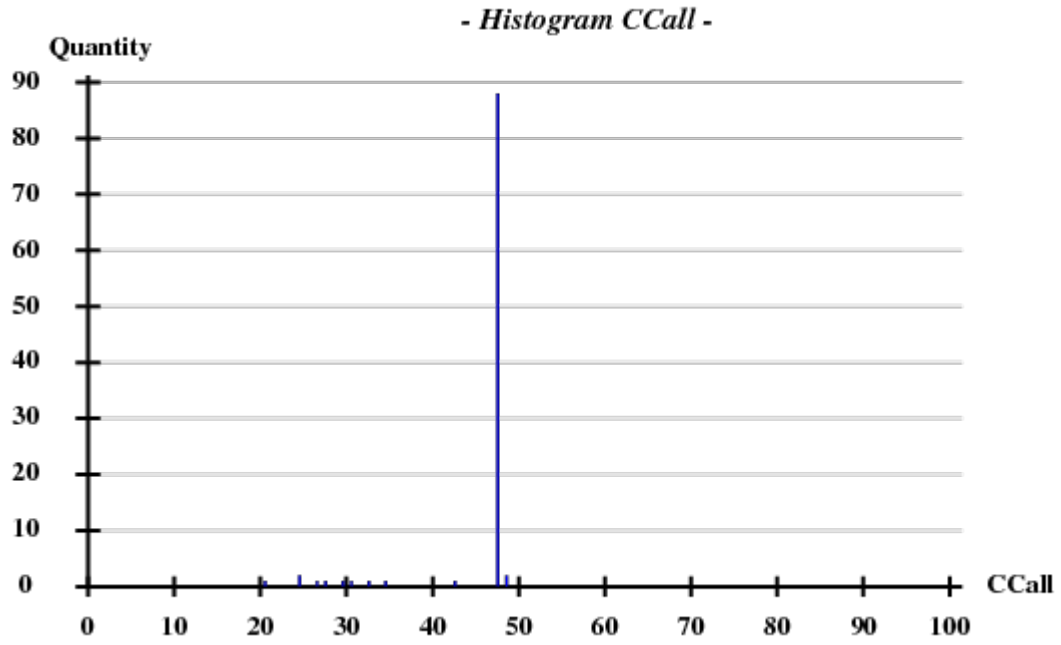
Solving the structure

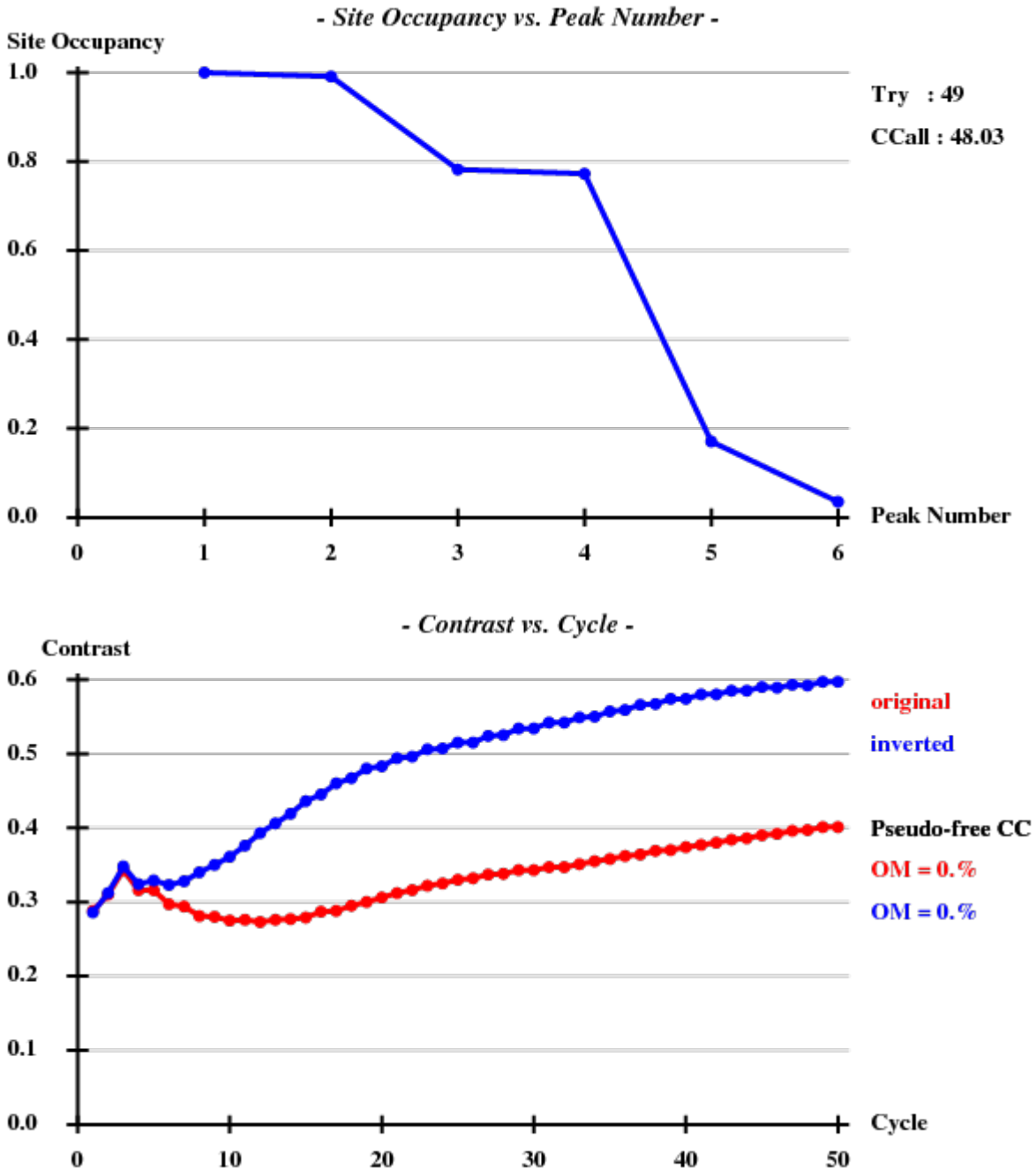
First, we repeat xscale after inserting FRIEDEL'S_LAW=FALSE into XSCALE.INP . This gives us

```
     NOTE:      Friedel pairs are treated as different reflections.

SUBSET OF INTENSITY DATA WITH SIGNAL/NOISE >= -3.0 AS FUNCTION OF RESOLUTION
RESOLUTION     NUMBER OF REFLECTIONS    COMPLETENESS R-FACTOR  R-FACTOR COMPARED I/SIGMA   R-meas
  LIMIT     OBSERVED  UNIQUE  POSSIBLE     OF DATA   observed  expected

    8.05          804     382       476       80.3%       3.1%      3.4%      665   24.13      3.9%
    5.69         1527     723       882       82.0%       3.4%      3.6%     1251   22.48      4.2%
    4.65         1956     938      1136       82.6%       3.4%      3.6%     1602   22.73      4.3%
    4.03         2400    1136      1357       83.7%       3.5%      3.6%     1943   22.62      4.4%
    3.60         2549    1261      1533       82.3%       3.4%      3.7%     2053   21.53      4.3%
    3.29         2867    1393      1694       82.2%       3.7%      3.9%     2347   21.22      4.7%
    3.04         3154    1507      1830       82.3%       4.5%      4.3%     2607   19.33      5.7%
    2.85         3389    1649      1979       83.3%       5.3%      5.2%     2761   16.37      6.7%
    2.68         3724    1757      2104       83.5%       6.5%      6.1%     3088   14.63      8.1%
    2.55         3720    1813      2197       82.5%       7.3%      7.6%     2999   12.84      9.2%
    2.43         4079    1933      2384       81.1%       9.0%      9.5%     3352   11.01     11.3%
    2.32         4199    2006      2420       82.9%      10.0%     10.5%     3474   10.17     12.7%
    2.23         4363    2099      2551       82.3%      10.6%     11.0%     3595    9.91     13.4%
    2.15         4651    2203      2634       83.6%      12.2%     12.5%     3827    9.29     15.3%
    2.08         4745    2248      2758       81.5%      14.2%     14.7%     3945    8.32     18.0%
    2.01         4744    2287      2843       80.4%      14.3%     14.6%     3896    7.92     18.1%
    1.95         5019    2429      2945       82.5%      18.5%     18.3%     4079    6.76     23.3%
    1.90         5210    2484      3000       82.8%      20.4%     21.0%     4282    6.06     25.6%
    1.85         5272    2569      3119       82.4%      27.8%     28.0%     4272    4.77     35.0%
    1.80         5054    2451      3171       77.3%      30.9%     31.1%     4092    4.20     39.0%
   total        73426   35268     43013       82.0%       6.5%      6.7%    60130   11.57      8.2%
```

One hint towards the contents of the "crystal" is that the information about the simulated data contained the strings "1g1c". This structure (spacegroup 19, cell axes 38.3, 78.6, 79.6) is available from the PDB; it contains 2 chains of 99 residues, and a chain has 2 Cys and 2 Met. Thus we assume that the simulated data may represent SeMet-SAD. Using hkl2map, we can easily find four sites with good CCall/CCweak:







I also tried the poly-Ala tracing feature of shelxe:

```
shelxe.beta -m40 -a -q -h -s0.54 -b -i -e -n 1g1c 1g1c_fa
```

but it traces only about 62 residues. The density looks somewhat reasonable, though.

The files xds-simulated-1g1c-I.mtz (ftp://turn5.biologie.uni-konstanz.de/pub/xds-datared/1g1c/xds-simulated-1g1c-I.mtz) and xds-simulated-1g1c-F.mtz (ftp://turn5.biologie.uni-konstanz.de/pub/xds-datared/1g1c/xds-simulated-1g1c-F.mtz) are available.

I refined against 1g1c.pdb:

```
phenix.refine xds-simulated-1g1c-F.mtz 1g1c.pdb refinement.input.xray_data.r_free_flags.generate=
```

The result was

```
Start R-work = 0.3453, R-free = 0.3501
Final R-work = 0.2170, R-free = 0.2596
```

which appears reasonable.