Data Processing with XDS

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Outline

1) **Introduction to XDS**

2) **Data processing** is the crucial link between your experiment and your structure

   * garbage in – garbage out!
   * for important data, do not rely on automatic data processing alone
   * manual checks are easily performed with *XDSGUI*
   * try to optimize data processing – this converts noise to signal, and may enable structure solution, and/or improve refinement
   * understand statistics (next talk)

3) **Process your data (afternoon, and during the week)**
   Tutors: Tiankun Zhou, Ralf Flaig, Clemens Vonrhein, me

The *XDS* program suite

- Original author: Wolfgang Kabsch (Max-Planck-Institute Heidelberg)
- Since ~1986
- I joined 2007

The *XDS*+ programs

- *XDS*: the main program - indexing, integrating, scaling, statistics
- *XSCALE*: scale several *XDS* intensity data sets together; zero-dose extrapolation; statistics
- *XDSCONV*: convert to MTZ / SHELX /... format (AIMLESS and CTRUNCATE are not needed!)

Programs independent from the *XDS* distribution:

- *XDS-Viewer*: inspect diagnostic images written by XDS, or (single) data frames (open source). *adxv* or *dials.image_viewer* may be used instead.
- *XDSSTAT*: additional statistics
- *XDSGUI*: graphical user interface for XDS, SHELX C/D/E, ARCIMBOLDO (open source)
- *XDSCC12*: (XDS) which frames are bad?
  (XSCALE) which data sets to re-index and merge?

Sources of information

- *XDS* main website: https://xds.mr.mpg.de ; download for Linux (WSL), Mac. complete, accurate, up-to-date documentation
- XDSwiki: http://strucbio.biologie.uni-konstanz.de/xdswiki
  Installation; data sets; documentation; download; links to e.g. Matthew J. Whitley's excellent tutorial given at CSHL 2018
- CCP4 bulletin board
- SBGrid talk (May 2020) at https://www.youtube.com/watch?v=3WU9NrILECo
- Making a difference in multi-data-set crystallography : simple and deterministic data-scaling/selection methods. Assmann, G.M., Wang, M., Diederichs, K. (2020) Acta Cryst D76, 636 (serial crystallography, *XDSCC12*)

Automatic processing with *XDS*

- beamline software (provides XDS.INP)
- scripts: *xia2* (CCP4), *autoPROC* (Globalphasing), *generate_XDS.INP* (XDSwiki), *fast_dp* (Diamond), *xdsme* (Soleil), *autoxds* (SSRL), *autoprocess* (CMCF), ...
- CCP4: *pointless, xdsconv* (type CCP4_I+F, or CCP4, or CCP4_I, or CCP4_F)
- SHELX: *shelxc* reads XDS_ASCII.HKL

Principle of *XDS* processing

- There is one JOB= line in XDS.INP which specifies a list of tasks:

JOB= XYCORR INIT COLSPOT IDXREF DEFPIX INTEGRATE CORRECT

- data reduction is divided into tasks in a **modular** way
- information storage/exchange/flow between tasks by data files which may be inspected/analyzed
- each task needs the result from the previous tasks
- fine-tuning of a task does *not* require previous tasks to be repeated
  - each task writes its output file <TASK>.LP

The tasks are ...

- XYCORR : write positional correction files (X-CORRECTIONS.cbf, Y-CORRECTIONS.cbf)
- INIT : find background pixels (defaults usually OK)
- COLSPOT: find reflection positions
- IDXREF : "index" reflections; user may supply/choose spacegroup
- XPLAN [not required] : strategy for data collection
- DEFPIX : mask shadows on detector (use *XDSGUI*!)
- INTEGRATE : evaluates intensities on all frames, writes INTEGRATE.HKL and FRAME.cbf
- CORRECT : scales, rejects outliers, statistics, writes scaled, unmerged XDS_ASCII.HKL (and other files)

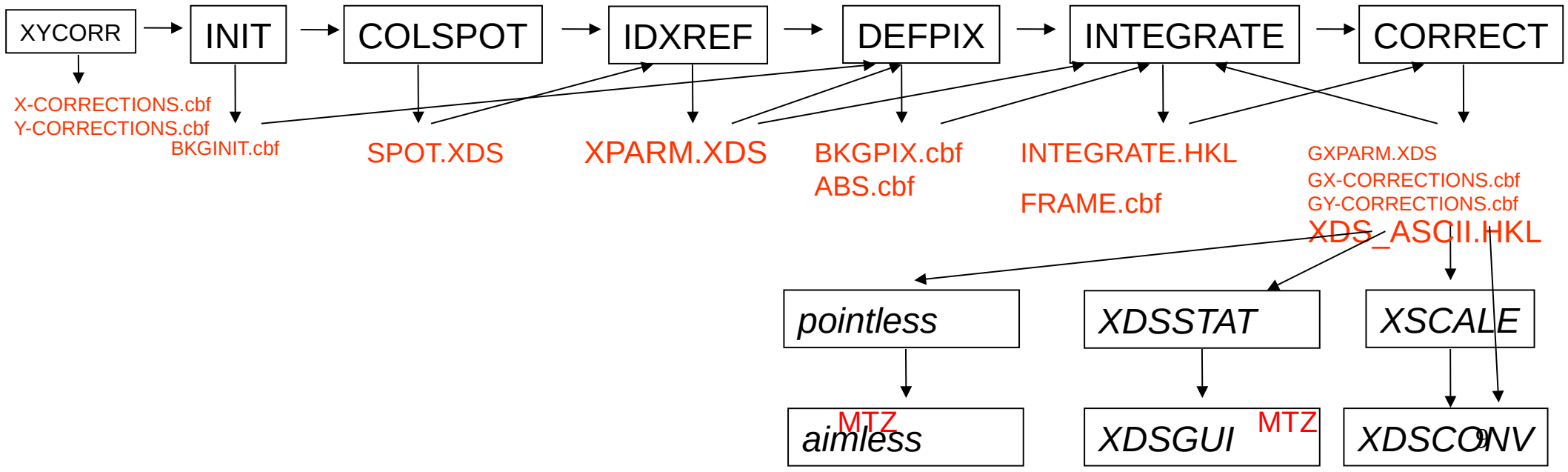
Information flow

NAME_TEMPLATE_OF_DATA_FRAMES
DETECTOR

OSCILLATION_RANGE
SEPMIN
STRONG_PIXEL

ORGX
ORGY
DETECTOR_DISTANCE
X_RAY_WAVELENGTH
SPACE_GROUP_NUMBER

DATA_RANGE



Example XDS.INP

```
JOB= XYCORR INIT COLSPOT IDXREF DEFPIX INTEGRATE CORRECT
ORGX=1546 ORGY=1552        !Detector origin (pixels); e.g. NX/2 NY/2
DETECTOR_DISTANCE=180      !(mm)
OSCILLATION_RANGE=0.50     !degrees (>0)
X-RAY_WAVELENGTH=0.980243 !Angstroem
NAME_TEMPLATE_OF_DATA_FRAMES=frms/wga2-27_1_???.img
DATA_RANGE=1 360           !Numbers of first and last data image collected
BACKGROUND_RANGE=1 10      !Numbers of first and last data image for background
SPACE_GROUP_NUMBER=  19    !0 for unknown crystals; cell constants are ignored.
UNIT_CELL_CONSTANTS= 44.4   86.4   104.5  90 90  90  ! not required if spgr=0
REFINE(IDXREF)=BEAM AXIS ORIENTATION CELL DISTANCE
REFINE(INTEGRATE)=DISTANCE BEAM ORIENTATION CELL ! AXIS
ROTATION_AXIS= 1.0 0.0 0.0
INCIDENT_BEAM_DIRECTION=0.0 0.0 1.0
FRACTION_OF_POLARIZATION=0.99                    ! SLS X06SA
POLARIZATION_PLANE_NORMAL= 0.0 1.0 0.0
DETECTOR=CCDCHESS        MINIMUM_VALID_PIXEL_VALUE=1     OVERLOAD=65000
DIRECTION_OF_DETECTOR_X-AXIS= 1.0 0.0 0.0
DIRECTION_OF_DETECTOR_Y-AXIS= 0.0 1.0 0.0
VALUE_RANGE_FOR_TRUSTED_DETECTOR_PIXELS= 7000 30000 !Used by DEFPIX
                                !for excluding shaded parts of the detector.
INCLUDE_RESOLUTION_RANGE=50.0 1.3 !Angstroem; used by DEFPIX,INTEGRATE,CORRECT
```

Bold keyword/parameter pairs are required. Complete documentation at xds.mr.mpg.de/html_doc/xds_parameters.html

Example XSCALE.INP

```
!============ EXAMPLE 3: specific reindexing of input data sets
!
!      Use of specific reindexing of input data sets for resolving
!      indexing ambiguities in the scaled output data set. This
!      happens if the crystal's space group symmetry is lower than
!      its lattice symmetry.
!
RESOLUTION_SHELLS= 100 10 6 4 3 2 1.9
SPACE_GROUP_NUMBER=78
UNIT_CELL_CONSTANTS=57.39 57.39 106.9   90 90 90
OUTPUT_FILE=scaf8_all_merged.hkl
MERGE=TRUE FRIEDEL'S_LAW=FALSE
STRICT_ABSORPTION_CORRECTION=TRUE
INPUT_FILE= ../xds-1_2/XDS_ASCII.HKL
REIDX_ISET= -1  0  0  0  0  1  0  0  0  0 -1  0
INPUT_FILE= ../xds-2_1/XDS_ASCII.HKL
INPUT_FILE= ../xds-3_1/XDS_ASCII.HKL
INPUT_FILE= ../xds-1_4/XDS_ASCII.HKL
INPUT_FILE=*../xds-5_1/XDS_ASCII.HKL
```

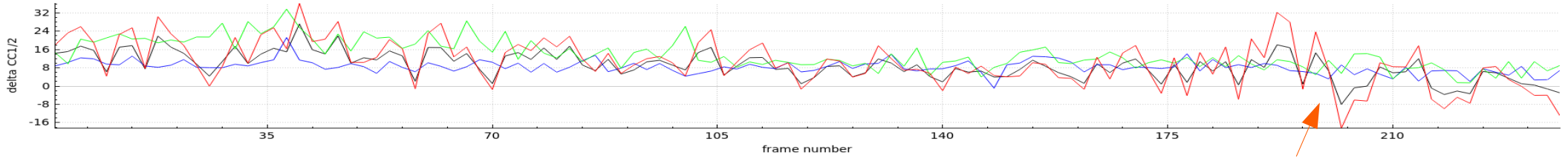
Bold keyword/parameter pairs are required. Complete documentation at xds.mr.mpg.de/html_doc/xscale_parameters.html

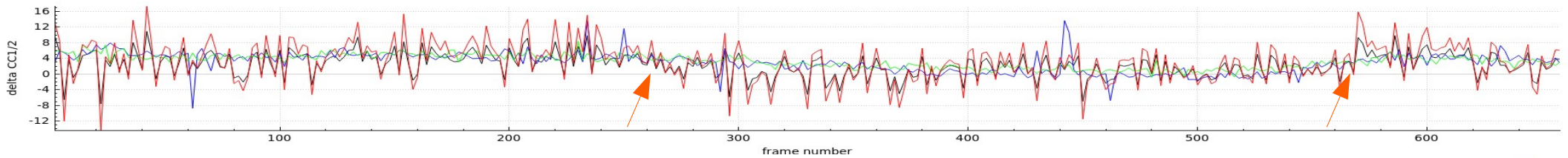
Example XDSCONV.INP

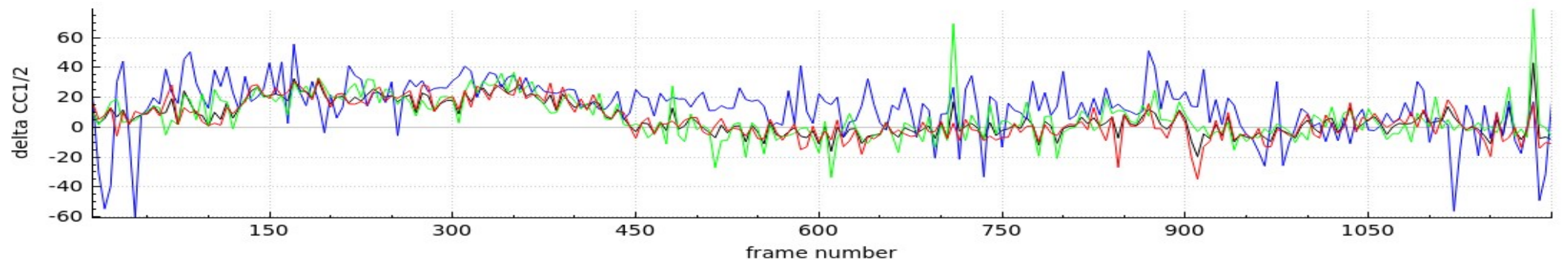
```
! UNIT_CELL_CONSTANTS= 10 20 30 90 90 90
! SPACE_GROUP_NUMBER= 96
! GENERATE_FRACTION_OF_TEST_REFLECTIONS=0.05

INPUT_FILE=XDS_ASCII.HKL
OUTPUT_FILE=temp.hkl CCP4_I+F ! or CCP4_I or CCP4_F or SHELX or CNS
FRIEDEL'S_LAW=FALSE ! store anomalous signal in output file even if weak
```

Bold keyword/parameter pairs are required. Complete documentation at xds.mr.mpg.de/html_doc/xdsconv_parameters.html

XDSCC12: calculates $\Delta CC_{1/2,i} = CC_{1/2,with\_i} - CC_{1/2,without\_i}$







Examples of single data sets (plots from *XDSGUI*)

three resolution ranges (blue=low green=medium red=high) - i refers to batches of width 1°

- find bad frame ranges
- radiation damage

XDSCC12 for selection of data sets for *XSCALE*

For important data, do not rely on automatic data processing

There are no clear-cut criteria for the quality of data set ("Table 1" is almost useless).

Synchrotrons typically run multiple pipelines, and the user has to choose …

What can go wrong in automatic data processing?

- does not handle radiation damage (discard frames towards the end of the data set)
- does not handle shadowed areas of detector
- does not handle indexing problems (multiple lattices, ice, …) flexibly
- does not optimize processing

Automatic processing with GlobalPhasing's *autoPROC* (and *xia2* for DLS data) is rather reliable for good data sets! But difficult data sets typically benefit from human insight.

Manual processing with *XDSGUI*

- problems in phasing and refinement
  often due to bad / wrong data processing
- visually inspect frames; mask shadows
- optimize parameters, frame range,
  resolution cutoff ..
- presents tables as plots
- interfaces to *XDS* through its files, e.g. XDS.INP
- user – extensible / modifiable commands

Manual checks are easily performed with *XDSGUI*

- before running *XDS*: check frames (*adxv*, *Albula*, *XDSGUI* ...)
- **Frame** tab: FRAME.cbf for match obs/calc, and masked areas
- **IDXREF** tab: for ice rings / indexed *vs* un-indexed reflections
- look at indexing in reciprocal space: **tools** tab/Further analyses/spot2pdb-coot command; see XDSwiki:XDSGUI#tools
- **statistics** tab: *XDSCC12* and *XDSSTAT*

Optimize data processing

- XDSwiki:Optimisation#Re-INTEGRATEing_with_the_correct_spacegroup.2C_refined_geometry_and_fine-slicing_of_profiles

  XDSwiki:Optimisation#using_the_refined_values_for_beam_divergence_and_mosaicity_for_re-integration

- **tools** tab: “Saving and comparing good results” and “Optimizing data quality”. After changing parameters, run “JOB=DEFPIX INTEGRATE CORRECT”, compare and save if better/restore old if worse.

- consider use of *StarAniso* if anisotropy

  … may make the difference between interpretable and non-interpretable map, substructure solution, …

Thank you!