XDS processing workflow. The links given like e.g. XDSGUI#Frame refer to the XDSwiki at https://wiki.uni-konstanz.de/xds/index.php/	**The programs must have been properly installed - see Installation. Troubleshooting hints are at Problems.**
Action	**why? what to look out for? what else to know?**
1. Set up environment. Open a terminal and position it on the left side of your screen. If you work with HDF5 data: `export NEGGIA_PATH= /usr/local/lib64/dectris-neggia.so`. For HDF5 data from Diamond, use `export DURIN_PATH= /usr/local/lib64/durin-plugin.so` instead (the path must match YOUR computer; the path given is just a typical one). Type `xdsgui` and move its window so that you still see the left half of the terminal window.	Keeping the terminal window to the left of the XDSGUI window makes it possible to see e.g. error messages from XDSGUI, or the `pointless` output. The path to the HDF5 library must appear in "Generic frame library" under `xdsgui / Preferences ../ Paths` on macOS, or `Menu / Settings / Paths` on Linux, and should appear after LIB= in `XDS.INP` (below). Optional: before typing `xdsgui` ,cd to an existing XDS directory, or create a new (empty) directory:`cd <toplevel-directory>; mkdir <xds-directory>; cd <xds-directory>`
2. Choose or create XDS project. Go to the `Projects` tab and either 1) choose an existing entry (if there is a list of previous projects), or 2) browse to an existing XDS directory, or 3) create a new (empty) directory	If XDS files exist in the XDS directory, they appear in the XDSGUI tabs. Note that the XDS directory name appears in the title bar of the XDSGUI window!
3. Load frame & set parameters. Go to the `Frame` tab and load a frame of your dataset (for HDF5, load `xxx_master.h5`). Click `generate XDS.INP` - this reads the header of that frame, and counts the frames of the dataset. Use `Zoom`, `Contrast` and `Brightness` and move around the frame to evaluate the shape and separation of the reflections: are they smeared or sharp, tiny or broad, regular or broken, symmetric or asymmetric? Look at other frames (selector is at upper right of window) as well!	Watch the green crosshair at ORGX ORGY, the green circle around it (lower INCLUDE_RESOLUTION_RANGE), the red UNTRUSTED_RECTANGLEs at the module borders, and the blue TRUSTED_REGION appear. The corresponding keyword=parameter lines in `XDS.INP` have the same colour code.
4. Define untrusted detector areas. Mask the shaded regions of the detector: at least the beamstop and its holder. There is a button `Untrusted areas (...)` towards the upper right with three tools: UNTRUSTED_ELLIPSE, UNTRUSTED_RECTANGLE, UNTRUSTED_QUADRILATERAL	This step is important, do not forget it! Reason is in the XDSGUI paper (reference below). More explanation of the tools is at XDSGUI#Frame . Unwanted UNTRUSTED_* areas can be removed by deleting their lines in `XDS.INP` .
5. Review and adjust XDS.INP. Go to the `XDS.INP` tab and inspect it. For a first XDS run, accept defaults, except increase MINIMUM_NUMBER_OF_PIXELS_IN_A_SPOT to 6 (rather than 3) for broad reflections with many pixels, i. In later runs, tweak parameters to optimize processing. JOB=XYCORR INIT COLSPOT IDXREF DEFPIX INTEGRATE CORRECT is only needed at the beginning i.e. for the first run.	The paradigm of manual processing is to repeat INTEGRATE and CORRECT with optimised parameters that are available after a completed XDS run. Note that geometry parameters used by INTEGRATE are in `XPARM.XDS`, not in `XDS.INP` !
6. Run XDS and handle errors. After changing `XDS.INP`, click `Save` (unless greyed out) and `Run XDS` . The tasks of the JOB keyword are run one after the other. Thus watch the adjacent tabs to the right flash yellow as they are being filled with text and graphics. Inspect the left (text) and right (graphics) sides of these tabs. Once the CORRECT tab is filled, the XDS run has completed, and the reflection file XDS_ASCII.HKL is available. The goal is to make sure that spacegroup and resolution are correct or at least reasonable, and that the processing is optimal.	If XDS stops after the IDXREF step (with ERROR in IDXREF.LP), this most often happens because it could index less than 50% of the spots only. This may be due to ice rings that obviously cannot be indexed, or due to additional lattices. In most cases, this should at least prompt you to think about the possible reasons. To continue, set JOB=DEFPIX INTEGRATE CORRECT in XDS.INP, `Save` and `Run XDS`.
7. First run of XDS: inspect and analyse diffraction. COLSPOT tab: is the "number of spots" evenly distributed among the frames? If not, it may be a sign of radiation damage or anisotropy, or plate-shaped crystal. Maybe see COLSPOT (https://wiki.uni-konstanz.de/xds/index.php?search=COLSPOT&title=Special%3ASearch&fulltext=1) . IDXREF tab: does the plot of spots appear elliptical - that would indicate anisotropy? Inspect the `predictions` in `Frame` . Do they match the observed reflections? *Visualize reflections in reciprocal space* : in `tools` go to `Further analyses` and click the second button from the top. This will load the indexed reflections (yellow) and non-indexed ones (pink) as pseudo-PDB files into `Coot`. Inspect the lattices: is the "yellow lattice" convincing, and/or do the pink reflections form their own lattice(s), or are they just random?	IDXREF tab: are the "CLUSTER INDICES" of the difference vectors integer numbers, or close to integers? Are the cell parameters reasonable? Is the first POPULATION of the first SUBTREE close to 3000? Ice rings? See IDXREF.LP and IDXREF. INTEGRATE tab: are the curves smooth (good) or are there jumps (bad)? Try to think of reasons for jumps/spikes! Could it be the beamline flux or the crystal changing? Are their straight red and green lines all along the "Beam divergence" and "Mosaicity" plots? If not, too few strong reflections were found (inspect the "THREE-DIMENSIONAL PROFILE" output in the text part) and you should add DELPHI=20 in `XDS.INP`, or increase the parameter if the keyword already exists.

8. Inspect scaling & statistics. In the CORRECT tab: Numerical values and plots are only meaningful if the spacegroup is correct (screw axes don't matter for the statistics, though). If the spacegroup is unknown, the text part reports the spacegroup that XDS determines automatically. To benefit from a more advanced (but not infallible) algorithm, in `tools / Further analyses` use `determine spacegroups with pointless`. Output is in the terminal window! Modify the SPACE_GROUP_NUMBER and UNIT_CELL_CONSTANTS in `XDS.INP` accordingly (unless you know better, of course). Often there are two enantiomorphic spacegroups possible (table), or a subgroup is correct; keep that in mind for the structure solution - the correct spacegroup is only confirmed when the structure is solved and well refined.	The first look should go to the the first plot (I/sigma unmerged data). The red horizontal line is ISa - what is its value? The exact numerical value is in the text part, but the plot is enough for a good estimate. If the value is less than 5, something (likely indexing or spacegroup) is severely wrong. Good values are 20 and higher. The blue line should be well below the red line, otherwise this is a sign of overexposure - in that case, the systematic error limits the quality of the data, not the random error.
9. Spacegroup and resolution cutoff. If the spacegroup that CORRECT determined differs from the one that pointless determined: in `XDS.INP`, fix SPACE_GROUP_NUMBER and UNIT_CELL_CONSTANTS, change the JOB=... line to JOB=CORRECT, and `Run XDS`. If the spacegroup is correct, decide about the high-resolution cutoff: go to the section after STATISTICS OF SAVED DATA SET "XDS_ASCII.HKL" and inspect the table SUBSET OF INTENSITY DATA WITH SIGNAL/NOISE >= -3.0 . A useful estimate of the high-resolution limit is the last resolution range that still gets a star "*" in the $CC_{1/2}$ column; you may also consider the <I/sigma> column. Put the upper resolution value into the INCLUDE_RESOLUTION_RANGE line in `XDS.INP`, and set JOB=CORRECT. Go to step 6.	Use FRIEDEL'_LAW=FALSE if the anomalous signal is so strong that you want to see the proper statistics (completeness ...). Use FRIEDEL'S_LAW= TRUE if scaling and merging statistics should not take the anomalous signal into account. Low resolution anomalous correlation above 60% is what I consider strong. Modify `XDS.INP` accordingly.
10. Optimize by iterative comparison. Second and further runs of XDS typically refine the upper resolution limit and optimize the geometric parameters. It is useful to compare, after each modification, the resulting CORRECT.LP with the best one previously available. This is achieved by items in `tools / Saving and comparing good results` and `tools / Optimizing data quality`	Thus, re-run INTEGRATE CORRECT or just CORRECT as needed (step 6). See Optimisation, XDSGUI#How to use XDSGUI
11. Statistics tab. The XDSCC12 and XDSSTAT programs give you additional statistics for the frames of the DATA_RANGE.	Look out for radiation damage. Bad frames have negative delta-$CC_{1/2}$.
12. **Creating MTZ file.** Use the XDSCONV tab. Un-comment GENERATE_FRACTION_OF_TEST_REFLECTIONS=0.05 if you intend to use the MTZ file for refinement.	FRIEDEL'S_LAW=FALSE is good even if little anomalous signal (FRIEDEL'S_LAW= TRUE in `XDS.INP`) since you may see metals or sulphur atoms in anomalous map.

The XDSGUI paper (Brehm, Triviño, Krahn, Usón and Diederichs (2023) XDSGUI: a graphical user interface for XDS, SHELX and ARCIMBOLDO. J. Appl. Cryst. 56) is open access at https://doi.org/10.1107/S1600576723007057 .
