Our Experiences with the Data Reduction Program XDS

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Let me tell you about our experiences with the data reduction program XDS as an alternative to the more widely used software packages. It is run by a script that is detector-specific and there are examples on Wolfgang Kabsch's web site: http://www.mpimf-heidelberg.mpg.de/~kabsch/xds/. We find it to be flexible and easy to use, which allows more experimenting with the raw X-ray data to achieve the best datasets.

Pick the appropriate script from the web site, paste it into an editor, and change a few lines in the script for your particular diffraction experiment: size of detector, wavelength, detector distance, and location/numbers/width of frames. We view the frames with Xdisplay to check the diffraction quality and to be sure that all the experimental parameters are correct. We often look at an .x file also, because they will have been brought back to the lab with the frames from the synchrotron. The .x files have parameters that were entered by the experimenter at the beamline and may be more correct than later estimates. We edit the XDS.INP script and then run XDS.

1. XDS makes a first pass through the data reading each frame and collecting strong pixels for autoindexing from the frames that the user specifies. We often allow it to "pick peaks" from all of the frames. This results in robust autoindexing.
2. XDS makes the second pass through the data reading each frame again, integrating, and profile fitting. If the space group is not specified, XDS integrates in P1 automatically. After autoindexing in P1, XDS writes a file with 44 possibilities with distortion values for the combination of lattice and cell constants. It includes the matrix for each of the 44 possibilities that can be used to reindex the P1 data. This is done by a simple edit of the XDS.INP file enabling one to quickly test the various symmetries of the new data set.
3. XDS automatically decompresses (.Z, .gz, etc) frames on the fly, so that frames can stay on the disk compressed if desired.
4. XDS automatically scales the data immediately after integrating and writes one file with all the reflections and one file, CORRECT.LP, with all the stats about the integration. Here the data is already scaled preliminarily and tables of redundancy, Rsym, Isig, and anomalous signal and correlations are ready to be digested by the user.
5. There is extensive documentation on the web site where each line in the script is defined and suggestions are given. The several modules that are called by XDS are described. Each module writes its results to a file that the next module uses as input. As various ideas come up, the whole integration does not need to be run again, just the modules that pertain to the new experiment. New versions of XDS are released on the web site several times a year.
6. The scaling program in the package, XSCALE, has a radiation damage correction algorithm that can work well in high symmetry space groups.
7. The program, XDSCONV, in the package converts integrated XDS data to an mtz file with Is or Fs, to CNS format, or to SHELX format for XPREP.

In one project, we had datasets from a crystal that seemed to be orthorhombic, but that we could not solve even with an excellent molecular replacement model. The low resolution Rsym values were about 5%, which seemed too high for the quality of diffraction. How to test if the data were monoclinic with a beta angle of 90? We integrated the data in P1 with XDS and used the matrices for each of the three monoclinic possibilities. The tables in CORRECT.LP were unambiguous in pointing to the monoclinic cell with a much lower Rsym than the orthorhombic and the two wrong monoclinic possibilities. This was quickly done.

We have found over the course of many projects and datasets that we sometimes achieve usable data to a higher resolution with XDS, than with other data reduction packages. This may be our own limitations in the operation of the other packages, but higher resolution is what we obtain.

There is a wiki at http://strucbio.biologie.uni-konstanz.de/xdswiki/index.php/XDS started by Kay Diederichs. There is a viewing program, VIEW, but we have found it to be less useful for judging diffraction quality than the viewing program associated with the HKL2000 package. We do use VIEW to examine the beam stop shadow. XDS does a decent job of blanking the beam stop automatically, but it usually needs some help to get the mask completely over the beam center.