

## Migrating the fast\_dp software package for Python 2 and 3 compatibility

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A great deal of existing crystallographic software in CCP4 and other packages has been successfully managed in a Python 2.7 environment for many years. Python 3 is significantly different from Python 2.7, which will soon no longer be maintained. That is why it is crucial to migrate MX software to Python 3. Fortunately, it is possible to write or upgrade Python code so that it can automatically detect the Python version within which it is being run and execute correctly in either environment. One very useful Python package for MX data processing is fast\_dp [1], which originated at Diamond Light Source and is used at many facilities for very rapid processing with XDS [2], Pointless [3] and Aimless [4]. We are converting the version of fast\_dp used at the AMX and FMX MX beamlines at NSLS-II to be able to function automatically in both Python 2.7 and Python 3 environments. This is an essential preliminary step in upgrading the processing pipelines, especially merging and serial crystallography pipelines such as Blend [2] and Kamo [3] to survive a Python 3 transition. We present examples of both the code conversion used and of applications to sample data.

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[1] Winter, G., McAuley, K.E., 2011. Automated data collection for macromolecular crystallography. *Methods in Structural Proteomics*, 55(1), pp. 81 – 93.

[2] Kabsch, W., 2010. XDS. *Acta Cryst.* D66(2), pp. 125 – 132.

[3] Evans, P.R., 2011. An introduction to data reduction: space-group determination, scaling and intensity statistics. *Acta Cryst.* D67(4), pp. 282 – 292.

[4] Evans, P.R., Murshudov, G.N., 2013. How good are my data and what is the resolution?. *Acta Cryst.* D69(7), pp. 1204 – 1214.

[5] Foadi, J., Aller, P., Alguel, Y., Cameron, A., Axford, D., Owen, R.L., Armour, W., Waterman, D.G., Iwata, S., Evans, G., 2013. Clustering procedures for the optimal selection of data sets from multiple crystals in macromolecular crystallography. *Acta Cryst.* D69(8), pp.1617 – 1632.

[6] Bernstein, H.J., Andrews, L.C., Foadi, J., Fuchs, M.R., Jakoncic, J., McSweeney, S., Schneider, D.K., Shi, W., Skinner, J., Soares, A., Yamada, Y., 2017. Serial Crystallography with Multi-stage Merging of 1000's of Images. *BioRxiv*, p.141770.