Poster

Work with serial crystallography data from CrystFEL and xia2.ssx in CCP4 suite

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The development of X-ray radiation sources, mainly the availability of the X-ray free electron lasers and the 4th generation synchrotrons, leads to increased interest in serial macromolecular crystallography. This method facilitates *e.g.* time-resolved studies, collection of data not affected by radiation damage, and pump and probe experiments, all at physiologically relevant room temperature. These novel approaches create new challenges for sample preparation, diffraction experiment setup and also *data processing and handling* which has triggered recent developments in the *CCP*4 suite [1].

A new *import_serial* task (Fig. 1) simplifies the import of merged data processed in *CrystFEL* [2] from its HKL text format to an MTZ format used in *CCP*4 [1]. The program adds required information about crystal symmetry, unit cell parameters and source wavelength to an output MTZ file. Moreover, data quality statistics are calculated and reported, including $CC_{1/2}$, R_{split} and multiplicity. The tool is available in the command line as well as a graphical interface in *CCP4i2* [1]. A merged MTZ data file from *xia2.ssx* [3] can be imported as well. Recently, a user case application of this program was published [4]. The code is available within *CCP*4 or stand-alone from a repository at *https://github.com/MartinMalyMM/import_serial* .

Support for *xia2.ssx* data processing pipeline [3] was also improved. Indexing and integration of reflections in serial crystallography are usually performed in computational clusters due to very demanding calculations. Nevertheless, subsequent scaling and merging can be done using a usual computer. For this purpose, a graphical interface for *xia2.ssx_reduce* has been implemented in *CCP4i2* to provide a user-friendly experience while tuning processing parameters.

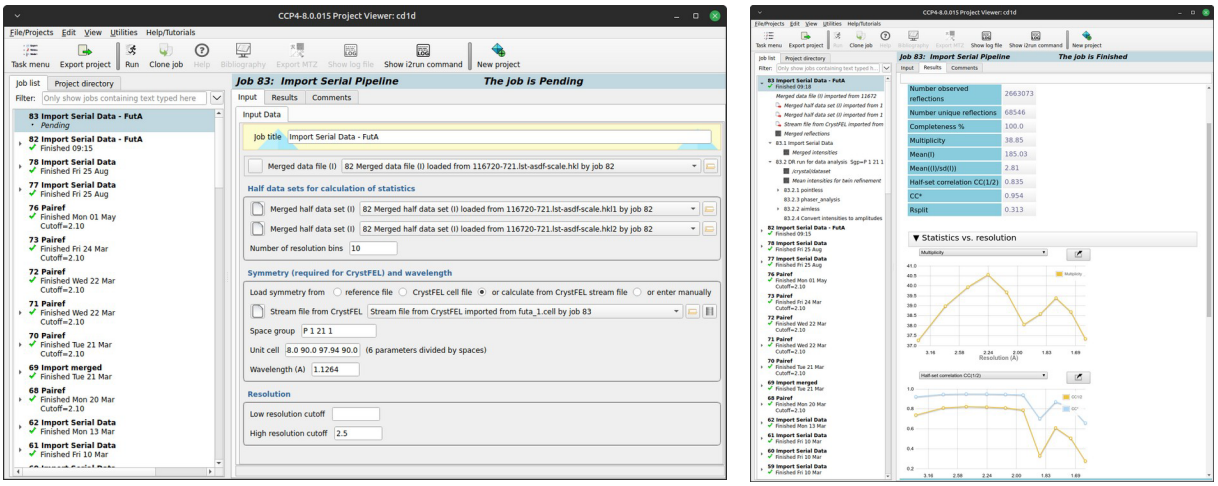

Figure 1. Graphical interface for the *import serial* data task in *CCP4I2* [1].

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[4] Stubbs, J., Hornsey, T., Hanrahan, N., Esteban, L. B., Bolton, R., Malý, M., Basu, S., Orlans, J., de Sanctis, D., Shim, J. U., Shaw Stewart, P. D., Orville, A. M., Tews, I. & West, J. (2024). *IUCrJ*, **11**, 237-248.

This work was funded by CCP4 & the Science and Technology Facilities Council (Collaboration Agreement Number CN8680) – project 521862101 "Serial Data Processing and Analysis in CCP4i2" at the University of Southampton (Martin Malý, Ivo Tews) and project R22512 "Development of the CCP4MG suite and CCP4i2" at the University of York (Stuart McNicholas).