Automation : Latest Developments and Future Prospects at the ESRF MX Beam-lines

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The production of three-dimensional crystallographic structural information of macromolecules can now be thought of as a pipeline which is being streamlined at every stage from protein cloning, expression and purification**,** through crystallisation to data collection and structure solution. Synchrotron X-ray beam-lines are a key section of this pipeline as they are where the X-ray diffraction data that ultimately leads to the elucidation of macromolecular structures are collected. The throughput of macromolecular crystallography (MX) beam-lines may be enhanced significantly with the automation of both their operation and of the experiments carried out on them. The automation of SRMX facilities can be split neatly into two different aspects: those which the user sees and feels directly and those hidden from view but which benefit both users and beamline staff.

Protocols and software for the automatic alignment of the optical elements of a SRMX facility are essential to ensure its smooth and efficient operation. Automatic beamline alignment (ABA) procedures to achieve this and a historical database that allows monitoring and correction of the optical element positions have been developed and will lead to a more reliable and user-friendly provision of an X-ray beam with the necessary characteristics for the experiment planned.

Sample identification, tracking and the handling of sample information known before an experiment commences will allow characterisation of each sample held in a sample changer (including the determination of unit cell dimensions, Laue Group, orientation matrix and data collection strategy), scoring and ranking of these samples and the collection and processing of diffraction data. Sample changer robots developed by the EMBL Grenoble Outstation and the ESRF hold up to 50 frozen samples and will be installed on all ESRF MX beam-lines by the end of 2005. The DNA software for automatic crystal characterisation, determination of optimal data collection parameters and the processing of diffraction data is already available on all MX beam-lines. Additionally all of the MX MAD beam-lines are already equipped with software for the automatic scanning of absorption edges. The beam-line experiment database (PXWeb/ISpyB) allows the submission and tracking of sample information and the exchange of data between the ESRF and the user home laboratory. Extensive tests of this data exchange pipeline are currently ongoing. The sample changer robots are compatible with the mini- and micro-diffractometers which have now been installed on nearly all the MX beam-lines (ID14-2,-3,-4, ID23-1, ID29). These diffractometers incorporate on-beam-axis visualisation of the sample, a high-precision air-bearing phi spindle and automatic sample centring and sample-to-beam alignment capabilities. A motorised mini-kappa system is under development as an add-on for the diffractometer. The current status of all of these recent developments will be discussed.