[MS21-02] Automated Processing of Datasets Obtained from Multiple Crystals

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A fundamental limitation of conventional macromolecular crystallography is the necessity of obtaining one or more crystals of sufficient size and quality to record a complete dataset. Frequently, particularly in the case of viruses and membrane proteins, only small, poor-quality crystals may be available.

Whilst the merging of partial datasets from multiple crystals to obtain a single complete dataset is not a recent concept [1, 2], with the advent of microfocus synchrotron beamlines such as I24 at Diamond Light Source, which can be used to collect data from crystals with dimensions smaller than 10 μm [3], it is becoming increasingly common to merge together datasets collected from many tens or hundreds of crystals [4, 5] in order to obtain a single complete dataset. Furthermore, Liu and co-workers have shown that merging data from multiple crystals can enhance weak anomalous signals giving improved results in SAD and MAD phasing [6].

Although there have been attempts to automate some aspects of the processing of multi-crystal datasets (xia2 [7] and BLEND [8]), processing of such data currently requires a significant amount of manual intervention to obtain the best results, particularly in more challenging cases. For example, it may only be possible to collect a highly incomplete dataset over a small oscillation range for each individual crystal before the diffraction quality is affected by radiation damage. Automatically processing such datasets can be challenging using existing software pipelines, particularly when faced with nonisomorphous crystals and severe radiation damage. Devising suitable procedures, and improving existing methods where necessary, is essential for making the collection and processing of multi-crystal datasets more routine.

Here we discuss in more detail some of the issues encountered when processing datasets from multiple crystals, and propose potential improvements to current procedures.

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