Poster Presentation

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A pipeline for the rapid generation of difference maps from protein crystals

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In 2013 MX beamlines at the Diamond synchrotron deployed an automated software pipeline, called DIMPLE, for rapid processing of crystals that contain a known protein and possibly a ligand bound. DIMPLE takes the already known "apo" structure for the target protein, compares it with the electron density map from X-ray diffraction images, and visualizes areas of the electron density unaccounted for by the structure model. When processing batches of crystals, such feedback allows the user to better decide what to measure next which leads to a more efficient use of the beam time. This year we've enhanced the pipeline to cover more complex cases, including changes in the space group and some changes in conformation. With multiple molecular replacement computations run in parallel, the time from shooting to viewing the difference map is still only a few minutes. While the software is developed primarily for use at synchrotron beamlines, it is included in the CCP4 suite and can be used as well for in-house automation.

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