MS4-P3 Latest developments in HKL2MAP 0.4

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HKL2MAP [1] is a graphical user interface (GUI) for the semi-automatic operation of the command-line-driven programs SHELXC/D/E [2]. These programs in combination with the GUI are widely used for macromolecular crystallographic phasing, not the least due to their runtime speed, and suited for on-the-fly assessment of diffraction data at synchrotron sources.

HKL2MAP allows for the selection of input files with diffraction data in various formats and automatically extracts unit cell parameters and space group for FA data preparation with SHELXC. Most importantly, it now supports input commands and result visualization regarding the latest SHELXC feature for multi-crystal SAD, where several data sets, also partial ones, can be merged for a maximization of multiplicity. Concerning substructure determination, HKL2MAP works with the multi-CPU version of SHELXD, where the achieved speed benefit is relevant for difficult cases that require a large number of solution trials. The program SHELXE for phase calculation and density modification (DM) underwent significant feature extensions during the last years, most prominently substructure site refinement for optimization of initial heavy-atom phases and peptide backbone auto-tracing for the iterative improvement of the DM steps. HKL2MAP renders the numerical SHELXE results graphically and thus facilitates the monitoring of phase quality. The line graphs for sequential progress visualization are now complemented by 3d ribbon graphs for the SHELXE poly-ala models. This automatically updated 3d view with continuous mouse rotation and zoom provides further information on phasing success by supporting the discrimination of map interpretability with respect to the two enantiomorph substructures. Furthermore, HKL2MAP employs COOT [3] as the graphical display program, so that the final poly-ala model and electron density map can be readily inspected post phasing.

The usage of HKL2MAP is demonstrated by means of practical examples, with a focus on multi-crystal SAD phasing scenarios. HKL2MAP is freely available for academic usage and can be downloaded from http://webapps.embl-hamburg.de.

References:

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Keywords: MX-Phasing, GUI, SHELXC/D/E

MS4-P4 Direct phase selection of initial phases from single-wavelength anomalous dispersion (SAD) for the improvement of electron density and *ab initio* structure determination

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The optimization of the initial phasing has been a decisive factor in the success of the subsequent electron density modification, model building and structure determination of biological macromolecules with the single-wavelength anomalous dispersion (SAD) method. Two possible phase solutions (Φ_1 and Φ_2) generated from two symmetric phase triangles in the Harker construction for the SAD method cause the well-known phase ambiguity. We have developed a novel *Direct phase selection method* utilizing the θ_{DS} list as a criterion to select optimized phases from Φ_1 or Φ_2 of a subset of reflections with the high *percentage of correct* phases to replace the corresponding initial SAD phases Φ_{SAD} [1]. Based on our work, the reflections with angle θ_{DS} in a range 35 – 145° are selected for an optimized improvement; θ_{DS} is the angle between the initial Φ_{SAD} phase and a preliminary density-modification (DM) phase Φ_{DM}. The results show that utilizing the additional direct phase selection step prior to simple solvent flattening without phase combination using the existing DM programs, such as *RESOLVE* or *CCP4 DM*, improves significantly the final phases, in terms of the increased correlation coefficient of electron-density maps and diminished mean phase errors. With the improved phases and density maps from our developed method of direct phase selection, the completeness of built residues with main chains and side chains of protein molecules is enhanced for efficient structure determination.

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