Keynote Lectures

[KN9] Charge flipping & Co.: dual space algorithms in crystallography.

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The charge-flipping algorithm [1-3] is a member of the diverse family of dual-space iterative phasing algorithms [e.g. 4-7]. These algorithms use alternating modifications in direct and reciprocal space to find a solution to the phase problem. Unlike other algorithms from the diverse family of ab initio structure solution methods, in dual space algorithms neither of the two spaces is dominant in the structure solution, but it is the iteration between the two that makes the structure solution possible. All dual space algorithms have in common the basic principle, but they differ in the exact definition of the modifications and in the way these modifications are combined together in an iteration scheme. The dual space algorithms bear strong relationship to the convex feasibility problem, but the constraint sets used in crystallography are not convex and therefore the convergence properties of the convex problems cannot be directly transferred to the solution of the phase problem in crystallography. As a result, the only truly reliable way of finding new and more efficient dual space algorithms is their extensive testing against realistic problems. It becomes more and more clear that there is no universal algorithm that is ideal for all applications, but different flavors are suited for different problems. Despite of these complications, the dual space algorithms have met considerable interest in the crystallographic community. Apart from the standard structure solution of small-molecule or inorganic compounds, the dual space algorithms, especially charge flipping, have been applied to specialized problems like the solution of complex structures from powder diffraction data, the solution of incommensurately modulated crystals and quasicrystals or solution of protein structures and heavy-atom substructures in macromolecular crystallography [8].

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