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Latest Improvements in Density Modification of Experimentally Phased Maps. Pavol Skubak, Willem-Jan Waterreus, Navraj S. Pannu. *Biophysical Structural Chemistry, Leiden University, PO Box 9502, 2300 RA Leiden, The Netherlands.*

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Current methods for phase combination in density modification assume independence of the experimental and density modified electron density map. This assumption often leads to a bias since the density modified map is obtained from the experimental map. Despite progress in developing methods to reduce the bias, it still plagues the density modification procedures as the underlying assumption of independence remains.

We have derived a multivariate equation that no longer assumes independence between the initial and density modified map, considers the observed diffraction data directly, and models the errors in a SAD experiment. The equation has been implemented and tested on almost a hundred real data sets. The method provides significantly improved maps over the current methods and leads to structures automatically built when current methods fail.

Despite the improvements, a great part of the bias has remained. We have analyzed this behaviour and developed a method for estimation of the bias and its subsequent suppression through a change in the parametrization of the function used in phase combination. As a result, the majority of the bias is removed which has several positive consequences: the figures of merit produced are a significantly better representation of the cosine of the phase error and the resulting density modified maps are slightly improved. Furthermore, significantly better results are obtained by model building iterated with MLHL refinement using the less biased phase probability distributions from density modification.

Keywords: density modification, phase combination, bias reduction

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The Use of Longer X-ray Wavelengths in Macromolecular Crystallography for Sulfur SAD Structure Determination. Manfred W. Weiss. *Helmholtz-Zentrum Berlin für Materialien und Energie, Institute F-12, Macromolecular Crystallography, Albert-Einstein-Str. 15, D-12489 Berlin, Germany.*

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The use of longer X-ray wavelengths ($\lambda = 1.5\text{-}3.0 \text{ \AA}$) in macromolecular crystallography has over the past few years almost become a routine tool for phase determination using the anomalous signal derived from the natively present sulfur and/or phosphorus atoms. Since the obtainable signal is very small, the experiment has to be conducted with great care. The challenges of the method are reviewed as well as some recent developments. Also, a survey about successful experiments carried out at beam lines and home sources around the world will be given.

Keywords: Macromolecular Crystallography, Long Wavelengths, Anomalous Signal, Sulfur SAD