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The development of computational methods and instrumentation for macromolecular crystallography has moved the focus of structural biology towards more challenging targets.

The phasing signal is usually low, thus sensitive to all kind of errors. Every physical phenomenon in the experiment not included into modeling adds up to uncertainty of the signal. Such phenomenon could be non-isomorphism between crystals, changes in the structure induced by X-rays, changes in anomalous signal and others. The optimal description of above effects is beneficial as it decreases uncertainty of the signal, and described components could be additional source of phase information. However, such analysis is not straightforward, as it creates correlated information about components. High-redundancy would reduce the correlation but this requirement is difficult to fulfill in many experimental situations. Without the high-redundancy, adding additional parameters during the merging procedure causes instabilities in numerical calculations resulting in non-optimal estimates of the signals and their uncertainties. Moreover, such non-optimal results propagate to phasing procedures and may reduce their efficiency.

The statistical description was developed and implemented to deal with described above situation. The results and their impact on the process of structure determination will be presented.