Poster Presentation

MS055.P06

Detection and analysis of resolution-(in)dependent systematic errors in crystallographic datasets

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Datasets collected from different crystals are often affected by systematic errors. Prior to merging, systematic errors need to be detected and analysed. An algorithm recently published [1] uses a multidimensional scaling approach of pairwise correlation coefficients CCij of the individual datasets to separate random and systematic errors. Systematic differences between datasets i,j are given by positions of the datasets in a unit sphere, at angles related to the amount of systematic deviation. A relation between the pairwise correlation coefficient CCij , the internal correlation coefficients CC1/2_i and CC1/2_j [2] of the datasets, and the angle between these datasets exists [1]. The difference between the product of the internal correlation coefficients (CC1/2_i *CC1/2_j), which is the maximum correlation possible, and the pairwise correlation coefficient calculated from both datasets CCij corresponds to the amount of systematic difference between the datasets. Comparison of the angle in a resolution dependent way allows conclusions about the types of systematic error found in this datasets.

[1] Diederichs, K. (2017) Acta Cryst. D73, https://doi.org/10.1107/S2059798317000699 (in the press)
[2] Karplus, A. & Diederichs, K. (2012) Science, 336, 1030-1033

Keywords: systematic error, CC1/2