MS44-P138 LATE | ON PHASING OF OVERSAMPLED DIFFRACTION DATA

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The latest progress in X-ray free-electron lasers demonstrated an ability to acquire continuous diffraction data for nanocrystals and non-periodic objects [1-2]. Most of the oversampling phasing algorithms are iterative and may require knowledge of a support to avoid stagnation. Therefore new approaches which benefit directly from intensity oversampling particulary for *de novo* phasing may be of interest. Thus, Elser [3] has developed phase recovery algorithm which employs intensity gradient extracted from the continuous intensity distribution around a Bragg peak.

We investigate a new approach to phase retrieval when continuous intensity is available. The method employs Whittaker-Shannon sampling theorem (ST) [4] for the structure factor (SF). The phases of reflections (for non-periodic objects reflections refer to an artificial unit cell constructed to embrace a particle) are permutated to give the best agreement between moduli of measured structure factors and calculated by means of the ST at non-integral points in the reciprocal space. Application of the ST to the points with close to zero intensity gives rise to approximate linear equations for SFs in the neigbourhood of these points. Preliminary results for simulated data will be presented.

[1] Chapman H.N. et al. (2011). Nature (London), 470, 73-77.
[2] Sun Z., Fan J., Li H., Jiang H. (2018). Appl. Sci., 8(1), 132.
[3] Elser V. (2013). Acta Cryst. A**69**, 559-569.
[4] Shannon C.E. (1949). Proc.IRE, 37, 10-21.