

MS3-01 The battle of signal vs noise, and how to tip the balance in your favor. James Holton, *University of California, San Francisco and Lawrence Berkeley National Laboratory, USA*
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The success or failure of any structure determination effort is dictated by the signal-to-noise ratio, so quantitative predictors of the both signal and noise on an absolute scale are needed for designing effective data collection strategies. There are three main classes of noise in the diffraction experiment: photon-counting error or “shot noise” which is proportional to the square root of the signal, noise that is independent of the signal such as detector read-out noise, and “fractional noise” that is proportional to the signal. This last class of error has many sources, including shutter jitter, incident beam flicker, sample vibration, detector calibration, and systematic errors such as the uncertainty in absorption correction factors and the uncorrectable “non-isomorphism” component of radiation damage. Procedures for independently measuring all these sources of error on a given instrument are described, and it was found that the dominant source of error in measurements of weak spots is the background-scattered photons that fall into the spot area, but the dominant source of error for anomalous difference measurements is fractional noise, which is usually 2-3%. Which of the many sources of fractional noise is most important depends on the particular experiment, and strategies for identifying and reducing the contribution of fractional noise will be discussed.

Keywords: diffracton simulation; MLFSOM; Elves; fake data

MS3-02 Extracting the maximum data from your samples – advanced sample evaluation at the ESRF. Matthew W. Bowler,^a *EMBL Grenoble, 6 Rue Jules Horowitz, BP 181, 38042 Grenoble CEDEX 9, France*
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Crystals of biological macromolecules often exhibit considerable *inter* and *intra* crystal variation in diffraction quality. This requires the evaluation of many samples prior to data collection, a practice already widespread in Macromolecular Crystallography. As sample evaluation, automation and micro-beams have become more widely available, more advanced screening methods have evolved. These include locating the best region of a crystal on which to perform data and the calculation of data collection strategies to collect from multiple positions and crystals in order to alleviate the limiting factor of radiation damage. Here we demonstrate workflows to identify the best diffraction volumes of crystals by mapping the diffraction quality heterogeneity [1]; methods to perform large scale automated evaluation of crystals in a number of supports and techniques to improve the diffraction quality of crystals [2].

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Keywords: sample evaluation; automation; beamline