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Validating single-particle x-ray laser reconstructions using orientation concurrence

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To date, experiments at x-ray free-electron lasers have generated a very large amount of raw diffraction data. Whilst current pulsed x-ray laser sources measure diffraction patterns at an already very fast rate, with unprecedented development in the instrumentation this data collection rate is projected to rise at least an order of magnitude over the next few years. These large datasets are typically processed and analyzed by many computational routines either in a sequential fashion or in more complicated feedback loops. Furthermore, these routines sometimes employ ad-hoc parameters that are hand tuned by a human operator.

In face of such large datasets, their accompanying processing workflows, and the large parameter space of the algorithms that compose these workflows, it has become practically impossible for peer-validation of single particle reconstructions.

This difficulty in validation is especially acute when imaging unknown structures or unknown conformations where "a true solution"for structural validation is absent. Moreover, the fact that the orientations of individual diffraction patterns are missing and have to be indirectly reconstructed makes it difficult to decide if a pair of patterns are different because they represent the same particle at different orientations or two particles with different structures.

Here we propose novel approach to validate any single particle reconstruction in orientation space, even though the orientations of individual patterns are unknown. Crucially, this approach is independent of the algorithm or dataset used for reconstructions. To do this, we recast the orientation-recovering process into a key-cracking exercise in cryptography: the "correctness"between two cracked keys can be measured by how consistently they decipher a common set of "sentinel messages".

Using realistic simulations of the single particle pipeline, we demonstrate how to measure an effective uncertainty in the reconstructions in a self-consistent manner. Furthermore, we show that it is possible to separate the negative impact on reconstructions either due to intrinsic noise in diffraction patterns or insufficient number of patterns.

Primary authors: Mr SHEN, Zhou; Dr TEO, Colin; Dr AYYER, Kartik; Dr LOH, N. Duane

Presenter: Mr SHEN, Zhou

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