Contribution ID: **48** Type: **Poster**

Shaking out Intrinsic Structural Variation in Femtosecond Protein Crystallography using Deep Learning

Friday 10 November 2023 12:35 (5 minutes)

Current femtosecond crystallography data processing routines such as CrystFEL by T. White generally assume that identical molecular structure for each of the tens of thousands of protein crystals used. This assumption is however known to be unphysical, and with the recent development of deep learning technology, we are exploring whether we can build a net capable of shaking out the subtle structural variation information hidden behind a cloud of noise. We report progress on the development of a variational autoencoder, with an architecture inspired both from work in particle physics and Cryo EM.

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Session Classification: Poster session and networking lunch