Recent Developments in Fluctuation X-ray Scattering at X-FELs

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Fluctuation X-ray scattering (FXS) is a biophysical technique that overcomes the low datato-parameter ratios encountered in traditional X-ray scattering methods used for studying noncrystalline samples [1]. In an FXS experiment solution scattering data are collected from particles in solution using ultrashort X-rays of pulse lengths shorter than the rotational diffusion time of the particles. The resulting data contains angularly varying information that yields structures with a greater level of detail than those obtained using tradition SAXS [2].

After successful application of FXS to single-particle data [3], we have recently demonstrated the experimental feasibility of this technique on data from an ensemble of PBCV-1 virus particles in solution [4, 5]. We found that by using advanced noise-filtering methods the required number of images to obtain decent correlation data is far lower than originally expected, thereby reducing the required data collection time to less than a few minutes. In this talk I will outline the data processing techniques for analysis of FXS data, and present an assessment of the effect of concentration and various sources of noise on experimental data.

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References

- [1] Kam Z, Koch MH, Bordas J. (1981). PNAS **78** (6), 3559–62.
- [2] Donatelli JJ, Zwart PH, Sethian JA. (2015). PNAS 112 (33), 10286-10291.
- [3] Kurta RP, et al. (2017). Phys Rev Lett., **119** (15), 158102.
- [4] Pande K, Donatelli JJ, Malmerberg E, Foucar L, Bostedt C, Schlichting I, Zwart PH. (2018). PNAS, 115 (46), 11772–11777.
- [5] Pande K, et al. (2018). Scientific Data, 5, 180201.