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Can XFEL facilities provide enough diffraction data for atomic resolution single particle imaging?

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The concept of single-particle-imaging (SPI) of macromolecules using ultrashort intense x-ray pulses (proposed [6] and studied in detail [5]) have been corroborated by a series of experimental demonstrations [2–4, 7]. These demonstrations focussed on different aspects of SPI (e.g. algorithms, signal to noise ratio, sample delivery, etc), but have been silent on the general and crucial question of data sufficiency. In simple terms: "how many diffraction patterns does an SPI experiment need given a target resolution?"

This problem of data sufficiency is particularly acute in SPI because macromolecules scatter weakly. Hence, many diffraction patterns have to be collected for the reconstructed volume to signal average to a desired three-dimensional resolution. As the pulse repetition rates at XFEL facilities continue to rise, without a general framework to assess SPI data sufficiency, the community struggles with experiment planning, instrument design, and prospect.

Estimating data sufficiency for macromolecular SPI in general is challenging because it is heavily influenced by beam intensity, scattering conditions, type of sample, delivery mechanism, reconstruction algorithm, etc. Nevertheless, despite these complicating factors, there should still be limits set by kinematic scattering and biological characteristics of macromolecules.

Here we use a minimal set of simplifying assumptions to establish a semi-empirical predictive equation for the upper bound of achievable resolution given SPI parameters at various XFEL facilities. For example, we found that 50 hours of continuous data collection for a 5 keV beamtime at the CXI endstation at LCLS, with a 1% particle hit rate (216k diffraction patterns), a 10-15 Angstrom resolution map should be possible for dessicated proteins whose radii are between 1-10 nm.

Finally, we speculate on the number of diffraction patterns required to reach 3 Angstrom resolution as laid out in the SPI initiative roadmap[1] and the role that future upgrades to XFEL facilities could play, with its increased pulse repetition rate.

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Primary authors: Dr TEO, Colin (Centre for Bio-imaging Sciences, National University of Singapore, Singapore); Mr SHEN, Zhou (Centre for Bio-imaging Sciences, National University of Singapore, Singapore); Dr AYYER, Kartik (Center for Free-Electron Laser Science, DESY, Hamburg, Germany); LOH, Duane (National University of Singapore)

Presenter: LOH, Duane (National University of Singapore)

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