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Towards real-time analysis of liquid jet alignment in SFX

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Serial femtosecond crystallography (SFX) enables atomic scale imaging of protein structures via X-ray diffraction measurements from large numbers of small crystals intersecting intense X-ray Free Electron Laser (XFEL) pulses. Sample injection typically involves continuous delivery of crystals to the pulsed XFEL beam via a liquid jet. Due to movement of the jet, which is often focused to further reduce its diameter using a gas virtual dynamic nozzle (GVDN), jet position is often adjusted multiple times during the experiment. This can result in loss of beamtime and significant manual intervention. Here we present a novel approach to the problem of liquid jet misalignment in SFX based on machine vision. We demonstrate automatic identification and classification of when there is overlap ('hit') and when there is not overlap ('miss') between the XFEL beam and jet. Our algorithm takes as its input optical images from the 'side microscope' located inside the X-ray hutch. This algorithm will be incorporated into the control system at the SFX/SPB beamline at the European XFEL where it will be used for in-situ 'alignment correction' via a continuous feedback loop with the stepper motors controlling the location of the nozzle within the chamber. Full automation of this process will result in a larger volume of useful data being collected. By increasing the efficiency and reducing the per experiment operational cost of SFX at the European XFEL a higher volume of experiments can be performed. In addition, via analysis of the feedback metrology we anticipate that optimised nozzle designs and jetting conditions could be achieved further benefitting the end user.

Level of Expertise

Student

Presenter Gender

Man

Pronouns

He/Him

Which facility did you use for your research

None of the above

Students Only - Are you interested in AINSE student funding

Yes

Do you wish to take part in the Student Poster Slam

Yes

Condition of submission

Yes

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