Integrated control of a chip scanner for time-resolved crystallography at the NSLS-II FMX beamline

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Abstract

The FMX (Frontier Microfocusing Macromolecular Crystallography) beamline at the NSLS-II light source has been developing a new experimental station for fixed target time-resolved serial crystallography on biological systems. We present here the controls-system for a chip scanner to enable the rapid collection of large numbers of room temperature crystallographic measurements on biological samples. In addition to static measurements, samples can be excited in a pump-probe scheme by the injection of compounds suspended in liquid through a microdrop dispensing system, at timed intervals preceding the measurement. Enabling this has required the implementation of a full stack integrated solution, involving direct programming of the powerPMAC motion controller, control of motion, triggering and detectors through EPICS, data collection through Ophyd/Bluesky, and the implementation of an optional GUI for control of the experiment.

Preliminary Results

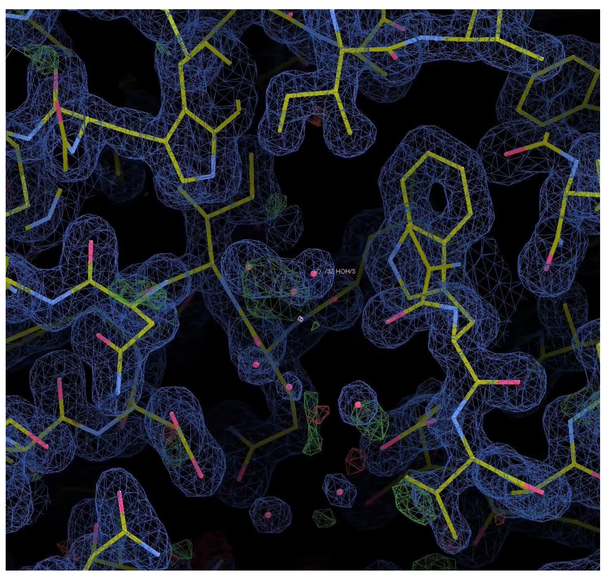

Figure 1. An image of the ligand binding site of hen egg lysozyme, collected with the chip scanner at FMX. A total of 20400 images were collected and 8851 images were indexed. Data shows excellent statistics.

Acknowledgments

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Layered Control System

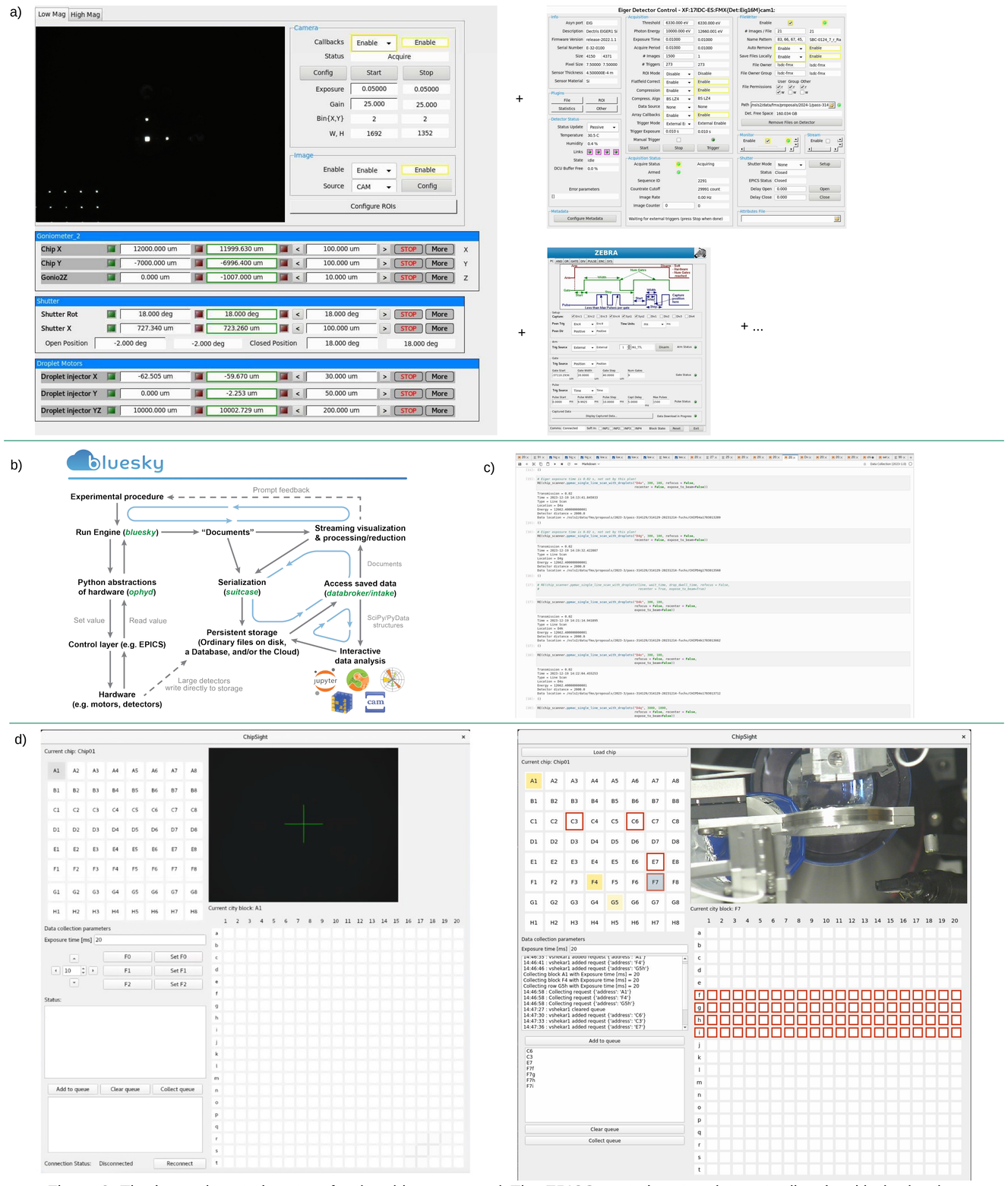

Figure 2. The layered control system for the chip scanner. a) The EPICS control system interacts directly with the hardware, directing motor control, cameras, detectors and timing hardware. b) Data collection is directed using the Ophyd/Bluesky middleware. Specific plans can be called for taking data with or without droplets, and over different subsets of the chip. c) These plans can be called through any pythonic interface (shown is the Jupyter interface which has been used widely). d) A user facing GUI has been developed, which simplifies usage and offers immediate visual feedback. On the left is a chip preparing for collection; on the right is a chip which has been partially collected.

Physical Setup

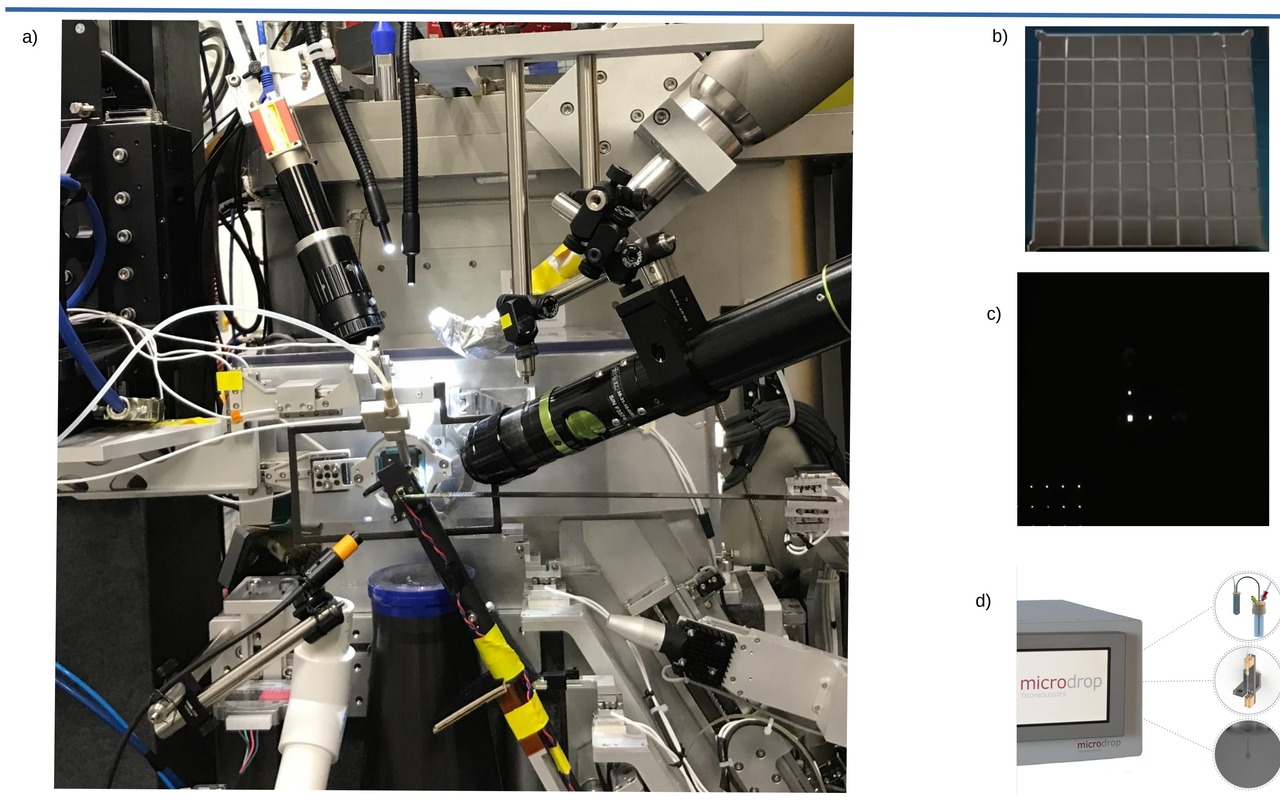

Figure 3. a) The chip setup at the FMX beamline. In addition to the chip itself, cameras and lighting are in place for alignment of the wells and droplets. A pipette is aligned to dispense droplets, driven by three motors. A curtain covers the chip to delay dehydration of the samples. b) A closer view of the chip. c) An image of the upper-right fiducial, showing a number of holes in which samples can be present. d) The droplets are dispensed by a Microdrop Technologies device.

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