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The Beauty of Not Being There: Integrating Interactive Screening with Offline Data Collection. James M. Holton, Univ. of California San Francisco and Lawrence Berkeley National Laboratory, Berkeley, CA 94720, George Meigs, Lawrence Berkeley National Laboratory, Berkeley, CA 94720.

At ALS 8.3.1 we are focusing on maintaining the advantages of screening crystals on-site and eliminating the need for users to stay up all night. Going home to sleep while your data are collected is already a common method of “remote” data collection, but it is impractical on beamlines bright enough to destroy the sample in half an hour. The obvious solution is to queue up data collection runs for many samples and change them out with a robot. However, the problem of automatically placing the crystal into the beam is a difficult one, and even the best crystal identification algorithms might not put the crystal where the user wants it.

Instead of solving the problem of finding the crystal in the loop, we have circumvented it. Users center their crystal as usual as they screen them. However, they now have the option to postpone data collection until after they go home. Digital photos of the centered sample are taken before the robot dismounts it. Early the next morning, the sample is re-mounted and these photos are used to reliably re-center the sample to within a few microns and a few degrees of where it was when the photos were taken. Data collection then commences as specified while the user sleeps.

This work is supported by the member of the ALS 8.3.1 Participating Research Team: University of California San Francisco, University of California Berkeley, Plexxikon Inc, The Alberta Synchrotron Institute and the MD Anderson Cancer Research Institute.