Automation of X-ray Diffraction Data Analysis at SSRL

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At SSRL, key services such as sample delivery, crystal screening, and data processing have been highly automated for many years. The global COVID-19 pandemic had accelerated the development of automated procedures and techniques at facilities worldwide, and prompted us to expand our repertoire of automated services, including – but not limited to – real-time data analysis with the in-house program Interceptor. Running on a dedicated data processing cluster, the Interceptor processes incoming images as they are collected; the current rate of data analysis copes well with the speed of data acquisition with the EIGER 16M and EIGER-2 16M XE detectors in use at SSRL microfocus beamlines. The results of this analysis are displayed to the user via the control software, providing crucial real-time information on data quality, crystal deterioration, and overall experimental success. Good to have for any experiment, these developments were especially useful to implementing serial crystallography options at SSRL microfocus beamlines and at LCLS-MFX. In addition to live data analysis during data collection, the Interceptor is utilized to locate mounted crystals, with applications in screening and crystal quality analysis currently in development.