Sample Centering Using Google Cloud Platform's AutoML Vision.

Scott Classen[1], James Holton[2], Shawfeng Dong[3], Feng Chen Liu[4], Giles Mullen[5]

[1]Advanced Light Source [2]UCSF/LBNL/SLAC, [3]LBNL, [4]LBNL, [5]Tetrahedron Technologies

sclassen@lbl.gov

Fully automated and unattended Macromolecular Crystallographic (MX) data collection relies on robust alignment of crystal samples within the X-ray beam. This step has historically been performed through a manual click-to-center strategy or traditional machine vision strategies based on edge detection and other rigid procedural techniques. Artificial Intelligence, Machine Learning, and Convolutional Neural Networks have also been used to achieve sample recognition steps, but often involved tools that are not readily accessible for non-experts. In this presentation I will outline our use of the AutoML Vision tool available from Google Cloud Platform (GCP). AutoML Vision is one of a number of AI/ML tools offered through an intuitive web-based user interface and designed for non-experts to take advantage of the immense potential of AI/ML tools. With AutoML you can train custom models for object classification and detection. The trained models can then be deployed on GCP and accessed remotely or downloaded and deployed on local compute resources. I will present details of the development and deployment of our AutoML-based sample centering software at beamline 8.3.1 at the Advanced Light Source.