

# APS Scientific Computation Seminar Series

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Title: SG-LIMS: A Laboratory Information Management System for Macromolecular Crystallography

Date: Monday, April 12, 2021

Time: 1:00 p.m. (Central Time)

Location: <https://bluejeans.com/150410242>

Hosts: Nicholas Schwarz and Mathew Cherukara

## Abstract:

Common use of Laboratory Information Management Systems (LIMS) includes the tracking shipments, the management of sample life cycle, the integration of test results, reporting, and management of customer relationships. Our group has built a custom LIMS to capture data of ANL structural biology pipelines. The web-based SG-LIMS is built using .NET technology and uses an Oracle database. It captures data from the beginning to the end of the pipeline, including cloning, small-scale clone evaluation, large-scale protein purification and crystallization. The data is synchronized with the public-facing website hosted at the University of Virginia.

The SG-LIMS was used to build ML-models to aid the design of clone variants that enhance the success rate of the pipeline. A live demonstration of the SG-LIMS will be followed with the results of the data mining strategies.