Title: High-performance computing applications in Biophysics

Abstract:
The UltraScan software has been developed to assist biophysicists with the analysis of analytical ultracentrifugation (AUC) experiments. It includes a desktop component written in C++, a web-based laboratory information management system with a MariaDB database backend written in PHP, and a high-performance computing backend using MPI, implemented on supercomputers around the world, and in particular on the US National Science Foundation's XSEDE infrastructure. A 4th component is the slurm-based Apache Airavata grid middleware that brokers analysis jobs to a variety of supercomputers publicly available to users of Ultrascan.

In this talk I will discuss several algorithms for AUC data fitting used in UltraScan, and how they are parallelized on supercomputers, and discuss the general architecture of UltraScan.