Computing Nanostructures at Scale

Dr. Abhinav Sarje
Lawrence Berkeley National Laboratory

Abstract

The inverse modeling, or structural fitting, problem of recovering nanostructures from X-ray scattering data obtained through experiments at light-source synchrotrons is an ideal example of a Big Data and Big Compute application. X-ray scattering based extraction of structural information from material samples is an important tool for nanostructure prediction through characterization of macromolecules and nanoparticle systems, applicable to numerous applications such as design of energy-relevant nano-devices. At Berkeley Lab, we are developing high-performance solutions for analysis of such raw data. In our work we exploit the use of massive parallelism available in clusters of GPUs, such as the Titan supercomputer, to gain efficiency in the reconstruction process. We explore the application of various numerical optimization algorithms ranging from simple gradient-based quasi-Newton methods, derivative-free trust-region-based methods, to the stochastic algorithms of Particle Swarm Optimization in a massively parallel fashion.