Reconstructing Nanostructures from X-Ray Scattering Data

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We consider the problem of reconstructing material nanostructures from grazing-incidence small-angle X-ray scattering (GISAXS) data obtained through experiments at synchrotron light-sources. Analysis of such experimentally collected data has been the primary bottleneck in this problem. X-ray scattering based extraction of structural information from material samples is an important tool for the characterization of macromolecules and nano-particle systems applicable to numerous applications such as design of energy-relevant nano-devices. We exploit massive parallelism available in clusters of multi/many-core/graphics processors to gain efficiency in the reconstruction process. To solve this inverse modeling problem, we explore various numerical optimization algorithms ranging from simple gradient-based methods, derivative-free trust region-based methods to stochastic algorithms. These include the quasi-Newton method LMVM, trust region based method POUNDerS, and Particle Swarm Optimization algorithms. We apply these in a massively parallel fashion and compare their performance in terms of both quality of solution and computational speed.