Acceleration of numerical methods for Coherent X-ray Diffractive Imaging

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X-ray imaging is a tool for characterizing nanoscale materials and devices that is capable of achieving nanoscale. An emerging 3D X-Ray imaging method is Coherent X-ray Diffractive Imaging (CXDI). CXDI is based on computational phase-retrieval of the X-ray diffraction patterns from the measured data of the magnitude. The reconstruction process involves multiple iterations, which evaluate the image in the real space and Fourier domains accounting for the constraints imposed on the sample under interest. Often the image reconstruction involves computer intensive tasks, which make the computations slow. The numerical aspects for enabling the rapid image reconstruction include imposing proper image constraints, computing the images in the reciprocal space rapidly, and utilizing sparsity of the image in the real and reciprocal domains.

Here, we present work towards enabling real-rime CXDI by accelerating the computations. Specifically, we address two aspects. In the first aspect, we accelerate the computations using Graphics Processing Units, which are well suited for CXDI. The GPU accelerations involves creating suitable data structure, properly addressing CPU and GPU memory, and executing operations in parallel. The GPU can accelerate the required Fourier transforms and products with 20-70-fold speed-up rates. We compare various approaches for the Fourier transforms, including out-of-place and in-place transforms for acceleration and memory consumption reduction as well as using alternative approaches. We also present work towards a virtual synchrotron framework, in which computational methods are used to simulate experimental image reconstruction and provide required constraints, using magnetic nanostructure as a testbed. In the presented work, a simulator for modeling the magnetization dynamics is used to predict expected images of a magnetic nanostructure. We obtain the reciprocal images using the forward transform framework and use them for verifying the computational methods for the GPU accelerated CXDI. Finally, we present how CXDI can be used for the study of nanoscale material composition via a set of examples.