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Department of Energy Conversion and Storage

Optimization for multi-scale 3D reconstruction of ptychographic X-ray tomography data

Azat M. Slyamov, **Tiago Ramos, Jens W. Andreasen**

Technical University of Denmark, Department of Energy Conversion and Storage, 4000 Roskilde, Denmark

Motivation

The structure of a large number of nano/microscale systems in material science is closely related with their physical and chemical properties. Ability to image such systems brings a better understanding of the structure-function correlations that can significantly increase their performance in applied fields. Here, we present a new method for 3D reconstruction of volumetric phase contrast from ptychographic coherent X-ray diffraction imaging (CDI). Direct reconstruction in 3D requires large computational recourses and/or time consuming reconstruction algorithms. Therefore, we propose a multi-scale approach for reducing convergence time by fast reconstruction of low-resolution image and its further application as an input guess for high-resolution reconstruction.

Coherent X-ray diffraction imaging

In CDI experiment an incident wave interacts with a sample experiencing refraction and attenuation and propagates into a far-field detector that measures its intensity, given by

$$I_{\Theta} \cong |\mathcal{F}\{\psi_{\Theta}\}|^2 = |\Psi_{\Theta}|^2,$$

where Θ is a set of relative orientation parameters between the incident wave and the sample, $\mathcal{F}$ is a Fourier transformation and $\psi_{\Theta} = PO_{\Theta}$ is an exit wave that formed after interaction of the incident wave P (probe function) and the sample O_{Θ} (object function). The latter can be described by its complex refractive index $n = \mathbf{1} - \delta + \mathbf{i}\beta$ as

$$O_{\Theta} = \exp\left[\mathbf{i}k \int_{\Theta} \boldsymbol{n} - \mathbf{1}\right],$$

where δ and β are refractive and absorptive parts of the refraction index.

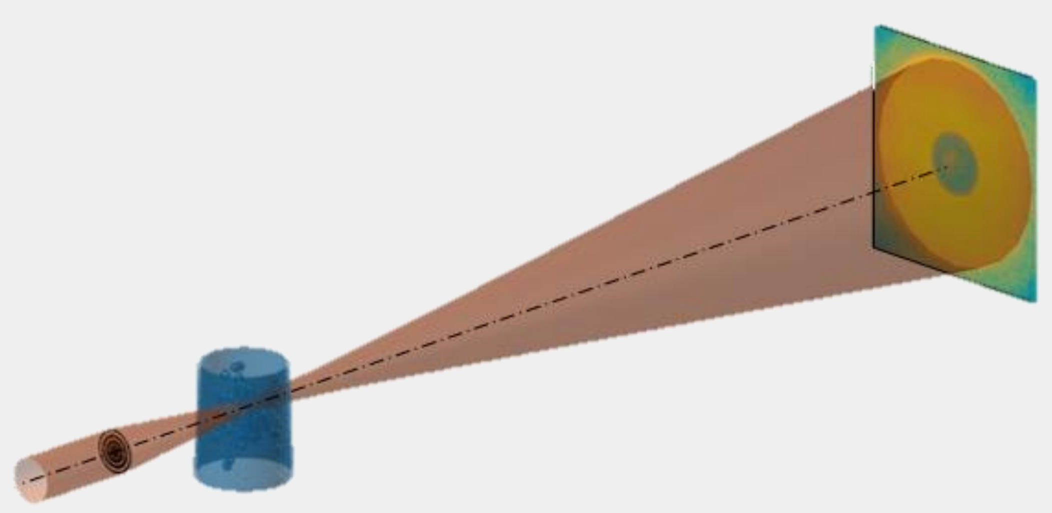

Figure 1: Schematic of coherent diffraction imaging.

Phase-retrieval algorithm

A reconstruction of the sample can be formulated as a least-squares optimization problem solved by iterative minimization of difference between measured and approximated (guessed) diffraction intensities.

$$\min(I^{g}_{\Theta} - I^{m}_{\Theta}).$$

Complex valued object function and squared modulus operation in the expression for intensity make the problem ill-posed and non-linear. Here, we use Levenberg-Marquardt algorithm (LMA) in combination with conjugate gradient method (CGM) to find the optimal solution.

Single-scale reconstruction

In order to present capabilities of developed algorithm we use a diffraction data of a solar cell phantom. The single-scale reconstruction from full diffraction data takes ~9000 seconds.

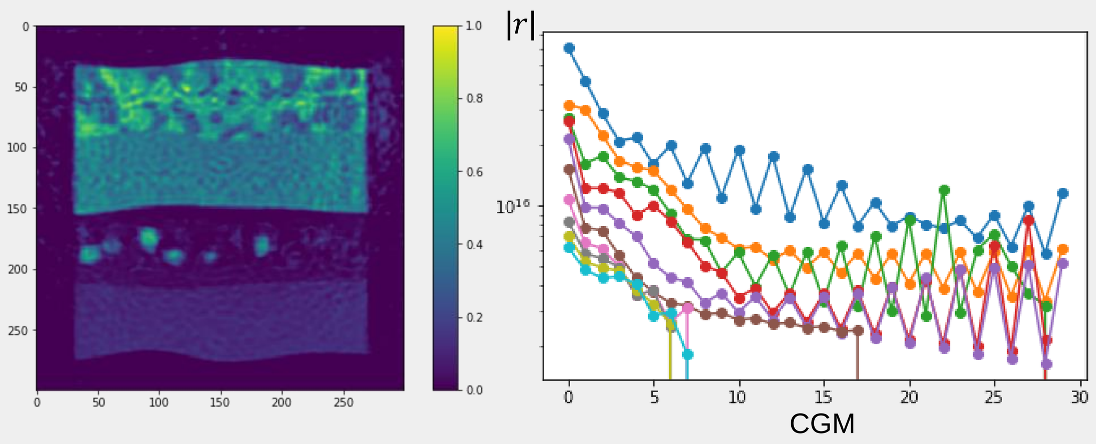

Figure 2: on the left: single-scale reconstruction from full data with zero-valued initial guess; on the right: residual value over LMA (curves) and CGM iterations.

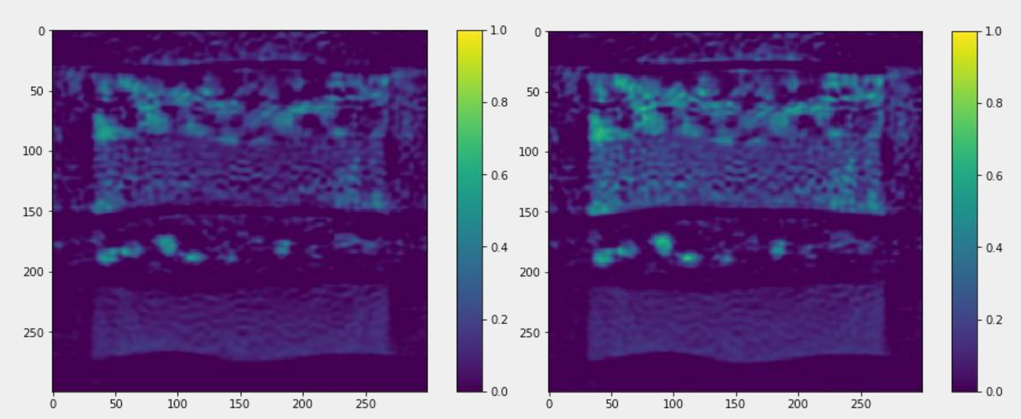

Figure 3: First two iterations of LMA for single-scale reconstruction, each takes ~1000 seconds.

Multi-scale reconstruction

The reconstruction from a half of the diffraction data takes ~2000 seconds. The obtained low-resolution image is then resized to the initial dimensions and used as an input guess for the reconstruction from full diffraction data.

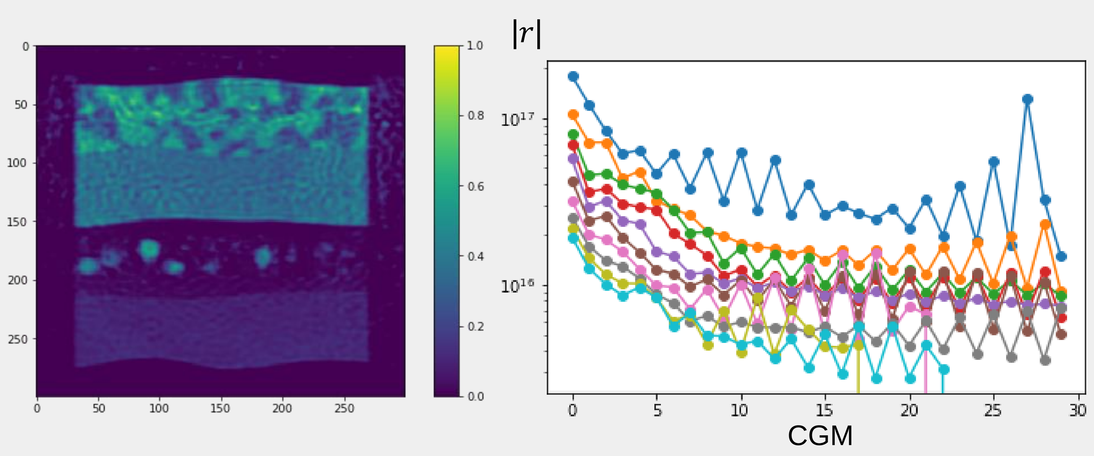

Figure 4: on the left: reconstruction from a half of the data with zero-valued initial guess; on the right: residual value over LMA (curves) and CGM iterations.

For comparison of convergence time of the algorithm we set up the same stopping criteria based on increment value of the residual update for both single and multi-scale cases.

Results

The multi-scale approach has shown to speed up the algorithm by ~30% (~3000 seconds) providing better initial input guess and more robust convergence of the reconstruction.

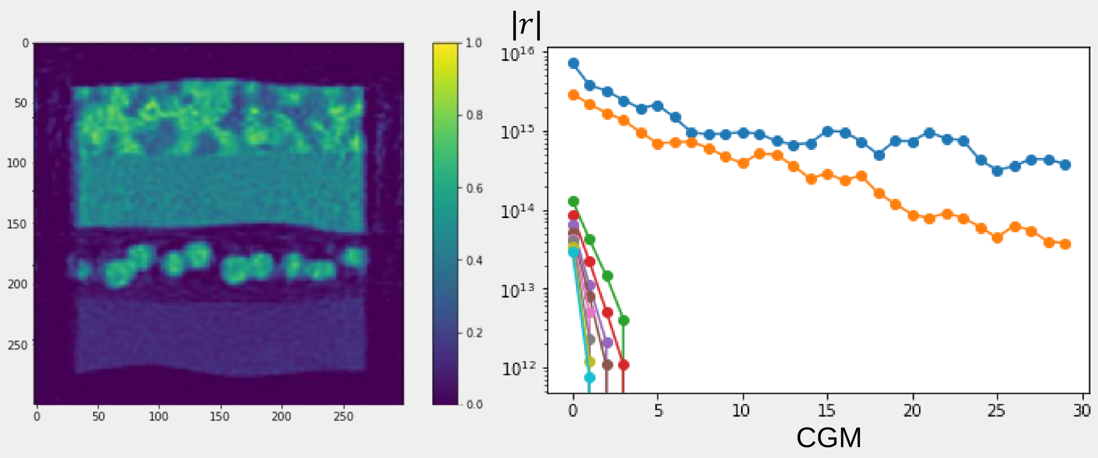

Figure 5: on the left: multi-scale reconstruction using low-resolution image as an input guess; on the right: residual value over LMA (curves) and CGM iterations.

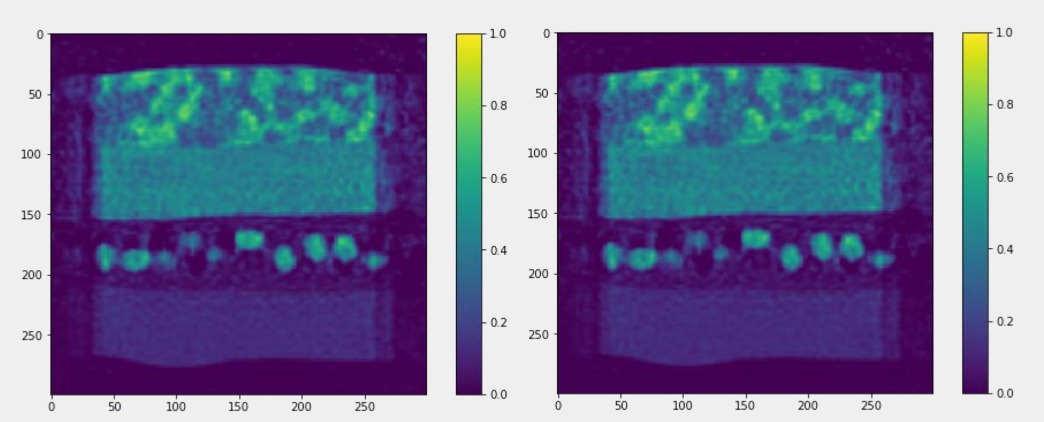

Figure 6: First two iterations of LMA for multi-scale reconstruction using low-resolution input guess.

Future work

Here, we present an extension of the direct 3D ptychographic reconstruction using multi-scale approach. The next step towards decreasing computational costs of the algorithm is to solve the problem of scanning path optimization with instrumental constraints. The final goal is to implement developed algorithm to a real data.

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Department of Energy Conversion and Storage
azslv@dtu.dk

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