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

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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

\[ I_\theta = |\mathcal{F}(\psi_\theta)|^2 = |\psi_\theta|^2, \]

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

\[ O_\theta = \exp \left[ i\frac{k}{\theta} \frac{n - 1}{n} \right], \]

where \( \delta \) and \( \beta \) are refractive and absorptive parts of the refraction index.

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.

\[ \min(I_\theta - I_\theta^m). \]

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 \(~9000 \text{ seconds.}\)

Multi-scale reconstruction
The reconstruction from a half of the diffraction data takes \(~2000 \text{ seconds.}\) 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.

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

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.

References