PyNX: a GPU-accelerated Coherent Imaging suite based on operators for CDI and Ptychography

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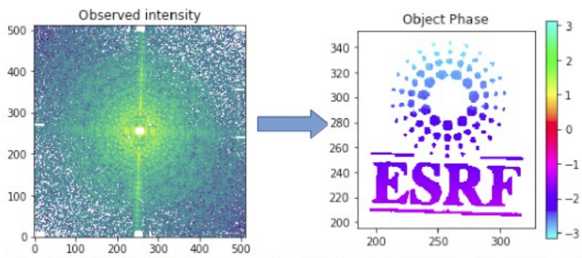
The advent of brighter, more coherent synchrotron sources requires the development of efficient and fast data analysis algorithms for synchrotron users, allowing live data analysis during the experiment as well as user-friendly packages.

For this purpose the use of GPU-accelerated software [1-3] has become a standard solution. However, a wide range of coherent imaging techniques exist, requiring complex developments using advanced parallel programming language. This complexity makes the development of improved algorithms difficult.

At ESRF, the chosen solution in the PyNX software [4] uses an operator-based approach [5]. Reconstructing an object can be *literally* written using the Python language by multiplying an object containing the diffraction data, by a series of operators performing basic mathematical operations (propagation to and from object or diffraction space, applying a support constraint or the observed diffraction amplitudes, ...). This approach allows to decompose complex algorithms in simple mathematical operators, which can then easily be combined to develop new algorithms. The operators are applied asynchronously in the GPU, allowing to fully exploit the available parallel processing speed, and providing more than two orders of magnitude speedup compared to running on a single CPU core.

We will present the applications of PyNX, which are available both as an open-source coherent imaging toolkit and end-user tools, for a wide range of coherent imaging techniques. We will discuss the current performance of algorithms for coherent diffraction imaging and ptychography in Bragg and small angle geometry, with current developments in phase contrast imaging.



cdi = ER200 * (SupportUpdate * HIO**20)**20 * cdi**

All coherent imaging algorithms can be described as a combination of mathematical operators allowing to reconstruct 2D or 3D objects from diffraction data. In PyNX, algorithms can *literally* be described as such a mathematical combination: in the above example the diffraction object (cdi) is transformed by 20 repetitions of 20 cycles of Hybrid Input/Output plus a support update, and finally 200 cycles of Error reduction. This approach is suitable to all coherent imaging techniques (CDI, Ptychography, ...) and algorithms (error reduction, HIO, RAAR, Maximum Likelihood, ...), and allows to customise algorithms as simple operator chains.

References

[1] Marchesini*et al.,J Appl. Cryst.***49** (2016)**,** 1245–1252

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[3] Mandula *et al.,J. Appl. Cryst.* **49**(2016)**,** 1842–1848

[4] PyNX, http://ftp.esrf.fr/pub/scisoft/PyNX/doc/

[5] Marchesini,*Rev. Sci. Instr.* **78** (2007), 011301