Parallel Ptychographic Reconstruction

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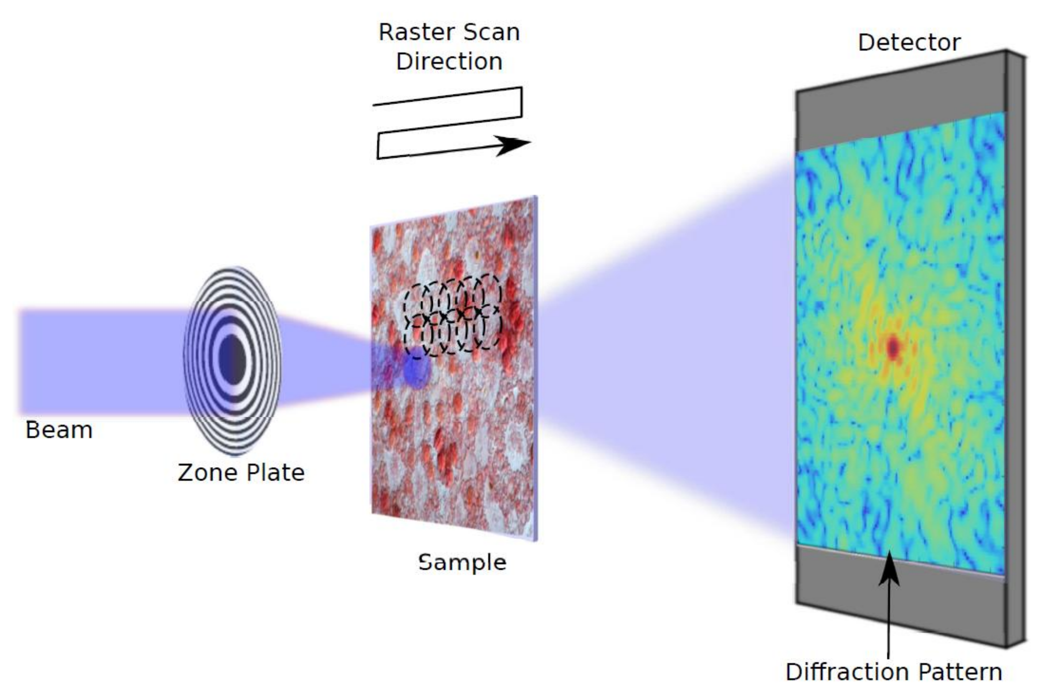
Introduction

Faster area detectors, brighter X-ray sources and increasingly higher resolution nanofocusing optics are leading to a rapid increase in the size of ptychography datasets. In practice these large ptychography datasets must be reconstructed in close to realtime in order to inform the progress of the experiment.



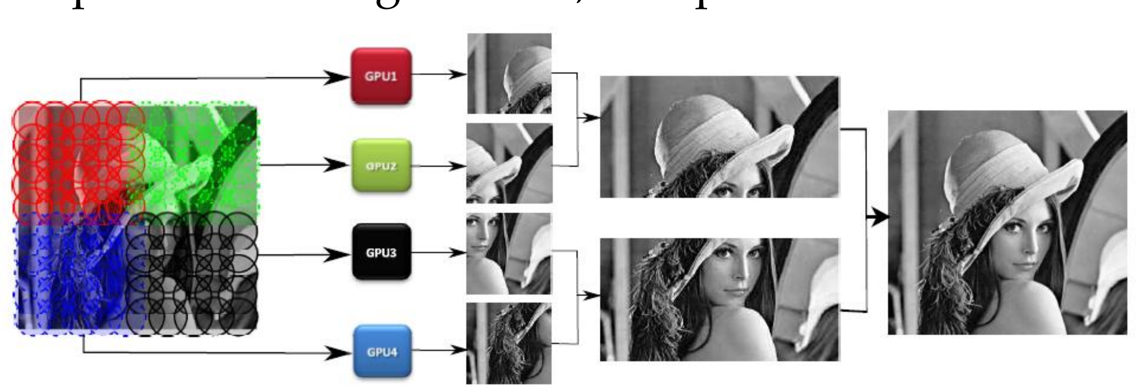
Simplified ptychography experiment setup

Multi-GPU Implementation

Asynchronous phase retrieval

Pros: Fast. No communication between GPUs. Only a parallel reduction-with-merge is needed in the stitching step.

Cons: Requires result registration, and phase normalization.

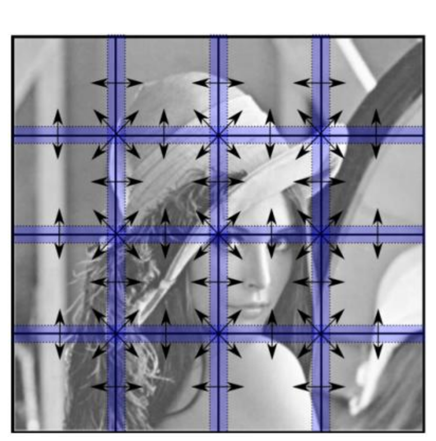


GPUs operate independently and their results are stitched in parallel at the end of the iterative reconstruction method

Synchronous phase retrieval

Pros: No need for registration or normalization; GPUs converge to a common phase and spatial offsets of the reconstruction.

Cons: GPU communication overhead. Can be mitigated using neighborhood and ROI sharing

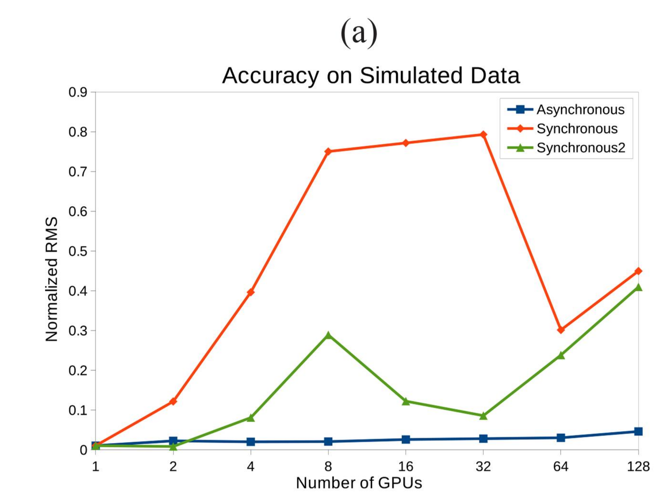


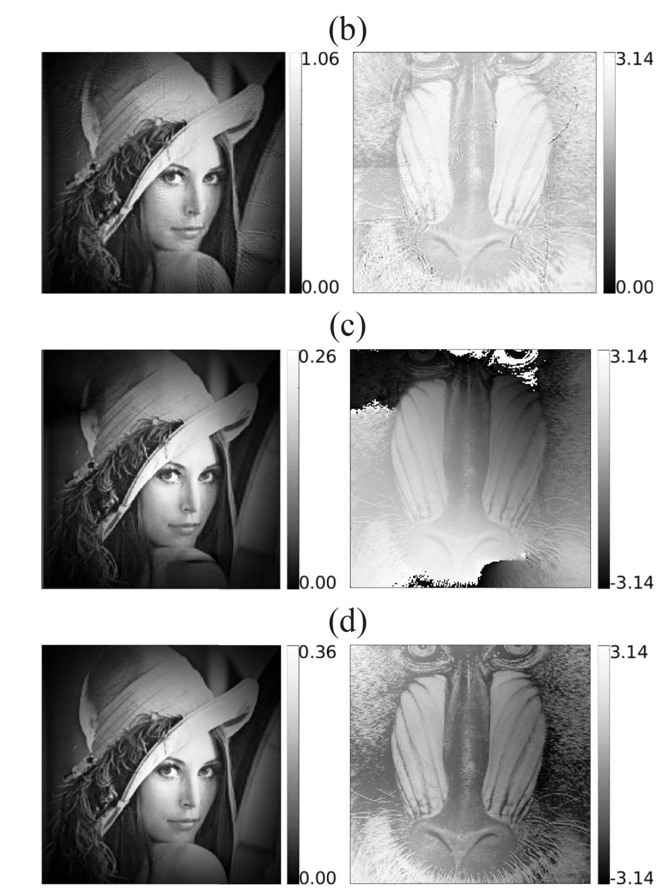
Object array sharing through neighborhood exchange between 16 GPUs.

Results

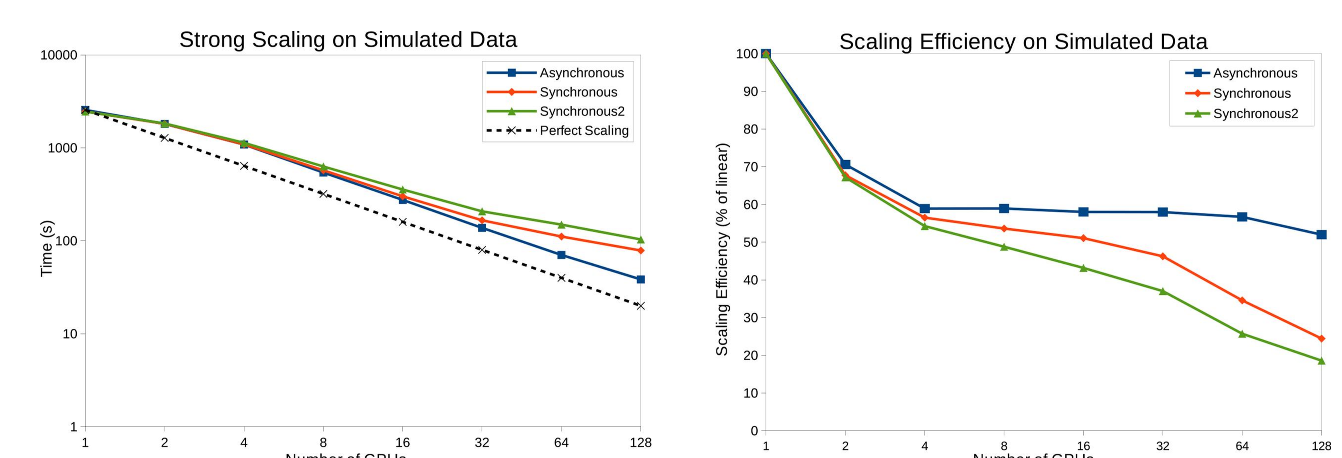
Two datasets of diffraction patterns were used for evaluation [1]. A synthetic sample, simulating the diffraction patterns from known images, and on real data acquired using the Bionanoprobe [2] at beamline 21-ID-D of the Advanced Photon Source (APS) at Argonne National Laboratory. Experiments were run on the *Tukey* cluster at the Argonne Leadership Computing Facility (ALCF).

Simulated data: Two 256×256 images, lena and baboon, were used to represent the object phase and magnitude profiles. A regular 175×120 Cartesian grid was used for the probe positions, generating 21,000 far-field diffraction patterns, totaling 5.12GB of single precision floating point raw data



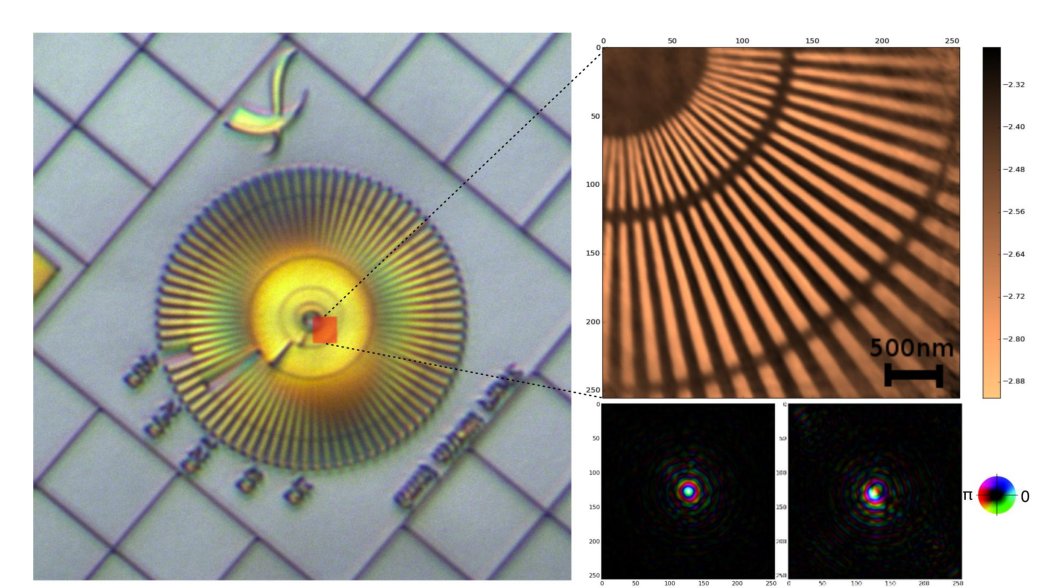


(a) Normalized RMS error of final reconstructions achieved by different GPU configurations. (b-d) Magnitude and phase of the object transmission retrieved from simulated data using the worst performing GPU configurations of the asynchronous and synchronous implementations



Performance plots on synthetic data. Left: Total running time (in seconds) of different GPU configurations. Right: The scaling efficiency plotted as a percentage of linear scaling

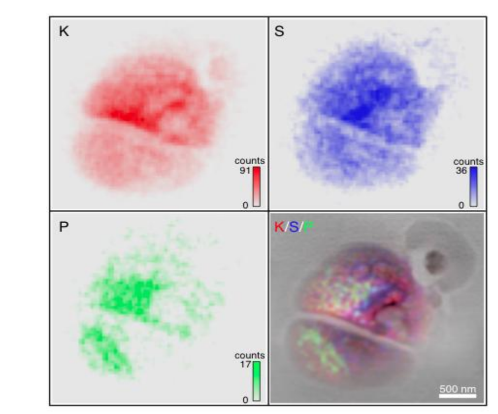
Real data: Gold test pattern, with 30 nm smallest feature size, was raster scanned through a 26×26 grid using a step size of 40 nm; the total scanning time was about 20 minutes, including positioning and computer overheads. The spoked region is 30 micron in diameter, each spoke is 180 nm thick, and the scan region highlighted in red is $1 \mu m \times 1 \mu m$.



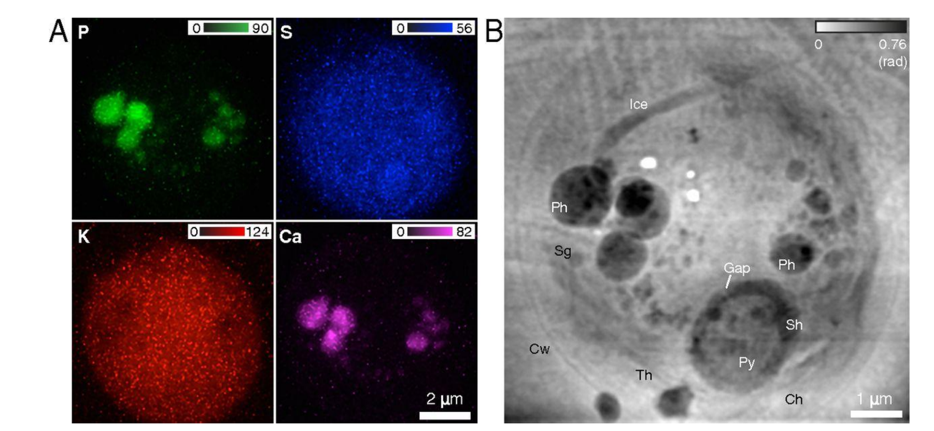
Left: An image of the Au Siemens star test pattern under an optical microscope where the scan region is highlighted in red. Top right: Phase image of the reconstructed object wavefront. Bottom right: The recovered illumination function of two probe modes.

Experiments

Simultaneous cryo X-ray ptychographic and fluorescence microscopy of green algae [3].

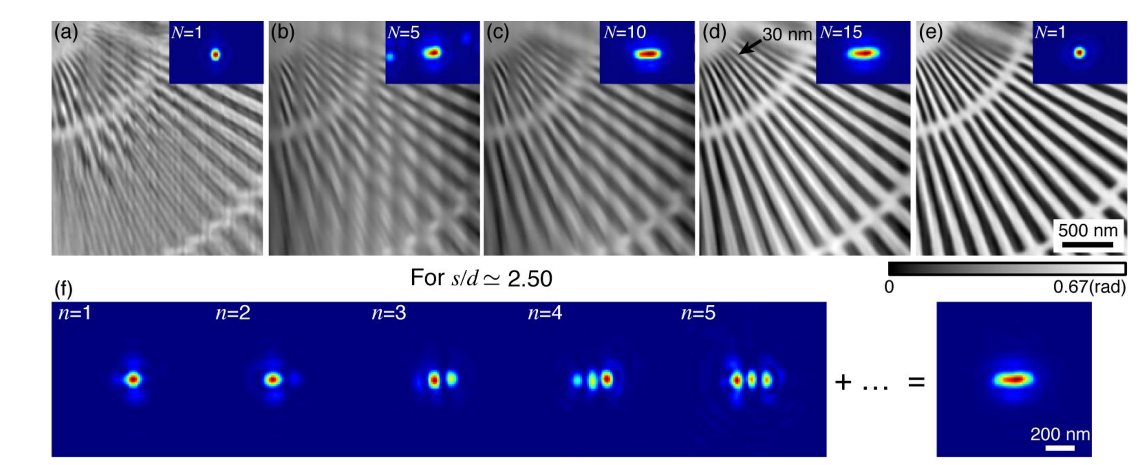


X-ray fluorescence maps of the distributions of the elements K, S, and P, along with their color composite overlay on the ptychographic image.



Fluorescence maps and ptychographic image of a frozen-hydrated alga obtained from 167×151 point scan data. (A) Elemental distributions of P, S, K and Ca within the cell. (B) Phase image reconstructed via ptychography

Continuous motion scan ptychography: characterization for increased speed in coherent x-ray imaging [4].



The improvement of fly-scan reconstruction quality using multiple probe modes. Images (a)–(d) were reconstructed using 1, 5, 10 and 15 probe modes, respectively. The first 5 individual probe modes in (d) case are shown in (f), along with the summed modes footprint at the right. The fly-scan reconstruction (d) is similar in quality to the step scan image (e)

Conclusion

Our running time using **one** GPU is **88% faster** than the data acquisition time. This marks the first time that our users have been able to reconstruct results while their imaging experiments were still running. It also enabled them experiment with new parameters and methods in post-processing their data.

Acknowledgements

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References

[1] Nashed, YSG., et al. (2014), Optics Express 22 (26), 32082–32097.
[2] Chen, S., et al. (2014). Journal of synchrotron radiation, 21 (1), 66–75.
[3] Deng, J., et al. (2015). PNAS, 112 (8), 2314–2319.
[4] Deng, J., et al. (2015), Optics Express 23 (5), 5438–5451.

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