Experience with Acceleration of Ptychographic Reconstruction

Jeffrey S. Kallman

LLNL-PRES-670518

Lawrence Livermore National Laboratory

Brief Introduction to Ptychography

- Coherent imaging technique
- Yields real (phase) and imaginary (attenuation) parts of refractive index
  - Phase is useful in biological imaging and may be able to image doping in semiconductors (important for chip assurance)
- Lensless technique
  - Good for probes (X-rays and particles) where it is hard to make good lenses
- Specimens are scanned with overlaps, unlike CT which uses multiple angular projections
- Works for 2D (thin) and layered 3D subjects
- Has been applied to
  - Biological imaging
  - Chips
- Requires numerical inversion
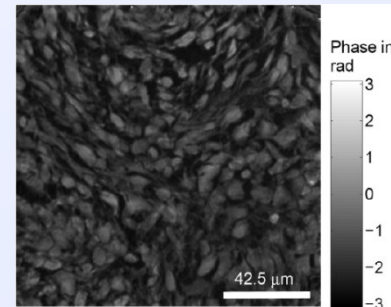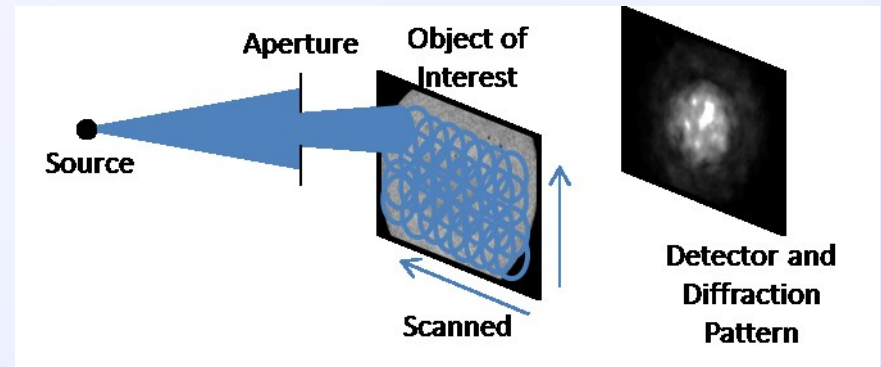
Mouse Tumor
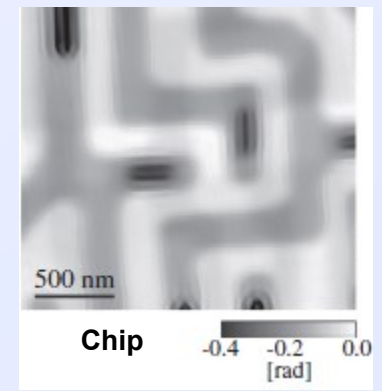
Chip

D. Claus, Proc. of SPIE Vol. 8001, 800109 (2011)

A. Shropp, Appl. Phys. Lett 100, 253112 (2012)

Why Are We Interested?

- We want to determine if ptychography is applicable to current or future NDE applications

  - Fairly new (first experimental paper published 2007*, at least 100 papers on the subject published since then)

- We want to research acceleration techniques (not exploiting parallelism) for ptychographic reconstruction algorithms. Investigate algorithm modifications based on prior experience in atmospheric propagation simulation (for SATRN SI LDRD)

Two Popular Reconstruction Techniques

Two of the popular techniques for ptychographic reconstruction are the ePIE and Difference Map methods

ePIE: A. M. Maiden and J. M. Rodenburg, "An improved ptychographical phase retrieval algorithm for diffractive imaging," Ultramicroscopy, Vol. 109, pp. 1256-1262 (2009).

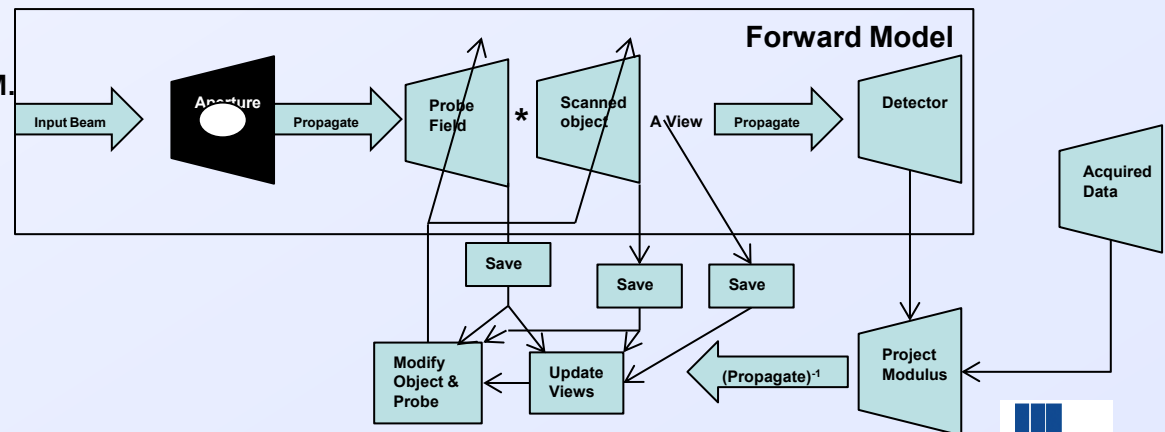Modification of object and probe are performed on an object position by object position basis
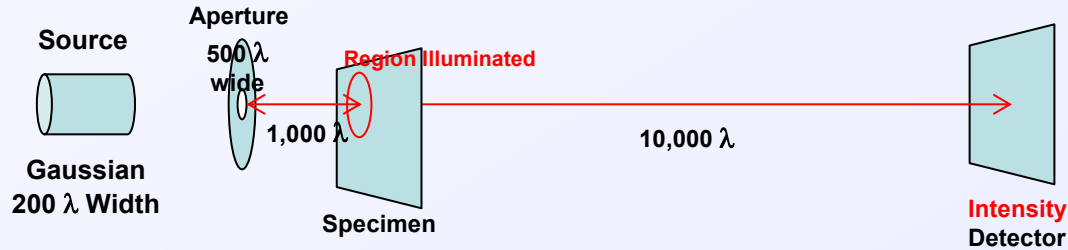
Amenable to dealing with layered 3D objects
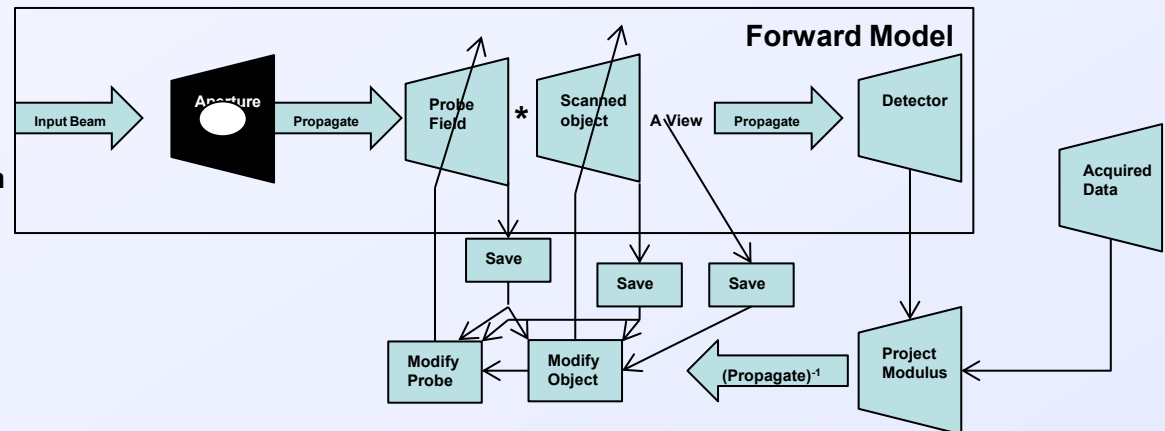
Difference Map Method: P. Thiabault, M. Dierolf, A. Menzel, O. Bunk, C. David, F. Pfeiffer, "High-Resolution Scanning X-ray Diffraction Microscopy," Science, Vol. 321, pp. 379-382 (2008). Details on the algorithm are in the supplementary material

Modification of the object and probe are performed once all views are updated

Not amenable to dealing with layered 3d objects
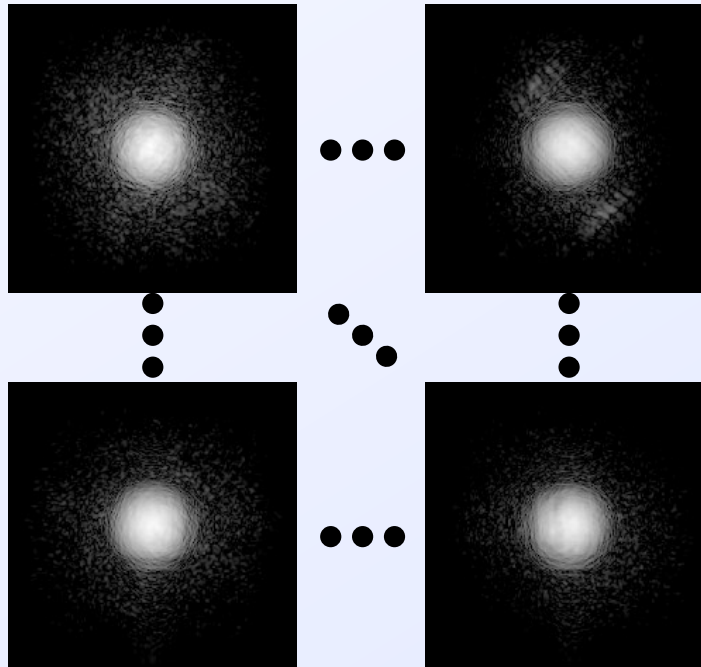
Simulated Example with Complex Specimen

Source — Gaussian 200 λ Width

Aperture 500 λ wide

Region Illuminated

1,000 λ

10,000 λ

Specimen

Intensity Detector

Complex Specimen

Specimen Real Part

2500 λ

Specimen Imag Part

11 X 11 Set of Detected Data (log scale)

Reconstruction using ePIE algorithm

Recon Real Part

Recon Imag Part

Potential Speedup

Forward Model

Aperture Field → **Propagate** → Probe Field * Object Region = Object Field → **Propagate** → Detector Field

Intensity Data

Modify Probe ← Modify Object ← Object Field ← **(Propagate)$^{-1}$** ← Modified Detector Field

Phase information

Amplitude Information
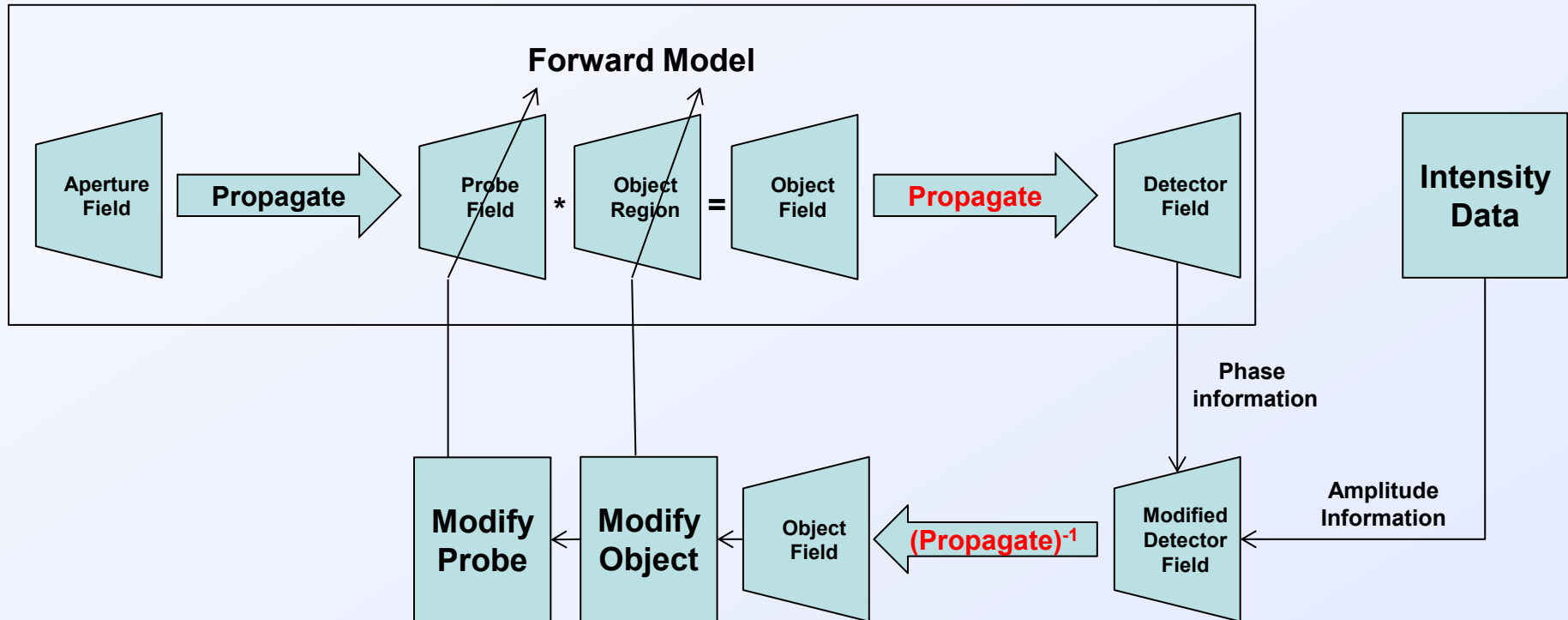
May be accelerated 2x – 5x by use of Talinov transform (used in SATRN SI LDRD)

Potential Speedup

- Talinov transform is used in conjunction with beam propagation techniques to follow changes in beam scale over a propagation step*:
  - Warp the phase of the beam at the beginning of the step
  - Propagate a scaled distance
  - Remove the residual warping of the phase on the propagated beam
  - The final propagated beam is in the newly scaled space.

- Talinov transform allows reductions in computational resolution and thus potentially speeds 2D and 3D reconstruction of ptychographic data.
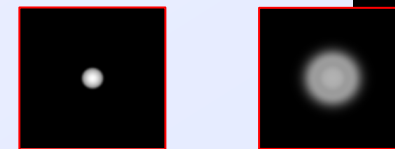
Optical System Example
Simulated using optical propagation code
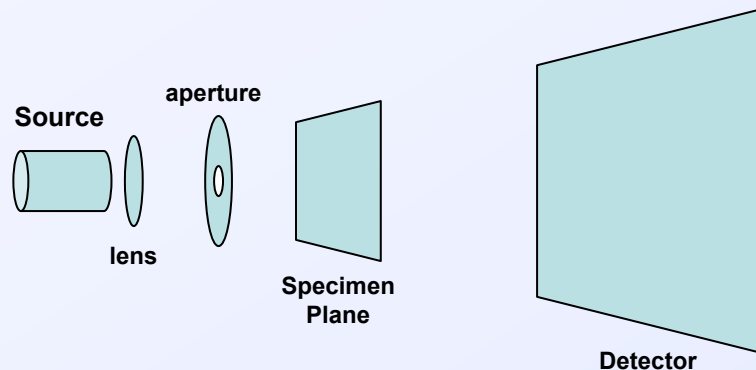
Aperture Plane **Specimen Plane** **Detector Plane**

Source **aperture**

lens

Specimen Plane

Without Talinov

Aliased

With Talinov

Detector

* E. Feigenbaum, R. A. Sacks, K. P. McCandless, and B. J. MacGowan, "Algorithm for Fourier propagation through the near-focal region," Applied Optics, V. 52, No. 20, pp. 5030-5035, July 10, 2013.

Reconstruction Software

- Written in C++
- Lenses, apertures, obscurations, moving stages, space, Talinov warped space, and projection to the far field are modeled as objects that operate on a complex wave field.
  - This allows many optical configurations of interest to be modeled
  - The optical configuration model is input via a model file
    - Both forward and reverse propagation models are derived from the same file
- Difference Map and ePIE method were implemented around the forward and reverse propagation models.
- I have implemented and explored the effects of the Talinov transform speedup with both ePIE and Difference Map methods. Expansions of space by a factor of 2 in each direction using the Talinov transform result in speedups by a factor of 4 in the reconstructions.
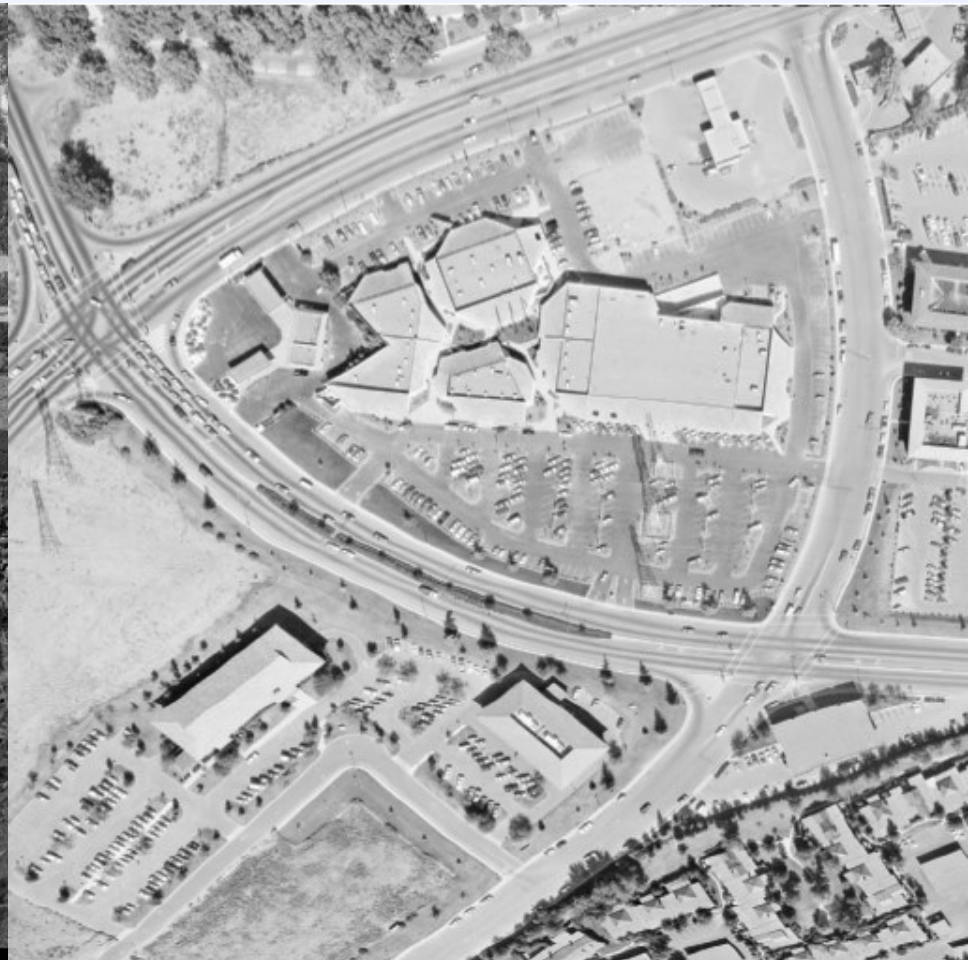
Test Images

Attenuation Image

Phase Image

Full resolution ePIE algorithm reconstruction

- Reconstruction was performed using ePIE algorithm

Full resolution ePIE algorithm reconstruction

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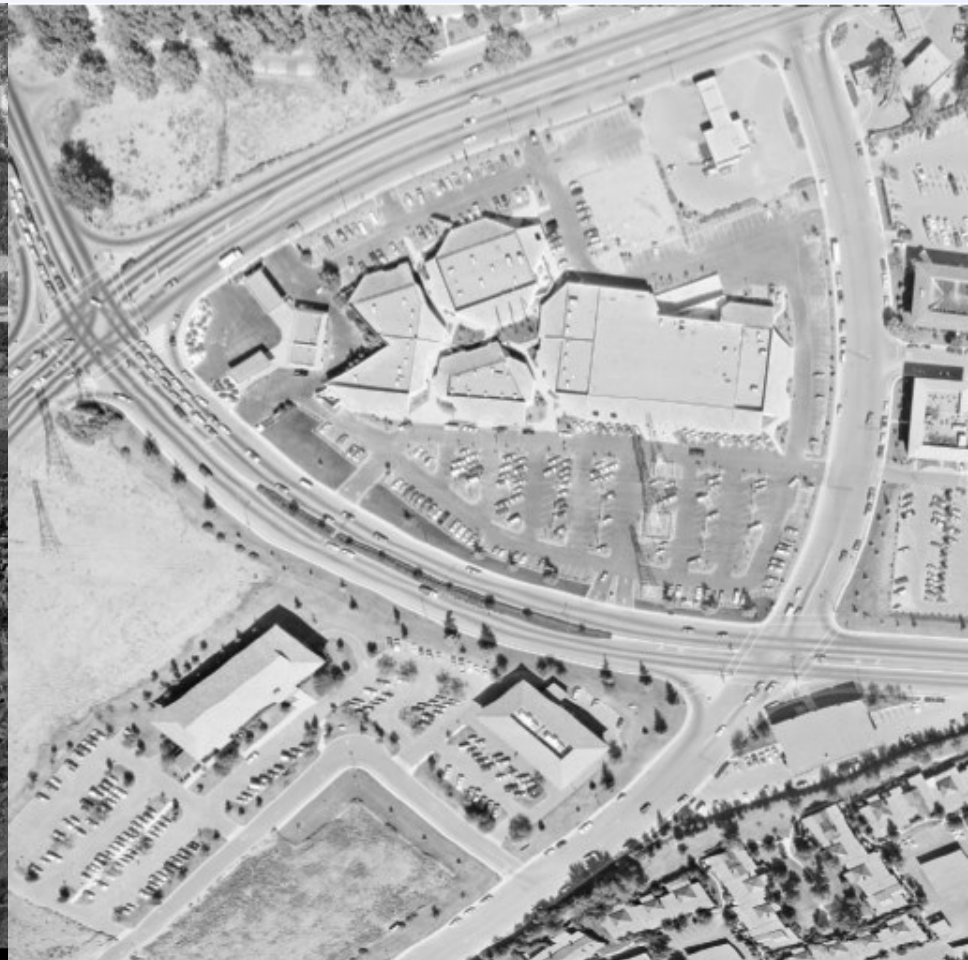
Test Images

Attenuation Image   Phase Image

Talinov transform cuts computation by a factor of four, but at a cost
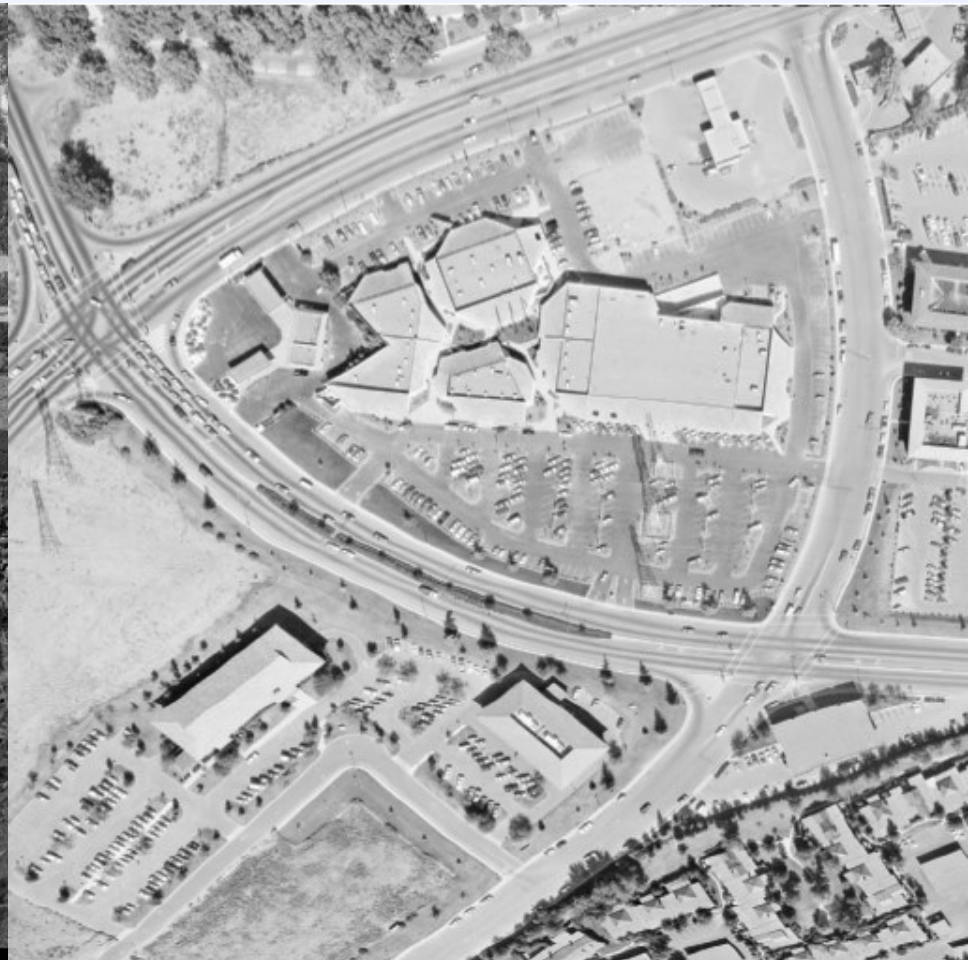
- Talinov transform was inserted into ePIE algorithm.

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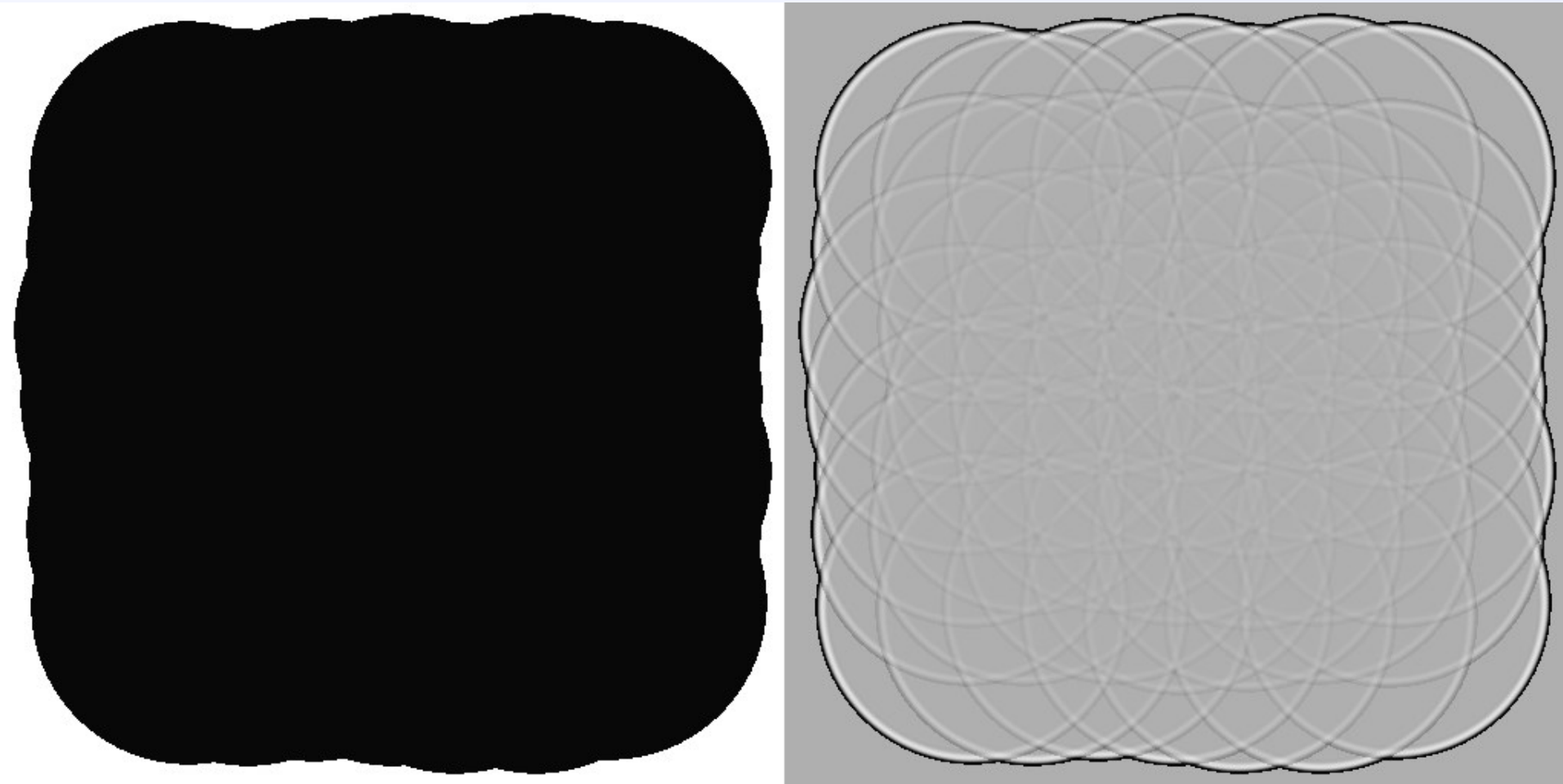
Test Images

Attenuation Image

Phase Image

Full Resolution Difference Map Reconstruction

- Reconstruction was performed using the Difference Map method

Full Resolution Difference Map Reconstruction

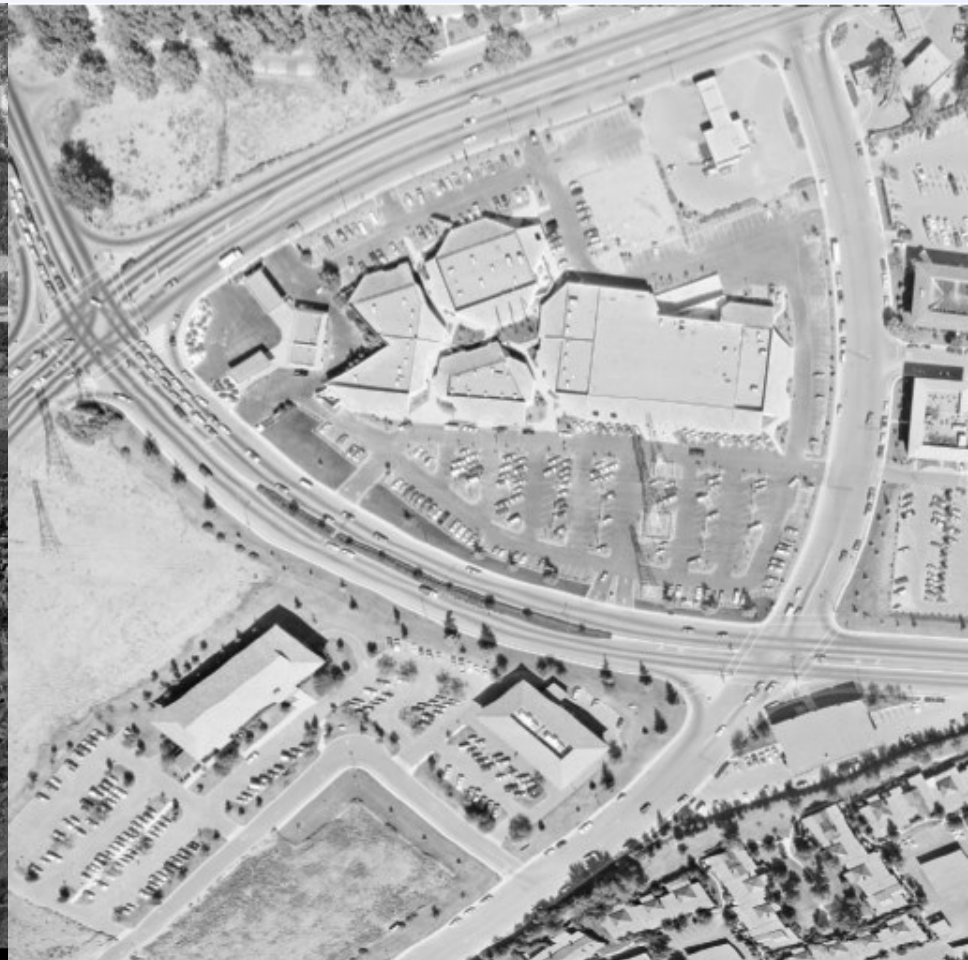- Reconstruction was performed using the Difference Map method
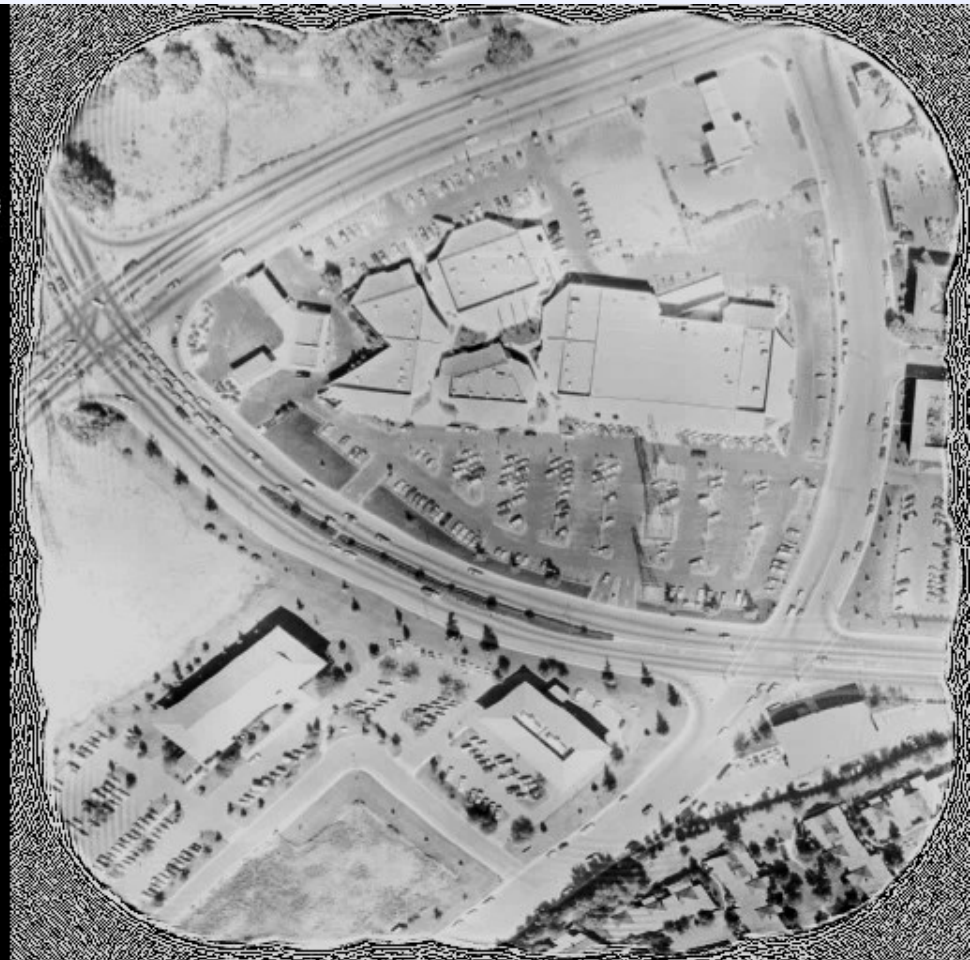
Test Images

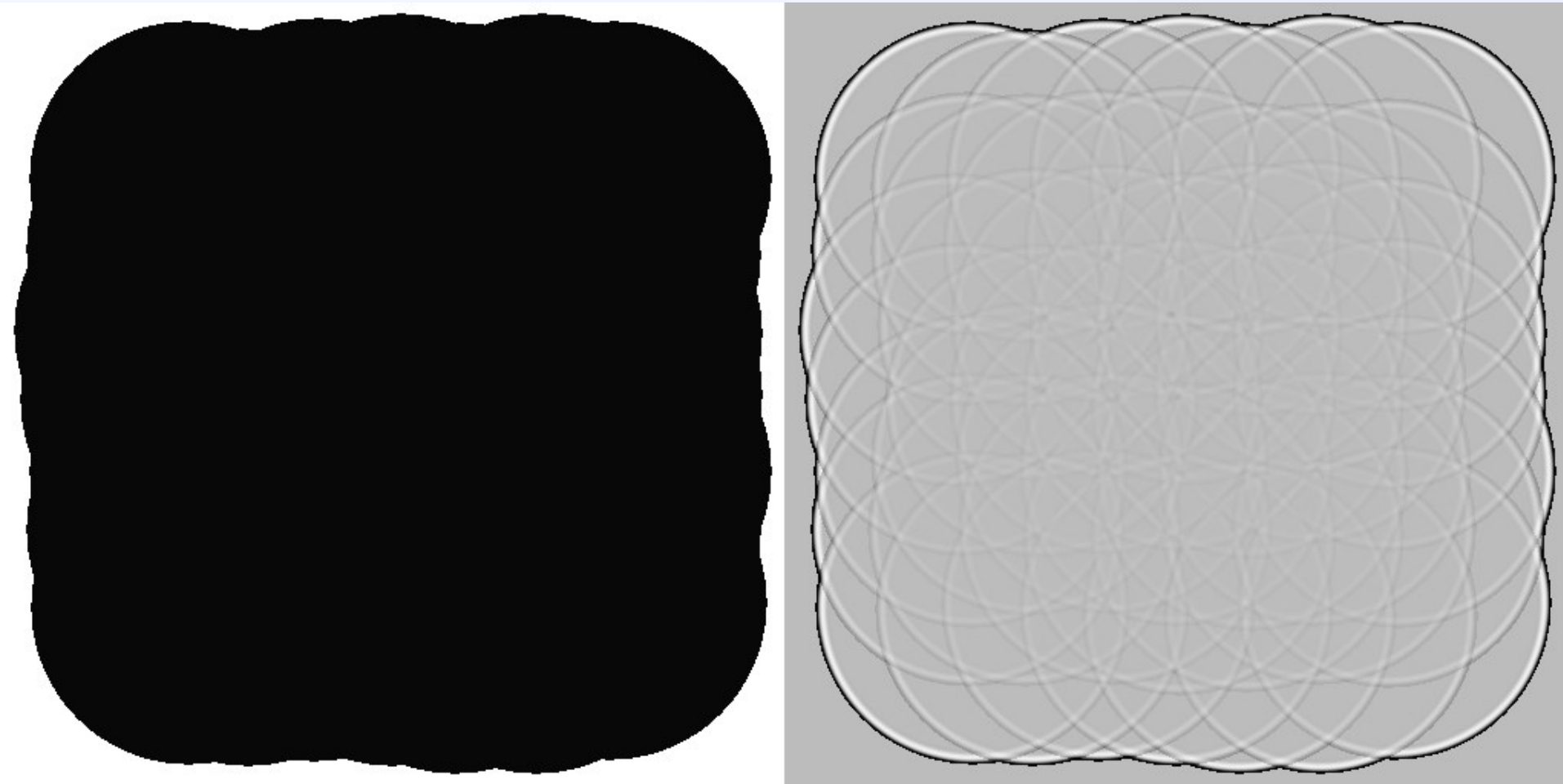Attenuation Image   Phase Image

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- Talinov transform was inserted into Difference Map algorithm.

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Talinov Transform Acceleration was Scooped

- In Applied optics, Vol. 54, No. 8, March 10, 2015 a paper by D. Claus and J. M. Rosenburg: "Pixel size adjustment in coherent diffractive imaging within the Rayleigh-Sommerfeld regime," was published.

- Essentially, the paper detailed the speedup and method of the Talinov Transform.

- Implementation in the paper was done using the ePIE algorithm.

Future work

- Build optical test bed so we can test these techniques using actual data.

- Implement conjugate gradient reconstruction scheme from: G. Guizar-Sicairos and J. R. Feinup, "Phase retrieval with transverse translation diversity: a nonlinear optimization approach," Optics Express, Vol. 16, No. 10, pp. 7264-7278, May 12, 2008.

  - There is another acceleration technique that can be applied here that may speed reconstruction by a factor of 10.

Summary

- I have built a C++ infrastructure for putting together ptychographic reconstruction codes and used it to implement the ePIE and Difference Map methods.

  - Difference Map method has problems with low frequencies and is slower to converge.

- I have incorporated the Talinov transform beam size following technique into the infrastructure

- Using the Talinov transform to quadruple the beam area reduces computation time by a factor of approximately 4.

  - ePIE reconstructions show high frequency leakage between the phase and the attenuation channels.

  - Difference Map reconstructions show less high frequency leakage between phase and amplitude channels

Acknowledgements

- This work is funded by LDRD 15-ERD-028

Disclaimer