

## INTRODUCTION AND MOTIVATION

- Coherence Diffraction imaging is a lensless approach to x-ray crystallography that enables structure determination of biological or noncrystalline samples.

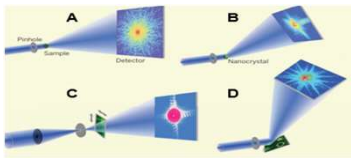


Figure 1. Different forms of CDI imaging methods a) Plane-wave CDI. b) Bragg's CDI. c) Fresnel CDI. d) Fresnel CDI. [2]

- A unique problem found within various fields of imaging and signal processing is the phase problem
- Another common problem found in CDI experiments using high intensity light is missing information when the center intensities are blocked by a beam stop
- Ultimate aims: Overcome the phase problem and various experimental setups such that result in missing information

## METHODOLOGY

- Using MATLAB to simulate CDI experiments to reconstruct an image from an object's diffraction pattern.
- Utilize a conventional HIO algorithm to account for the phase problem and reconstruct an image object.
- Utilize a modified HIO algorithm to overcome missing information such as due to a central beam stop.

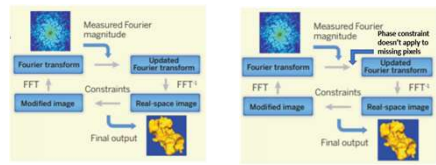


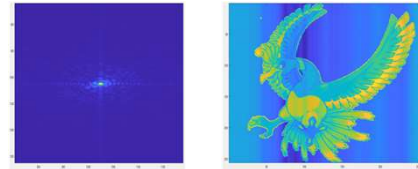
Figure 2. a) Concept behind HIO algorithm, enforcing real space constraints as well as Fourier space constraints b) Concept behind modified HIO algorithm, enforcing added Fourier space constraint on pixels with missing information[2].

## OVERSAMPLED PURE PHASE IMAGE RECONSTRUCTION

- A coherent light source is shone on a pure phase object with an opaque rectangular support
- The light is diffracted an infinite distance and detected by a 2048x2048 pixel array detector
- Thus, the detector measures the Fourier transform of the original image leading the well described phase problem [1]
- The rectangular support can be determined by analyzing the fringes in the diffraction pattern measured by the detector (Figure 3a.)
- With the support size the phase information can be recovered through the HIO algorithm [1] and
- The quality of a reconstructed image can be quantified by an R factor which for an accurate reconstructed image converges to zero (Equation 1)

$$f_{i+1}(x) = \begin{cases} f'_{i+1}(x) & f_i(x) \in S \& \text{imag}(f_i(x)) \geq 0 \\ f_i(x) - \beta f'_{i+1}(x) & \text{else} \end{cases}$$

Equation 1. The updating scheme for the HIO algorithm. This scheme forces the pixels outside of the support and those with negative imaginary values to zero. This is slightly different that the error reduction algorithm as the speed of changing the values to zero is controllable with beta.



$$R_{i+1} = \frac{\sum_{\text{pixels}} |G_{i+1}(k)| - \sum_{\text{pixels}} |G_i(k)|}{\sum_{\text{pixels}} |G_{i+1}(k)|}$$

Equation 2. The R factor is given by the difference between two consecutive reconstructed images in Fourier space. As the algorithm completes more iterations the R factor should drop to zero.

Figure 3. a) Original diffraction pattern. b) Reconstructed image with original HIO algorithm. c) Reconstructed image with modified HIO algorithm.

## RECONSTRUCTION OF BACTERIOPHAGE MS2 DIFFRACTION PATTERN WITH MISSING LOW FREQUENCY INFORMATION

- A similar diffraction pattern to that of the oversampled pure phase but with the center pixels change to have a zero value
- The center of the diffraction pattern contains low frequency information and is commonly blocked by way of a beam stop
- This is common practice to block the direct beam with a beam stop to protect the detector and avoid oversaturation pixels [3][4]
- The HIO algorithm can be updated to neglect the pixels blocked by the beam stop in order to accurately retrieve the phase information (Equation 3)
- The modified HIO algorithm was tested on a known diffraction pattern with a simulated beam stop and accurately reconstructed the image (Figure 4) and was able to accurately recreate the MS2 virus (Figure 5)

$$G'_{i+1}(k) = \begin{cases} G_{i+1}(k) & k \notin D \\ |F(k)|e^{i\phi} & \text{else} \end{cases}$$

\*  $k \notin D$  represents pixels blocked by beamstop  
\*  $e^{i\phi}$  represents the phase term of  $G_{i+1}(k)$

Equation 3. The updating scheme for the HIO algorithm. This scheme forces the pixels outside of the support and those with negative imaginary values to zero. This is slightly different that the error reduction algorithm as the speed of changing the values to zero is controllable with beta.

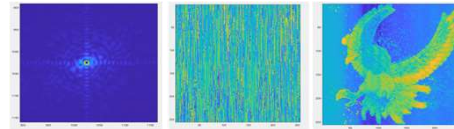


Figure 4. a) Original diffraction with the 4x4 pixel center manually set to value zero. b) Reconstructed image with original HIO algorithm. c) Reconstructed image with modified HIO algorithm.

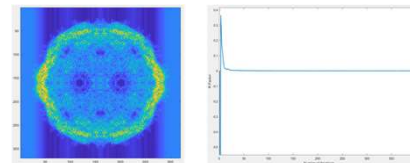


Figure 5. a) MS2 Virus image reconstruction with  $\beta = 0.15$ , 2000 iterations b) R factor for the MS2 Virus image reconstruction

## RECONSTRUCTION OF EXPERIMENTAL X-RAY DIFFRACTION FROM SCHIZOSACCHAROMYCES POMBE SPORE (YEAST)

- The experimental X-Ray diffraction image is like that of the MS2 diffraction pattern in that the low frequency phase information is lost due to the beam stop. Our treatment of this problem is the same as before.
- In our analysis of the yeast cell, we neglected absorption and considered only real electron density, forcing the imaginary terms in the reconstruction to zero (Equation 4)
- For the yeast reconstruction the erf F function was used to quantify the quality of reconstruction (Equation 5)(Figure 6)

$$f_{i+1}(x) = \begin{cases} f'_{i+1}(x) & f_i(x) \in S \& \text{real}(f_i(x)) \geq 0 \\ f_i(x) - \beta f'_{i+1}(x) & \text{else} \end{cases}$$

Equation 4. Modified HIO algorithm where the only values that aren't forced to zero are those inside the support with real-positive values

Equation 5. Error function for the ith iteration

$$\text{erf } F_i = \frac{|\sum_{\text{pixels}} F_i(k)| - |\sum_{\text{pixels}} F(k)|}{|\sum_{\text{pixels}} F(k)|}$$

\*  $H(k)$  represents the Fourier transform of the current iteration outside the beam stop

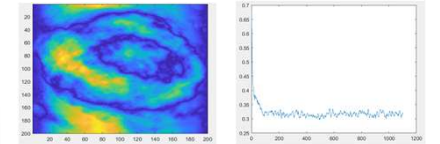


Figure 5. a) Yeast cell image reconstruction with  $\beta = 0.50$ , 2000 iterations b) erf F for the Yeast cell image reconstruction

## SUMMARY

Problem	Solution
Oversampled pure phase object scattered at far field.	Original HIO algorithm.[1]
MS2 virus image with missing low frequency information at center of diffraction pattern.	Modified HIO algorithm. $G'_{i+1}(k) = \begin{cases} G_{i+1}(k) & k \notin D \\  F(k) e^{i\phi} & \text{else} \end{cases}$
Yeast cell image from experimental X-Ray diffraction with missing low frequency information.	Updated modified HIO algorithm that enforces real-positive value constraint in real space.

Table 1. Overview of unique problems with phase retrieval experiments and our solutions.

## References

- [1] J. Miao, D. Sayre, and H. N. Chapman, Journal of the Optical Society of America A **15**, 1662 (1998).
- [2] J. Miao, T. Ishikawa, I. K. Robinson, and M. M. Murnane, Science **348**, 530 (2015).
- [3] C.-C. Chen, J. Miao, C. W. Wang, and T. K. Lee, Physical Review B **76**, (2007).
- [4] H. Jiang, C. Song, C.-C. Chen, R. Xu, K. S. Ramesh, B. P. Fahimian, C.-H. Lu, T. K. Lee, A. Nakashima, J. Urano, T. Ishikawa, F. Tamanoi, and J. Miao, Proceedings of the National Academy of Sciences **107**, 11234 (2010).