X-Ray Beam Characterization by Robust Phase Retrieval with Transverse Translation Diversity

James R. Fienup
Robert E. Hopkins Professor of Optics
Gregory R. Brady and Manuel Guizar-Sicairos
University of Rochester
Institute of Optics

Presented at
Workshop on X-ray Science
at the Femtosecond to Attosecond Frontier
UCLA, May 19, 2009
Outline

- Phase retrieval background (prequel to Keith Nugent’s talk)
  - Image reconstruction -- CDI
  - Optical metrology / wavefront sensing / beam characterization

- Transverse translation diversity in the focused beam
  - Results of x-ray experiments

- Transverse translation diversity in the pupil plane
  - Results of optical experiments
Phase Retrieval Basics

Fourier transform: \( F(u,v) = \int \int_{-\infty}^{\infty} f(x,y) e^{-i2\pi(ux + vy)} dx \, dy \)

\[ = |F(u,v)| e^{i\psi(u,v)} = \mathcal{F}[f(x,y)] \]

Inverse transform: \( f(x,y) = \int \int_{-\infty}^{\infty} F(u,v) e^{i2\pi(ux + vy)} du \, dv = \mathcal{F}^{-1}[F(u,v)] \)

Phase retrieval problem:

| Given \( |F(u,v)| \) and some constraints on \( f(x,y) \),
| Reconstruct \( f(x,y) \), or equivalently retrieve \( \psi(u,v) \) |

\( |F(u,v)| = |\mathcal{F}[f(x,y)]| = |\mathcal{F}[e^{i\psi} f(x-x_0, y-y_0)]| = |\mathcal{F}[e^{i\psi} f^* (-x-x_0, -y-y_0)]| \)

(Inherent ambiguities: phase constant, images shifts, twin image all result in same data)

Autocorrelation:

\[ r_f(x,y) = \int \int_{-\infty}^{\infty} f(x',y') f^* (x' - x, y' - y) dx' \, dy' = \mathcal{F}^{-1}[|F(u,v)|^2] \]

- Patterson function in crystallography is an aliased version of the autocorrelation
- Simply need Nyquist sampling of the Fourier intensity to avoid aliasing
Constraints in Phase Retrieval

- **Nonnegativity constraint:** $f(x, y) \geq 0$
  - True for ordinary incoherent imaging, *x-ray diffraction, MRI*, etc.
  - Not true for wavefront sensing or coherent imaging

- **The support of an object** is the set of points over which it is nonzero
  - Meaningful for imaging objects on dark backgrounds
  - Wavefront sensing through a known aperture
  - A good support constraint is essential for complex-valued objects
    - Coherent imaging or wave front sensing

- **Atomiticity when have angstrom-level resolution**
  - For crystals -- *not* applicable for coarser-resolution, single-particle

- **Object intensity constraint** (wish to reconstruct object phase)
  - E.g., measure wavefront intensity in two+ planes (*Gerchberg-Saxton*)
  - If available, supercedes support constraint
Example on Real X-Ray Data
(Data from M. Howells/LBNL and H. Chapman/LLNL)

(a) X-ray data
(b) Autocorrelation from (a)
(c) Initial Support constraint computed from (b)
(d) Electron micrograph of object
Iterative Transform Algorithm

\[ g_{k+1}(x, y) = \begin{cases} 
  g'_k(x, y), & g'_k(x, y) \text{ satisfies constraints} \\
  g_k(x, y) - \beta g'_k(x, y), & g'_k(x, y) \text{ violates constraints}
\end{cases} \]
First Phase Retrieval Result

(a) Original object, (b) Fourier modulus data, (c) Initial estimate
(d) – (f) Reconstructed images — number of iterations: (d) 20, (e) 230, (f) 600

Image Reconstruction from Simulated Speckle Interferometry Data

Labeyrie’s stellar speckle interferometry gives this

Phase retrieval from experimental far-field speckle data

J. N. Cederquist, J. R. Fienup, J. C. Marron, and R. G. Paxman

Optical Science Laboratory, Advanced Concepts Division, Environmental Research Institute of Michigan, P.O. Box 8618, Ann Arbor, Michigan 48107

Received March 11, 1988; accepted May 20, 1988

Phase retrieval from experimental (laboratory) data has been successfully demonstrated. A diffuse object was coherently illuminated and Fourier intensity data were collected by a charge-coupled device detector and a video digitizer. By using the data and an a priori triangular image support constraint, an iterative Fourier-transform algorithm was used to estimate the phase of the Fourier transform of the object. The reconstructed image compares favorably with a conventional image with the same spatial-frequency bandwidth.

Predates x-ray by > 1 decade
PROCLAIM 3-D Imaging Concept
Phase Retrieval with Opacity Constraint LAser IMaging

- tunable laser
- direct-detection array
- collected data set
- initial estimate from locator set
- phase retrieval algorithm
- 3-D FFT
- reconstructed object
ST Object. The three concentric discs forming a pyramid can be seen as dark circles at their edges. The small piece on one of the two lower legs was removed before this photograph was taken.

3-D Laser Fourier Intensity
Laboratory Data

Data cube:
1024x1024 CCD pixels x 64 wavelengths

Shown at right:
128x128x64 sub-cube
(128x128 CCD pixels at each of 64 wavelengths)
Coherent Image Reconstructed by ITA from One 128x128x64 Sub-Cube
Measurements & Constraints:
- Pupil plane: known aperture shape
  phase error fairly smooth function
- Focal plane: measured PSF intensity

Wavefronts in pupil plane and focal plane are related by a Fourier Transform
Nonlinear Optimization Algorithms
Employing Gradients

Minimize Error Metric, e.g.: \[ E = \sum_u W(u)[|G(u)| - |F(u)|]^2 \]

Contour Plot of Error Metric

pupil model: \[ g(x) = |g(x)| e^{i\phi(x)} , \quad G(u) = F[g(x)] \]

Repeat three steps:

1. Compute gradient:
   \[ \frac{\partial E}{\partial p_1}, \frac{\partial E}{\partial p_2}, \ldots \]

2. Compute direction of search

3. Perform line search

Gradient methods:
(Steepest Descent)
Conjugate Gradient
BFGS/Quasi-Newton

\[ e(x) = \sum g(x) = \sum g(x) e^{i\phi(x)} \]
Analytic Gradients with Phase Values as Parameters

\[ E = \sum_u W(u)[|G(u)| - |F(u)|]^2 \]
\[ G(u) = P[g(x)] \]

Optimizing over \( g(x) = g_R(x) + i g_I(x) = m_o(x)e^{i\theta(x)}, \ \theta(x) = \sum_{j=1}^{J} a_j Z_j(x) \)

For point-by-point pixel (complex) value, \( g(x) \),
\[ \frac{\partial E}{\partial g(x)} = 2 \text{ Im}\left\{g^W*(x)\right\} \]

For point-by-point phase map, \( \theta(x) \),
\[ \frac{\partial E}{\partial \theta(x)} = 2 \text{ Im}\left\{g(x)g^W*(x)\right\} \]

For Zernike polynomial coefficients,
\[ \frac{\partial E}{\partial a_j} = 2 \text{ Im}\left\{\sum_x g(x)g^W*(x)Z_j(x)\right\} \]

where
\[ G^W(u) = W(u) \left[ |F(u)| \frac{G(u)}{|G(u)|} - G(u) \right] \]

\( P[*] \) can be a single FFT or multiple-plane Fresnel transforms with phase factors and obscurations

Analytic gradients very fast compared with calculation by finite differences

Optical wave fronts (phase) can be measured by many forms of interferometry.

Novel wave front sensor: a bare CCD detector array, detects reflected intensity.

Wave front reconstructed in the computer by phase retrieval algorithm.

Approach:

Simulation Results:
- PSF at z=333um: True Phase
- PSF at z=500um: Retrieved Phase
- PSF1: Actual wrapped phase
- PSF2: Reconstructed wrapped phase
Reconstructing Pupil Phase and Amplitude

-60mm

-40mm

-25mm

Circular pupil
dia. = 10mm

f = 500mm
Complex Pupil Function Reconstructions

<table>
<thead>
<tr>
<th></th>
<th>Two measurement planes</th>
<th>Three measurement planes</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Actual</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Amplitude</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Phase (waves)</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Guess</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Retrieved</strong></td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>RMS reconstruction error</strong></td>
<td>0.029λ</td>
<td>0.017λ</td>
</tr>
</tbody>
</table>

G. Brady, U.R.
Phase Retrieval with Transverse Translation Diversity for Coherent Diffractive Imaging and X-ray Beam Characterization

Manuel Guizar-Sicairos and James R. Fienup

The Institute of Optics, University of Rochester,
Rochester, NY, 14627
Transverse translation diversity
(Ptychography)

Moving the sample with respect to a known illumination pattern can provide suitably diverse measurements

Makes phase retrieval more robust to noise and ambiguities

Problem statement

\( o(x,y) \)  
\( p(x,y) \)  
\( f_n(x,y) \)

Unknown object
Known illumination function
Field for \( n \)-th position of \( o(x,y) \)

\[
f_n(x, y) = o(x - x_n, y - y_n) p(x, y)
\]

\[
I_n(u, v) = |F_n(u, v)|^2
\]

Measure the far-field intensity for different object positions

\( p(x,y) \) can be:
- An aperture close to the object
- The beam diffracted from an aperture
- A focused beam
Ptychographical iterative engine (PIE)

PIE is an iterative transform reconstruction method.

Closely related to a steepest descent search for the $n$-th diversity field

J. M. Rodenburg et al.,
Reconstruction with the PIE – Noiseless simulation

Known aperture
Object Amplitude Phase

[-0.4 0.4] rads

Reconstruction Amplitude Phase

172x210 portions of 256x256 arrays
Introducing errors in \textit{a priori} known information

RMSE in translations $\Delta r = 0.8$ pixels

Aperture radius 52 pixels (instead of 50)

Either from not knowing the aperture or the distance to the detector exactly

Assumed illumination

True illumination

Object

Amplitude

Phase

Reconstruction with the PIE

Amplitude

Phase
Nonlinear optimization approach

It allows to include nonideal experimental scenarios and optimize over inaccurately known parameters

Error metric

\[ \varepsilon = \sum_{n=1}^{q} \sum_{u,v} W_n(u,v) \left\{ \left[ |\hat{F}_n(u,v)|^2 + \delta \right]^{\gamma} - \left[ I_n(u,v) + \delta \right]^{\gamma} \right\}^2 \]

- Weighting
- Field estimate
- Measured data

we use \( \gamma = 0.5 \), \( \delta \ll I_n(u,v) \)

Field estimate for the nth diversity image

\[ \hat{F}_n = \text{DFT} \left\{ \hat{f}_n(x, y) \right\} = \text{DFT} \left\{ \hat{o}(x - \hat{x}_n, y - \hat{y}_n) \hat{p}(x, y) \right\} \]

- Estimate of object transmittance
- Known illumination pattern
Analytic expressions for the gradients

Gradient of error metric w.r.t. object and system parameters allows joint optimization

\[
\frac{\partial \varepsilon}{\partial \hat{\varOmega}_R(x, y)} + i \frac{\partial \varepsilon}{\partial \hat{\varOmega}_I(x, y)} = 4 \sum_{n=1}^{q} \hat{p}^*(x + \hat{x}_n, y + \hat{y}_n) \text{IDFT}\left\{ W_n \left[ \left( |\hat{F}_n|^2 + \delta \right)^\gamma - \left( I_n + \delta \right)^\gamma \right] \right.
\]
\[
\times \gamma \left( |\hat{F}_n|^2 + \delta \right)^{\gamma^{-1}} \hat{F}_n \exp \left[i2\pi \left( \frac{u\hat{x}_n}{M} + \frac{v\hat{y}_n}{N} \right) \right] \bigg\}
\]

\[
\frac{\partial \varepsilon}{\partial \hat{p}_R(x, y)} + i \frac{\partial \varepsilon}{\partial \hat{p}_I(x, y)} = 4 \sum_{n=1}^{q} \hat{\varphi}^*(x - \hat{x}_n, y - \hat{y}_n) \text{IDFT}\left\{ W_n \left[ \left( |\hat{F}_n|^2 + \delta \right)^\gamma - \left( I_n + \delta \right)^\gamma \right] \right.
\]
\[
\times \gamma \left( |\hat{F}_n|^2 + \delta \right)^{\gamma^{-1}} \hat{F}_n \bigg\}
\]

\[
\frac{\partial \varepsilon}{\partial \hat{x}_n} = \frac{8\pi}{M} \sum_{u, v} W_n \left[ \left( |\hat{F}_n|^2 + \delta \right)^\gamma - \left( I_n + \delta \right)^\gamma \right] \gamma \left( |\hat{F}_n|^2 + \delta \right)^{\gamma^{-1}}
\]
\[
\times \text{Im} \left[ \hat{F}_n^* \text{DFT} \left( \hat{p}(x, y) \text{IDFT} \left\{ u' \hat{\varphi}(u', v') \exp \left[-i2\pi \left( \frac{u'\hat{x}_n}{M} + \frac{v'\hat{y}_n}{N} \right) \right] \right\} \right) \right] \bigg]\]

Reconstructions with errors in a priori known information

PIE reconstruction

NL optimization (conjugate gradient)

True illumination

Initial estimate

After joint optimization
Numerical simulation

Illumination function is the field propagated from an aperture

\[ p(x, y) \]
\[ o(x, y) \]

Added photon noise \(-10^5\) photons on the brightest pixel in the diffraction pattern

Original image courtesy of Brainmaps.org
Reconstruction with errors in the \textit{a priori} known parameters

\[ r = 1.762 \text{ pixel (RMS)} \]

Reconstruction with PIE

Reconstruction with NL optimization
**Reconstruction of a 1D focus**

**Reverse of ptychography**: use structure in beam to characterize unknown beam rather than known beam to reconstruct unknown structure.

Numerical simulations show that 1D phase retrieval with a moveable structure yields robust reconstructions.

An experiment was performed at Argonne for comparing results from 1D phase retrieval and fluorescent scanning.


\[ \lambda = 0.1 \text{ nm} \]

\[ f = 10 \text{ cm} \]

\[ D = 200 \mu m \]

Reconstruction of a 1D focus

Numerical simulations show that 1D phase retrieval with a moveable structure yields robust reconstructions.

An experiment was performed at Argonne for comparing results from 1D phase retrieval and fluorescent scanning.

Data collected by Kenneth Evans-Lutterodt, A. Stein, A. Isakovic, J. Warren (BNL), A. Sandy, S. Narayanan and M. Sprung (ID8 beamline).

Point detector to measure fluorescence from chrome

\( \lambda = 0.1 \text{ nm} \)

SEM image of the structure

30 nm chrome slab

40 nm steps
Reconstruction of a 1D focus

Numerical simulations show that 1D phase retrieval with a moveable structure yields robust reconstructions.

An experiment was performed at Argonne for comparing results from 1D phase retrieval and fluorescent scanning.

Data collected by Kenneth Evans-Lutterodt, A. Stein, A. Isakovic, J. Warren (BNL), A. Sandy, S. Narayanan and M. Sprung (ID8 beamline).

$\lambda = 0.1 \text{ nm}$

30 nm chrome slab

Silicon

YAG crystal

Objective

Point detector to measure fluorescence from chrome

CCD
A diffraction pattern was recorded for each position of the structure
Deconvolution by Wiener filter

Intensity patterns are severely blurred by the spatial response of the YAG crystal.

We estimated the PSF and deconvolved each frame.
Integrated measurement

We integrate data along the non-focusing direction for input to the 1D phase retrieval algorithm.

1D intensity data for phase retrieval

Removed additional “bias”, a residual convolution effect.
Reconstruction vs. fluorescent scanning

Intensity

Fluorescence
Phase retrieval
Initial estimate

Phase

Radians

y [μm]

y [μm]
Numerical propagation

Independent scan  Reconstruction plane

Intensity

\( y [\mu m] \)

\( z [\mu m] \)

Fluorescence  Phase retrieval

\( y [\mu m] \)
Phase retrieval with transverse translation diversity can be used for **coherent lensless imaging** and to **characterize a focused x-ray beam in situ**

- Reconstructions are robust to noise, stagnation and ambiguities
- Structure and translations can be much larger than the resolution to achieve
- Reconstructed field can be propagated to a plane of interest
- We expect a great improvement on the reconstructions by bare CCD detection or by carefully characterizing the detection PSF

Joint optimization allows for object reconstruction and simultaneous refinement of the **illumination pattern** and object **translations**

- Each iteration takes ~ 4 times longer than the PIE (~ 6 times when jointly optimizing)

Error metric can include experimental non-ideal scenarios

- Detector misalignments or drift
- Different bias or scaling factors on the diffraction patterns
Optical Wavefront Measurement Using Transverse-Translation-Diverse Phase Retrieval

Gregory R. Brady*, Manuel Guizar-Sicairos and James R. Fienup

The Institute of Optics
University of Rochester
Rochester, NY, USA 14627

*Now with Sandia National Laboratories
PO Box 5800
Albuquerque, NM, USA 87111

The support of the Center for Electronic Imaging Systems (CEIS) / New York State Office of Science, Technology, and Academic Research (NYSTAR) and Corning Tropel Corporation is gratefully acknowledged
Motivation

- Phase retrieval is limited by the sampling of the measured intensity distribution and the size of the detector array.
- Beams that converge at a large angle produce high frequency features, which must be sampled adequately by the detector array.
  - Defines a limit on f-number or numerical aperture:
    \[
    \frac{f}{\#} \geq \frac{2d_\xi}{\lambda} \quad \text{and} \quad NA \leq \frac{\lambda}{4d_\xi}
    \]
- Wavefront aberrations increase the size of the spot on the detector, so the size of the detector limits the amount of aberration:
  \[
  \left[ \frac{\partial W(\rho)}{\partial \rho} \right]_{\text{max}} \leq \frac{\lambda N}{8}
  \]
- If we decrease the diameter of the aperture under test, f-number increases, numerical aperture decreases, and wavefront slope decreases.
- Allows us to perform phase retrieval on the measured data, but only measure a small region – How do we measure the whole wavefront?

Transverse Translation Diversity

- Take many measurements using different subaperture positions, reconstructing single underlying wavefront
- Optimize field over entire clear aperture using all subaperture measurements jointly
- Allows for measurement of faster beams, more wavefront error, more robust
- Insensitive to positioning errors of subaperture (optimized for)
- Can solve for phase only or amplitude and phase of both the wavefront being measured and the subaperture

![Diagram of Transverse Translation Diversity](image_url)
TDD PR Algorithm

• Model the field immediately after the subaperture in the \(n\)th position as the product of the field of interest \(h\) and the subaperture pupil function \(a\)

\[
g_n(x, y) = h(x + x_n, y + y_n) a(x, y)
\]

• For each position the field is propagated to the detector plane using scalar diffraction techniques, represented by the operator \(P[\ ]\)

\[
G_n(u, v) = P\left[ g_n(x, y) \right]
\]

• In this work, the model used was a Fresnel propagation to the focal plane and angular spectrum propagation from there to the plane of the CCD:

\[
G_n^f(u', v') = \exp \left\{ \frac{i\pi}{\lambda z} \left[ (u'd_u)^2 + (v'd_v)^2 \right] \right\} \text{DFT} \left[ g_n(x, y) \right],
\]

\[
G_n(u, v) = \text{IDFT} \left[ \text{DFT} \left[ G_n^f(u', v') \right]\exp \left\{ i2\pi\Delta z \left[ \frac{1}{\lambda^2} - \left( \frac{r}{Nd_u} \right)^2 - \left( \frac{s}{Nd_v} \right)^2 \right]^{\frac{1}{2}} \right\} \right],
\]
From the measured intensity patterns we have the field magnitudes
\[ |F_n(u,v)| = \sqrt{I_n(u,v)} \]

Compare the measured amplitudes to the computed ones using an error metric
\[ E = \sum_{n=1}^{q} \sum W_n(u,v) \left[ |F_n(u,v)| - |G_n(u,v)| \right]^2, \]

The metric is minimized with an optimization algorithm (e.g. conjugate gradient) that varies parameters describing the subaperture field, \( g_n(x,y) \)

Compute derivatives required by the algorithm using analytical expressions

These make repeated use of a few terms, which we define here:

\[ G_n^w(u,v) = W_n(u,v) \left[ |F_n(u,v)| \frac{G_n(u,v)}{|G_n(u,v)|} - G_n(u,v) \right], \]

\[ g_n^w(x,y) = P^\dagger \left[ G_n^w(u,v) \right] \]

where the operator \( P^\dagger[\ ] \) is the inverse of the operator \( P[\ ] \)
Analytic Derivatives

• Example: Phase of the field of interest

\[
\frac{\partial E}{\partial \theta_h(x', y')} = 2 \text{Im} \left[ \sum_{n=1}^{q} g_n^w(x' - x_n, y' - y_n) h(x', y') a(x' - x_n, y' - y_n) \right].
\]

• Example: Amplitude of the field of interest

\[
\frac{\partial E}{\partial |h(x', y')|} = -2 \text{Re} \left[ \sum_{n=1}^{q} g_n^w(x' - x_n, y' - y_n) a(x' - x_n, y' - y_n) \exp \left[ i \theta_h(x', y') \right] \right].
\]

• Can write similar expressions for the subaperture, \(a\), including phases

• Finally, the subaperture positions \((x_n, y_n)\) can also be free parameters

\[
\frac{\partial E}{\partial x_n'} = \frac{4\pi}{M} \text{Im} \left\{ \sum_{x,y} g_n^w(x, y) a(x, y) \text{DFT} \left[ u' \exp \left[ i2\pi \left( \frac{x_n' u'}{M} + \frac{y_n' v'}{M} \right) \right] \right] \text{DFT} \left[ h(x, y) \right] \right\}.
\]

• For more details and other parameterizations see the reference below

Experimental Arrangement

- HeNe Laser
- ND Filter
- Pinhole
- Microscope Objective: f=250 mm
- Clear Aperture
- Lens
- Moving Subaperture
- Stage (two axes)
- Lens in mount
- Moving subaperture
- Stage (one axis)
- CCD Camera
- Image of subaperture: 9.9 mm
• Measured lens over 33.32 mm diameter aperture using 43 positions of a 9.9 mm subaperture
• F-number of 9.1, would be undersampled if it was a full aperture measurement
Reconstructed Amplitude and Phase

Scratches on the lens were reconstructed
Comparison of Independent Measurement

- Took 17 intensity measurements covering central region of previous larger aperture result
- Performed reconstruction using same algorithm with this independent data

RMS Difference = 0.0107 waves
Summary (Greg Brady)

- For highly aspheric beams, smaller subaperture limits field extent for **adequate sampling and capturing intensity**, needed by phase retrieval
- Multiple **transverse translations** of the subaperture map out entire area of interest
- Intensity patterns from are collected and the phase retrieval algorithm optimizes over them **jointly**
- Optimize over multiple unknowns
  - Field of interest \((h)\)
    - Zernike coefficients, real and imaginary parts etc.
  - Subaperture \((a)\)
  - Translations of the subaperture
- Experimentally verified
  - Two independent collections and retrievals agreed to about \(\lambda/100\)
Phase Retrieval and Imaging Science Group