X-ray wave propagation in PETSc

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Outline

Introduction

Synchrotron light sources

- Accelerate electrons close to speed of light, then bend the beam to produce "bright" x-rays.

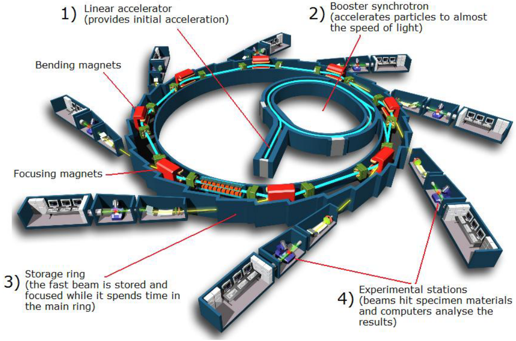
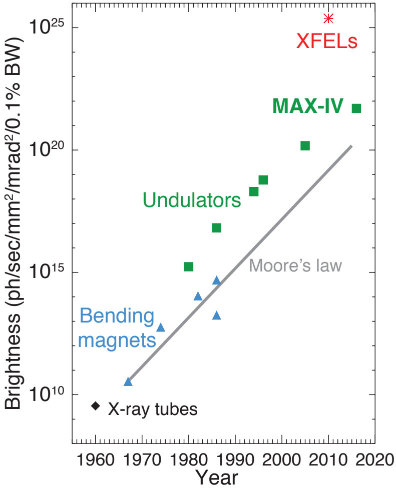


Figure: Synchtrotron schematic[1]

[1] https://dc.edu.au/hsc-physics-quanta-to-quarks/

More than Moore! [2]



[2] Jacobsen [2016]

Zone Plates

Focusing X-Rays

- Ref. index$\rightarrow$ complex,slightly < 1
- Zone plates$\rightarrow$ monochromatic diffractive optics.
- Consist of alternate rings of low and high refractive index materials placed such that the outgoing waves constructively interfere with each other at the focal spot.

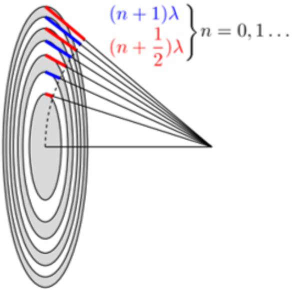


Figure: Illustration of zone plate [3]

[3] Jacobsen [2019]

Zone plates in action!

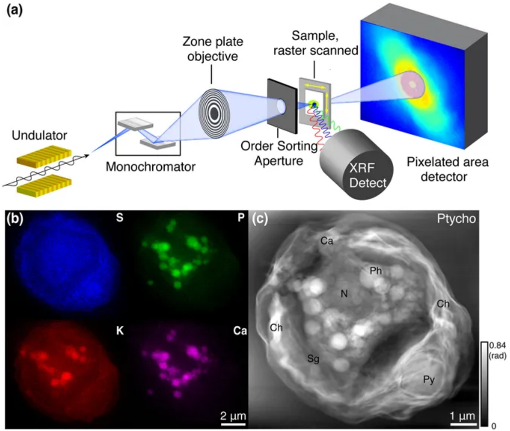


Figure: Simultaenous Ptychography and fluoresence imaging [4]

[4] Deng et al. [2017]

Factors affecting efficiency & resolution

- Efficiency of zone plate depends on refractive index.
- Zones must be thick enough along beam direction to produce a phase shift of π, several um at hard x-ray energy.
- Spatial resolution limited to finest, outermost zone width.

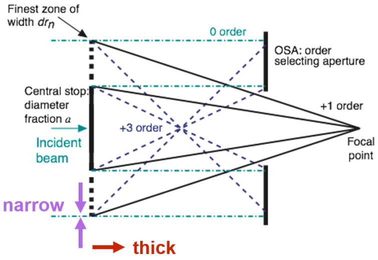


Figure: Thickness vs efficiency [5]

[5] Jacobsen [2019]

Scalar theory is not enough

- Scalar approximation assumption → interaction between x-rays and the optic can be treated as one-step diffraction.
- Clearly, waveguide effects need to be taken into account.
- Thick zone plate → test object.
- Klein-Cook param. : Q_{K-C} indicator of "diffraction regime"[6].

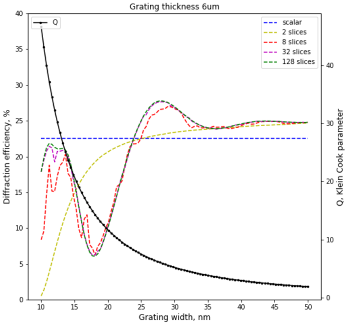


Figure: Volume effects in 1d gratings

Beyond Depth of Focus imaging

What is DoF?

- Can be thought of as the longitudinal spread of focal spot
- Goes like $\approx 5(\text{transverse res.})/\lambda^2$, 30nm/25keV$\rightarrow$90um.

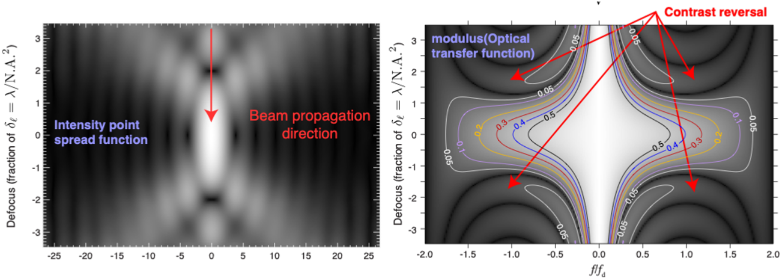


Figure: Optical Transfer Function in real and frequecny space [7]

[7] Jacobsen [2019]

Current Imaging schemes

- Object within DoF
- No modulation of input wave within the object

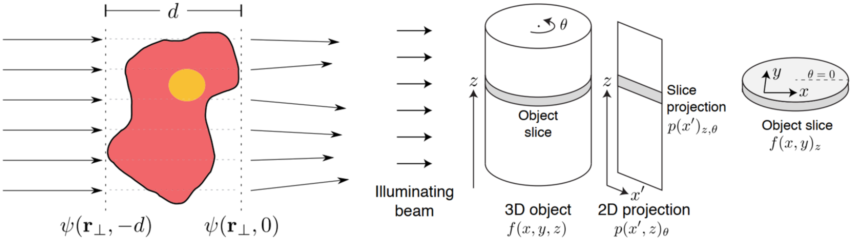


Figure: (Left) Pure Projection Approximation[8], (Right) Each slice is projected onto a 2D plane. All planes are independent of each other [9]

[8] Krenkel [2015]

[9] Jacobsen [2019]

Current Imaging schemes

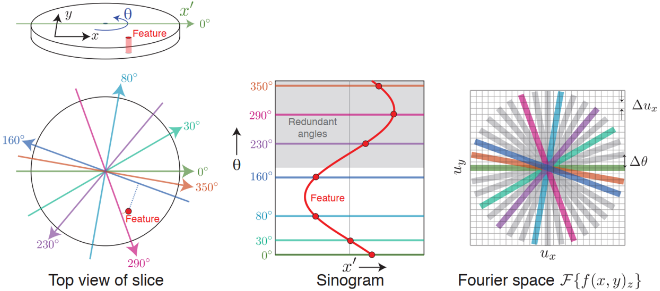


Figure: Spinning the object to obatin "sinograms", reconstruct each slice independently [10]

[10] Jacobsen [2019]

New reconstruction schemes

- "Thick" objects that extend beyond depth of focus → Pure Projection Approximation is not valid!
- New approaches → optimization of cost function[11], neural networks[12], etc.
- We will compare the relative merits of two approaches to solve the forward problem.

[12] Gilles et al. [2018]; Li und Maiden [2018]; Öztürk et al. [2018]; Shimomura et al. [2015]; Tsai et al. [2016]

[12] Goy et al. [2018]; Rivenson et al. [2018]; Scott W. Paine [2019]; Sun et al. [2018]

Multi-slice method

Multislice

- "Slice" the object into multiple thin sections. [13].
- Agrees with rigorous coupled wave theory [14].
- At pixel ≈ 0.25 feature size, need $\approx Q_{K-C}$ steps.

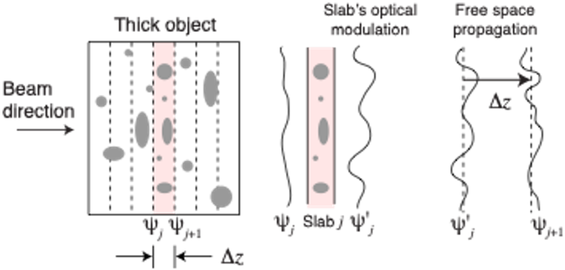


Figure: Multi-slice schematic [15]

[13] Cowley und Moodie [1957]; Li et al. [2017]; Roey et al. [1981]

[14] Li et al. [2017]

[15] Jacobsen [2019]

Implementation

- Slab modulation $\rightarrow$ point-wise multiply with the transmission matrix (a point-wise function of refractive indices)[16].
- Free Space propagation is given by Fresnel Transform which is implemented numerically by [17]:

$$\psi_{out} = \mathcal{F}^{-1}\{\mathcal{F}\psi_{in} * TF\}$$

$$TF(x, y) = exp(\frac{-i2\pi\delta z}{\lambda})\sqrt{1 - \lambda^2(u_x^2 + u_y^2)}$$

- Where λ is wavelength, δz is step size, u_x/u_y are the x/y co-ordinates.

[16] Cowley und Moodie [1957]; Li et al. [2017]; Roey et al. [1981]

[17] Goodman [2017]

Finite Difference methods for wave propagation

FD-basics

- Directly solve the Helmholtz equation for scalar diffraction in inhomogenous matter:

  $$\nabla^2\psi + k^2 n^2(x, y, z)\psi = 0$$

  ($k = \frac{2\pi}{\lambda}$ and $n(x, y, z)$ is the refractive index)
- Approximate the wavefunction with plane wave and osciallating parts:

  $$\psi(x, y, z) = u(x, y, z)exp(-ikz)$$

FD-basics

- Substituting this in the Helmholtz equation and neglecting the derivative of u along the direction of propagation, we get the following equation :

$$-2ik\frac{\partial}{\partial z}u + \left(\frac{\partial^2}{\partial x} + \frac{\partial^2}{\partial y}\right)u + k^2(n^2 - 1) = 0$$

- Defining $a = \frac{-i}{2k}$ and $F(x, y, z) = \frac{-ik}{2}(n^2(x, y, z) - 1)$; PDE now becomes [18] :

$$\frac{\partial u}{\partial z} = \mathrm{a}\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right) + \mathrm{F(x,y,z)}u$$

- In scaled units, u is $\approx 1e^1$, $|a|$ is $\approx 1e^2$ and $|F|$ is $\approx 1e^{-3}$.

[18] Fuhse [2006]; Kopylov et al. [1995]

Results from literature

- Need second-order integration along direction of propagation for accuracy [19].
- A recent implementation [20] was in C++ with a Python front end where ADI [21] was used.
- Preferred method[22] :
  free-space $\rightarrow$ MS,
  waveguides (inhomogenous matter) $\rightarrow$ FD

[19] Fuhse [2006]; Melchior und Salditt [2017]
[20] Melchior und Salditt [2017]
[21] Alt und Rubinoff [1962]
[22] Melchior und Salditt [2017]

PETSc Implementation

PETSc Implementation [23]

- For the FD method : Standard 5-point stencil.

$$DMDA + CN/GMRES/GAMG$$

- For the MS method : Using the PETSc-FFTW interface which maps FFT/IFFT $\rightarrow$ MatMult,MatMultTranspose

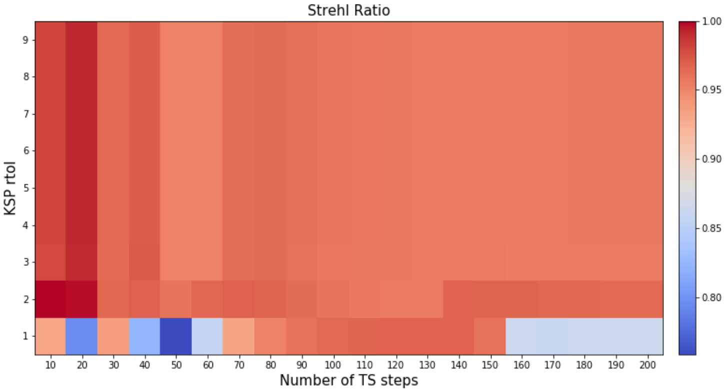
$$\text{Loop } \{VecView/2DFFT/VecPointwiseMult/2DIFFT\}$$

- PETSc vastly simplifies parallel IO, pointwise mult and FFT integration!

[23] https://github.com/s-sajid-ali/xwp_petsc

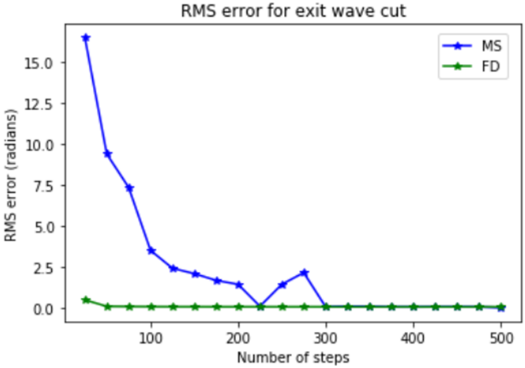
Sensitivity sweep

- Test a zone plate of size $2^{14}x2^{14}$, $Q_{K-C} = 500$.
- Vary number of TS steps and KSP Rtol.
- A relative tolerance of $1e-5$ suffices!



Zone plate results

- Test a zone plate of size $2^{15}x2^{15}$; $Q_{K-C} = 1500$.
- FD converges in fewer steps, but needs more memory.



Zone plate results

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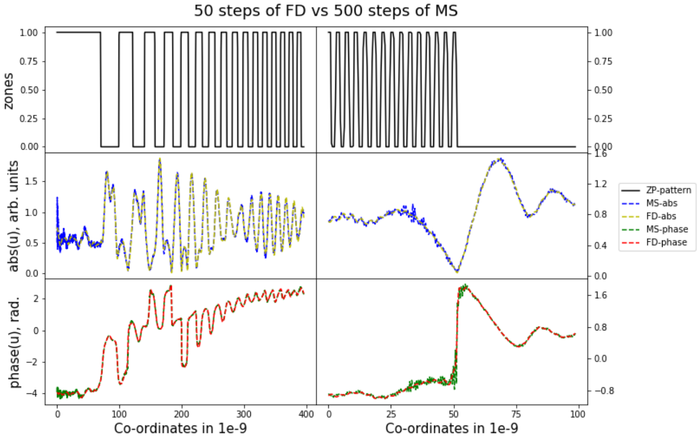

Next Steps

- Simulate tomography (essentially *MatMult* + wave propagation); for $\theta_i \subset (0, \pi)$, $TS(A_{\theta_i} * x) \rightarrow y_{\theta_i}$.
- Solve the inverse problem with *TAO* using adjoints given by *TSAdjoint*; Given $y'_{\theta_i}s$ for $\theta_i \subset (0, \pi)$ get x!

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