X-ray wave propagation

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8 Aug 2018

Outline

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Fresnel Propagation

- Approximation of the Huygens propagation.
- Equation : $A(x) = \int_{-\infty}^{\infty} h_{space}(x, x^{'}, k) t(x^{'}) dx^{'}$ [1] [2]
- Kernel : $h_{space}(x, x^{'}, k) = exp(i\frac{2\pi z}{\lambda})\sqrt{\frac{1}{i\lambda z}} exp(i\frac{\pi}{\lambda z}(x - x^{'})^2)$

[1] $k = 2\pi/\lambda$ and λ is the wavelength, primed co-ordinates denote source plane and unprime co-ordiantes denote observation plane

[2] [HSSA11]

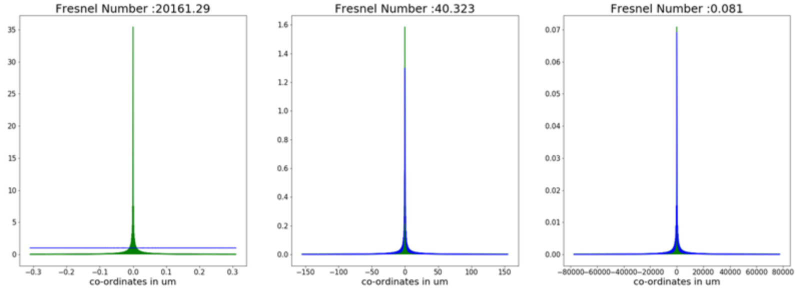
Outline

Fraunhofer Propagation

- Further approximation of the Huygens propagation valid at very large propagation distances.
- Valid when $\frac{W^2}{L\lambda} << 1$ or Fresnel number, $N_F << 1$ [3]
- Equation : $A(x) = \int_{-\infty}^{\infty} \psi(x^{'}) \exp(i2\pi \frac{xx^{'}}{\lambda z}) dx^{'}$
- This can be seen as a scaled Fourier Transform and implemented using FFT.

[3] Fresnel Number is defined as $N_F = \frac{a^2}{\lambda L}$, where a is the aperture, L is the distance of propagation and λ is the wavelength.

Fraunhofer propagator - accuracy[4]



[4] Green plots represent the result of the propagator and blue ones represent the results of exact evaluation

Outline

Evaluation Methods

- Direct computation
- Spectral methods

Fresnel Propagation : Direct computation

- Naive method :
  $A(x) = \frac{\delta X}{\sqrt{j\lambda z}} exp(\frac{j\pi x^2}{\lambda z}) \left\{ \sum_{n=1}^{\infty} U_n exp(\frac{j\pi X_n^2}{\lambda z}) exp(\frac{-j2\pi x X_n}{\lambda z}) \right\}$ [5]
- Complexity is $O(N^2)$ (assuming length of input and output arrays are the same)
- Rapidly oscillating quadratic phase factor forces use of large arrays.
- Advanced integral schemes have been developed to deal with the phase issue.[6]

[5] [Kel14]
[6] [KOH10]

Spectral Methods

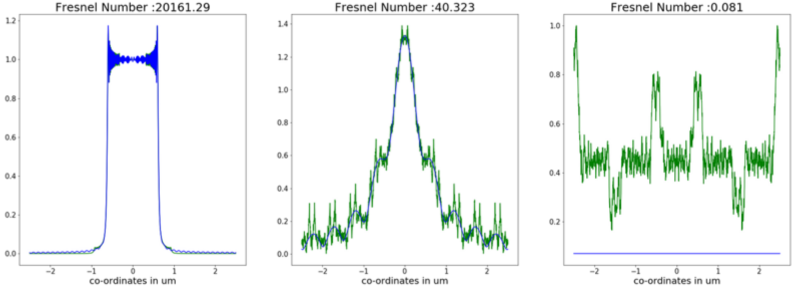
- Approximations to the Fresnel integral that make use of the Fast Fourier Transform
- They include the Transfer Function, Impulse Response and Single Fourier Transform methods.
- Each method is valid only in a small range

Transfer Function

- This method involves taking the FT of the signal and multiplying it with the "transfer function" in frequency space and finally applying an inverse FT to the product to bring it to real space.
- Equation : $\mathcal{F}^{-1}(\mathcal{F}(f(x))H(fx))$
- Transfer fuction is $H(fx) = e^{jkz}exp(-j\pi\lambda zfx^2)$
- Valid for small distances since as distance increases, the transfer function become undersampled[7].

[7] [VR09]

Transfer Function propagator - accuracy[8]



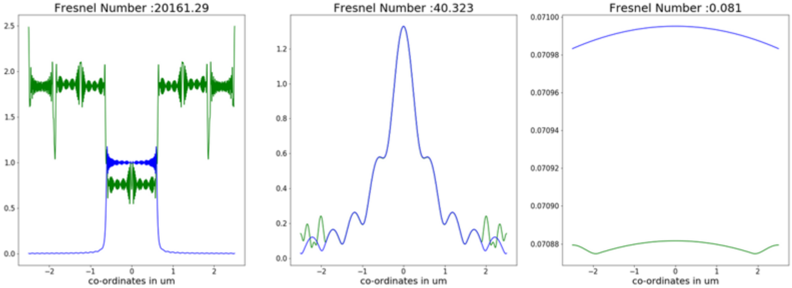
[8]Green plots represent the result of the propagator and blue ones represent the results of exact evaluation

Impulse Response

- This method involves calcuating the "impulse response" in real space before taking transforming it to Fourier space and multiplying it with the input FT. This product is then brought back into real space by performing an inverse FT.
- Equation: $\mathcal{F}^{-1}(\mathcal{F}(f(x))\mathcal{F}(h(x)))$
- Impulse Response function is $h(x) = \frac{e^{jkz}}{jkz} exp(\frac{jk}{2\pi}x^2)$
- Valid for large distances since as distance decrease, the impulse response function become undersampled[9].

[9] [VR09]

IR - accuracy

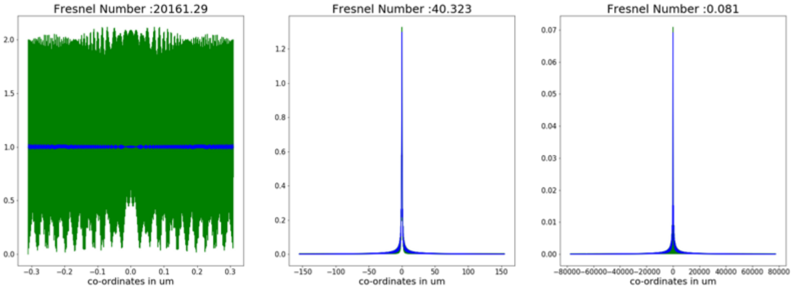

Fresnel Number :20161.29
co-ordinates in um
Fresnel Number :40.323
co-ordinates in um
Fresnel Number :0.081
co-ordinates in um

Fresnel Single Transform

- Modify the input wave by multiplying it with an input plane chirp function (quadratic phase factor) and take a fourier transform. Modify this with a second output plane chirp.
- Equation: $\frac{e^{jkz}}{j\lambda z} exp(j\frac{k}{2z}x_2^2)\mathcal{F}(f(x)exp(j\frac{k}{2z}(x_1^2)))$
- Valid for only one distance beacuse either the source plane chrip is undersampled or the output plane chirp is[10].
- Used when only amplitude is necessary and not the phase.

[10] [VR09]

Fresnel Single Transform propagator - accuracy[11]



[11] Green plots represent the result of the propagator and blue ones represent the results of exact evaluation

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Fractonal Fourier Transform

- FrFT is a generalization of the Fourier Transform. The FT transforms a function from real space to frequency space. The FrFT can transform the function to anything in between.
- $f_a(x) = \int_{-\infty}^{\infty} K_a(x, x^{'}) f(x^{'}) dx^{'}$[12]
- $K_a(x, x^{'}) = \sqrt{\frac{1 - icot(\alpha)}{2\pi}} exp(i0.5(x^2 cot(\alpha) - 2xx^{'} csc(\alpha) + x^{'} cot(\alpha)))$ where $\alpha = \frac{\pi a}{2}$
- $K_a(x, x^{'}) = \delta(x \pm x^{'})$ when a is an odd/even multiple of π.

[12] [HSSA11]

Fresnel integral in terms of FrFT

- Fresnel integral can be stated in terms of Fractional Fourier Transform
- Given an input wave $t(x)$ Hanna et al,[13] examined the expression for Fresnel Transform and came up with the following mapping for the output wave:

$$A(x) = \sqrt{\frac{1}{1+itan(\alpha)}} * exp(i(\frac{2\pi L}{\lambda})^2 tan(\alpha))$$
$$exp[i0.25sin(2\alpha)(\frac{x}{L})^2] * t_a^s(\frac{x}{L}cos(\alpha))$$

- where t^s is a scaled input wave given by $t(Lx)$ and $t_a^s(x)$ is the ath order Fractional Fourier transform ot $t^s(x)$ and α, the order of the transform is given by $tan^{-1}(\frac{\lambda d}{2\pi L^2})$
- An alternate mapping first transforms the input and output wave to spherical references and describes the propagation between these spherical references via FrFT[14].

[13] [HSSA11]
[14] [OM95]

Outline

Linear Canonical Transform

- Fresnel Transform and FrFT are in fact just two specific cases of the more general Linear Canonical Transform.
- The LCT is a an integral transform defined by three parameters α, β, γ as[15]
$$u_{\alpha,\beta,\gamma} = L_{\alpha,\beta,\gamma}u(x)(x') = exp(\frac{-j\pi}{4})\sqrt{\beta}\int_{-\infty}^{\infty} u(x)$$
$$*exp[j\pi(\alpha x^2 - 2\beta xx' + \gamma x'^2)]dx$$
- The LCT can be described by an abcd matrix which transform the Wigner Distribution as $W(x, k) \rightarrow W(ax + bk, cx + dk)$ with relations between a,b,c,d that limiting them to three degrees of freedom.

[15] [HS05]

LCT continued...

- The LCT acting in phase space is equivalent to a rotation in phase space according to[16]

$$\begin{bmatrix} x' \\ k' \end{bmatrix} = \begin{bmatrix} a & b \\ c & d \end{bmatrix} \begin{bmatrix} x \\ k \end{bmatrix}$$

- The Fresnel transform is now described by the matrix[17]

$$\begin{bmatrix} a & b \\ c & d \end{bmatrix} = \begin{bmatrix} 1 & \lambda z \\ 0 & 1 \end{bmatrix}$$

[16] [HS05]
[17] [HS05]

Fresnel transform written as successive LCT's

- The Fresnel transform can be "decomposed" into a set of LCT's as two LCT's can be cascaded together. Two such methods are listed below.[18]
- Spectral Method (FFT, Chirp multiplication, FFT):

$$\begin{bmatrix} 1 & \lambda z \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} 0 & -1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ -\lambda z & 1 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix}$$

- Direct Method (Chirp multiplication, optical Fourier Transform, Chirp multiplication):

$$\begin{bmatrix} 1 & \lambda z \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ \frac{1}{\lambda z} & 1 \end{bmatrix} \begin{bmatrix} \lambda z & 0 \\ 0 & \frac{1}{\lambda z} \end{bmatrix} \begin{bmatrix} 0 & 1 \\ -1 & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ \frac{1}{\lambda z} & 1 \end{bmatrix}$$

[18] [HS05]

Fresnel Transform in terms of LCT

- Fresenl Transform is just a shear of the Wigner Distribution of the signal along the space co-ordinate.
- The chirp convolution shears the signal's bandwidth which increases the sampling requirement.
- When the sampling requiremnts for each operator are taken into account, any decomposition gives accurate results. The preferable methods are those that reduce the amount of up and downsampling of the signal.

Outline

FrFT on XeonPhi

- The newest cluster at ALCF is θ which has Xeon Phi nodes. Each Xeon Phi 7230 chip has 64 cores and ≈250 threads. Each core is lightweight but has AVX-512 enabled VPU.
- Given that there are multiple methods to evaluate - sampling of FRFT, linear combination, eigenvalue decomposition, how do we pick one that's appropriate for Xeon Phi ?
- To preseve properties like index additivity or prefer speed ? Does any method have benefits for the inverse problem?

Acknowledgements

- Chris Jacobsen XSD, APS.
- Kenan Li SLAC National Accelerator Laboratory.

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