Non-uniform sampled scalar diffraction calculation 
using non-uniform fast Fourier transform

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Scalar diffraction calculations such as the angular spectrum method (ASM) and Fresnel diffraction are widely used in the research fields of optics, X-rays, electron beams, and ultrasonics. It is possible to accelerate the calculation using fast Fourier transform (FFT); unfortunately, acceleration of the calculation of non-uniform sampled planes is limited due to the property of the FFT that imposes uniform sampling. In addition, it gives rise to wasteful sampling data if we calculate a plane having locally low and high spatial frequencies. In this paper, we developed non-uniform sampled ASM and Fresnel diffraction to improve the problem using the non-uniform FFT.

Formulae

\[ u_2(x_2) = \int u_1(x_1) h_z(x_2 - x_1) dx_1 = \mathcal{F}^{-1} \left[ \mathcal{F} \left[ u_1(x_1) \right] H_z(f) \right], \]

where \( \mathcal{F}[\cdot] \) and \( \mathcal{F}^{-1}[\cdot] \) are forward and inverse Fourier transforms, \( u_1(x_1) \) and \( u_2(x_2) \) are the source and destination planes, \( f = (f_x, f_y) \) is the position vector in the Fourier domain, and \( z \) is the propagation distance between the source and destination planes, \( h_z(x_2 - x_1) \) is the impulse response, and \( H_z(f) = \mathcal{F}[h_z(x_1)] \) is the transfer function.

ASM is expressed as the following equations:

\[ u_2(x_2) = \mathcal{F} \left[ u_1(x_1) \right] \exp \left( 2\pi i z \sqrt{\frac{f}{\lambda^2} - |f|^2} \right) \times \exp \left( 2\pi i f x_2 \right) df = \mathcal{F}^{-1} \left[ \mathcal{F} \left[ u_1(x_1) \right] H_z(f) \right], \]

where \( H_z(f) = \exp \left( 2\pi i z \sqrt{\frac{1}{\lambda^2} - |f|^2} \right) \) is the transfer function of ASM. In numerical calculation, it is possible to accelerate the calculation using fast Fourier transform (FFT) as follows:

\[ u_2(m_2) = \text{FFT}^{-1} \left[ \text{FFT} \left[ u_1(m_1) \right] H_z(m_f) \right], \]

where, \( m_1 = (m_1, n_1) \) and \( m_2 = (m_2, n_2) \) are the position vector on the spatial domain as integer. \( m_f = (m_f, n_f) \) is the position vector on the frequency domain as integer. The source, destination planes and frequency domain are sampled by the rates of \( \Delta_1, \Delta_2 \) and \( \Delta_f \), respectively. The operators FFT\(^{-1}[\cdot]\) and FFT\(^{-1}[\cdot]\) are forward and inverse FFTs, respectively. The transfer function \( H_{z,\Delta}(m_f) \) is defined by:

\[ H_{z,\Delta}(m_f) = \exp \left( 2\pi i \left( om_f + z \sqrt{\frac{1}{\lambda^2} - |m_f\Delta|^2} \right) \right) \times \text{Rect} \left( \frac{m_f - c_m}{w_m}, \frac{n_f - c_n}{w_n} \right) \]

where \( \Delta \) is the sampling rate, and the offset parameter \( \mathbf{o} = (o_x, o_y) \) is for off-axis calculation. The two-dimensional rectangle function Rect(\( \cdot \)) is capable of calculating long propagation of ASM, respectively. \( (w_m, w_n) \) and \( (c_m, c_n) \) are the band-widths and the center of the band widths, respectively. See Ref. [2] for the determination of these parameters. Likewise, we can calculate Fresnel diffraction using the following transfer function:

\[ H_{z,\Delta}(m_f) = \text{FFT} \left[ \exp \left( ikz \exp \left( \frac{i(m_f\Delta + o)^2}{\lambda z^2} \right) \right) \right]. \]

Note that we have to expand the calculation size by zero-padding to \( N' \times N' \) where \( N' = 2N \) (\( N \) is the horizontal and vertical pixel numbers of planes) in order to avoid wraparound by the circular convolution of Eq.(3). Therefore, the sampling rate \( \Delta \) in the transfer functions is \( \Delta = 1/(N'\Delta_1) \).

However, using FFT imposes the same sampling rates on the source and destination planes (\( \Delta_1 = \Delta_2 \)). In order to solve this restriction, scaled-Fresnel diffraction [3–7] and scaled-ASMs [8–10] that can address different sampling rates on source and destination planes were proposed. In Refs. [3–8,10], chirp-z transform (a.k.a. scaled...
Fourier transform) is used instead of normal FFT. In Ref. [9], non-uniform sampling FFT (NUFFT) [11] is used. The scaling operation is, for example, useful for lensless zoomable holographic projection [12, 13], digital holographic microscopy [14] and fast CGH calculation [15]. Even though scaled-ASMs can address different sampling rates on source and destination planes, each plane still requires uniform-sampling.

In this paper, we develop non-uniform sampled ASM (NU-ASM) and Fresnel diffraction (NU-FRE) to overcome the restriction using the non-uniform FFT. The uniform-sampled scalar diffractions give rise to wasteful sampling data if we calculate a plane having locally low and high spatial frequencies. In contrast, NU-ASM and NU-FRE are expected to be useful for the situation. NU-ASM is a generalized version of the scaled-ASM of Ref. [9].

First, we consider NU-ASM. We need three types of NU-ASM, that is, the first NU-ASM1 calculates ASM from a non-uniform sampled source plane to the uniform-sampled destination plane. The second NU-ASM2 is the opposite version of the first. The third NU-ASM3, calculates ASM on both non-uniform sampled source and destination planes.

By applying NUFFT to Eq.(3) to a source plane, we can straightforwardly obtain NU-ASM1:

\[
 u_2(m_2) = \text{NUASM}_1 \left[ u_1(x_1) \right] = \text{FFT}^{-1} \left[ \text{NUFFT}_1 \left[ u_1(x_1) \right] H_{z,\Delta}(m_f) \right], \tag{6}
\]

where NUFFT1[·] is the type 1 of NUFFT, \( \Delta = 1/(N'\Delta_1) \) and \( u_1(x_1) \) is the non-uniform sampled source plane. Several implementations of NUFFT were proposed. We used Greengard and Lee’s NUFFT [11]. Two types of NUFFT are defined. NUFFT type 1 is defined as follows:

\[
 F(m_f) = \text{NUFFT}_1 \left[ f(x'_1) \right] = \sum_{x'_1} f(x'_1) \exp(-i\pi m_f x'_1), \tag{7}
\]

where, \( m_f \) is uniform sampled with the integer value on the frequency domain. Practically, the right-side of the equation is accelerated by FFT, gridding algorithm and deconvolution [11].

Due to the NUFFT property, we need to normalize the coordinate of the source plane as shown in Fig.1. The original coordinate system of the source plane \( x_1 \) is defined as \( x_1 \in [-N/2, N/2] \times [-N/2, N/2] \) as shown in Fig.1(a). The NUFFT requires the range of the coordinate, \( x'_1 \in [0, 2\pi) \times [0, 2\pi) \) as shown in Fig.1(b). Therefore, we convert the coordinate system by \( x'_1 = 2\pi(o' + x_1)/N \) where \( o' = (N/2, N/2) \).

NUFFT type 2 is defined as follows:

\[
 f(x'_2) = \text{NUFFT}_2 \left[ F(m_f) \right] = \sum_{m_f} F(m_f) \exp(i\pi m_f x'_2), \tag{8}
\]

where \( f(x'_2) \) is the non-uniform sampled plane. Note that we need to normalize the coordinate of the destination plane for the same reason as that of NUFFT1. For more details, see [11].

Likewise, NU-ASM2 is obtained as follows:

\[
 u_2(x_2) = \text{NUASM}_2 \left[ u_1(x_1) \right], \tag{9}
\]

where \( x_2 \) is non-uniform sampled and the range is \( x_2 \in [-N', N'] \times [-N', N'] \). The NUFFT2 requires the range of the coordinate, \( x'_2 \in [0, 2\pi) \times [0, 2\pi) \). Therefore, we convert the coordinate system by \( x'_2 = 2\pi(o' + x_2)/N \).

We obtain NU-ASM3 by combining NU-ASM1 and NU-ASM2. In addition, using Eq.(5) instead of the transfer functions of NU-ASM, we can straightforwardly derive three types of NU-FRE, that is, NU-FRE1, NU-FRE2 and NU-FRE3.

Let us compare the NU-ASM and NU-FRE with Rayleigh-Sommerfeld (RS) diffraction. RS diffraction is rigorous scalar diffraction and is expressed as,

\[
 u_2(x_2) = \frac{1}{2\pi} \int \int u_1(x_1) \left\{ \frac{z}{r} \left[ 1 - ikr \right] \frac{\exp(ikr)}{r^2} \right\} \, dx_1, \tag{10}
\]

where \( k \) is the wave number and \( r = \sqrt{|x_1 - x_2|^2 + z^2} \). RS diffraction with non-uniform sampled planes is calculated by directly numerical integration, which has the complexity of \( O(N^4) \).

We use Fig.2 as the non-uniform sampled source plane with 256 \times 256 pixels. The image “Lenna” is the am-
The amplitude distribution of the source plane, and the image “Mandrill” is the phase distribution where the pixel value 0 corresponds to the phase value \(-\pi/2\) and the pixel value 255 corresponds to the phase value \(+\pi/2\).

The calculation condition is as follows: the wavelength is 500 nm and the sampling rate on the uniform-sampled destination plane is \(\Delta_2 = 5 \mu m\). The source plane is non-uniform-sampled, where the sampling rates on the first to fourth quadrants are 0.9\(\Delta_2\), 0.8\(\Delta_2\), 0.7\(\Delta_2\) and \(\Delta_2\), respectively.

Figure 3(a) and (b) are the amplitude and phase on the diffracted result by RS diffraction at \(z = 8mm\). Figure 3(c) and (d) are the amplitude and phase on the diffracted result by NU-ASM\(_1\). In Fig. 4, we measure the error of NU-ASM\(_1\) and NU-FRE\(_1\) to RS diffraction, which is the criteria, by the signal-to-noise ratio (SNR). At short distance propagation, the SNR of NU-ASM\(_1\) is good quality, while that of NU-FRE\(_1\) is poor quality. Whereas, at long distance propagation, the SNR of NU-ASM\(_1\) is decreased because the band-limited transfer function of Eq.(4) has a small area, which is pointed out by Ref. [16]. While, the SNR of NU-FRE\(_1\) is increased. The average calculation time of the NU-ASM\(_1\) is about 46 ms, while that of RS diffraction is about 76 s. We use an Intel Core i7-2600S CPU and eight CPU threads, and multi-thread version of FFTW [17] as the FFT library.

Figure 5 shows diffracted results from a uniform-sampled source plane to non-uniform-sampled destination plane by RS diffraction and NU-ASM\(_2\). We use Fig.2 as the uniform-sampled source plane at the sampling rate \(\Delta_1 = 5 \mu m\). The destination plane is non-uniform-sampled, where the sampling rates on the first to fourth quadrants are 0.9\(\Delta_1\), 0.8\(\Delta_1\), 0.7\(\Delta_1\) and \(\Delta_1\), respectively. Figure 5(a) and (b) are the amplitude and phase on the diffracted result by RS diffraction at \(z = 8mm\). Figure 5(c) and (d) are the amplitude and phase on the diffracted result by NU-ASM\(_2\). The SNR is maintained at approximately 32 dB.

We conclude this work. This paper proposes the non-uniform sampled scalar diffractions, NU-ASM and NU-FRE, based on NUFFT. These diffractions are categorized into three types: type 1 is the diffraction from a non-uniform sampled source plane to a uniform sampled destination plane, the type 2 is the opposite situation of type 1; and type 3 is the diffraction between a non-uniform sampled source and destination planes. NU-ASM is suitable for the short propagation, while NU-FRE are suitable for the long propagation. In addition, the calculation times of NU-ASM and NU-FRE is faster than RS diffraction. In future, we will attempt to apply the non-uniform sampled scalar diffractions to CGH calculation, the design of optical elements, and optical encryption and watermarking. These diffraction calculations will be provided in our open-source library: CWO++ library [18].

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