SAND2015-5784C

Big-Data X-ray Phase Contrast Imaging System Simulation

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ABSTRACT

This position paper describes a potential implementation of a large-scale grating-based X-ray Phase Contrast Imaging System (XPCI) simulation tool along with the associated challenges in its implementation. This work proposes an implementation based off of an implementation by Peterzol et. al. where each grating is treated as an object being imaged in the field-of-view. Two main challenges exist; the first is the required sampling and information management in object space due to the micron-scale periods of each grating propagating over significant distances. The second is maintaining algorithmic numerical stability for imaging systems relevant to industrial applications. We present preliminary results for a numerical stability study using a simplified algorithm that performs Talbot imaging in a big-data context.

1. INTRODUCTION

The purpose of developing an big-data centric X-ray Phase Contrast Imaging (BDXPCI) system simulation tool is threefold. First, this tool would assist in quantifying performance of experimental designs virtually rather than spending significant time and resources to fabricate several candidate prototypes. Second, the simulation tool would help the influence of as-built imperfections of the various components components within an XPCI system. Lastly, an BDXPCI simulation tool may also serve as a forward-projector for a BDXPCI computed tomography iterative reconstruction algorithm.

Developing a full 3D imaging system simulation is immensely computationally daunting, frequently requiring significant computational resources to reasonably resolve the system behaviour. For this work, it was decided that an incremental approach to building a complex system was most reasonable to help identify challenges early-on and at a smaller scale for which there exists extensive studies.[1–4] One of the appealing features of XPCI is its greater sensitivity to density and material variations; however, greater sensitivity in a system may imply that a greater level of caution is needed when designing algorithms for a BDXPCI simulation tool. Particular caution must be exercised when attempting to design algorithm that will operate on big data as a small error can propagate through the algorithm- increasing as more information is processed by the method.

For background on grating-based XPCI or XPCI in general, the reader is referred to the scientific literature[5–8] and will not be discussed in this work. Instead, this will will focus on describing a proposed approach as well as the challenges that are associated with such an approach, along with proposed solutions with preliminary results.

2. BACKGROUND

A survey of the literature yielded many informative and interesting approaches to XPCI simulation. The methods spanned various approaches and implementations with varying degrees of success. Unfortunately, the survey could not find any efforts in large-scale simulation as most efforts either restricted the simulation to very small fields-of-view, compressed information in object-space, or short propagation lengths.

Work by Peterzol et. al.[1] describes a robust and deterministic implementation with a large field-of-view to perform XPCI without gratings on Complex 3D objects based on Fresnel-Kirchhoff diffraction theory. Peterzol et. al. achieve these potentially large-scale simulations by representing the imaged object with a set of CAD models. While CAD model-based representations using Non-uniform rational B-splines (NURBS),[9] as is done in

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this work, greatly reduces the computational burden, it also reduces the range of objects that can be simulated using this approach. One potential example would be representing objects that exhibit a gradual material composition transition across an interface as well as object that exhibit slight defects, imperfections, and/or variation that may be difficult to represent with a set of NURBS basis functions. This method is appealing as it is not restricted to monochromatic radiation and can model system spatial resolution properties.

Work done by Wolf et. al. describes a fast XPCI simulation that greatly reduces computational resource requirements by decomposing a 2D plane wave into a set of 1D lines and can be processed in parallel efficiently. Wolf et. al. correctly point out that fully representing the XPCI system would require tremendous memory resources (over 16 terabytes for their mammography application). The work exploits efficiency by the decomposition as well by only up-sampling the object to the resolution of the plane wave line when it is in use. Although Wolf et. al. improved efficiency by approximately three orders-of-magnitude using a high-end 48 core server with 512 GB of system memory, the pixel processing rate was still well below 100 pixels processed per second. It is unclear if the same benefits are realizable if the Wolf et. al. approach is adapted for spherical waves as the decomposition potentially becomes more complex as well as the potential for irregular memory access patterns severely degrading performance as demonstrated by Jimenez et. al.[10] and Perez et. al.[11] for other big-data x-ray imaging applications.

To other interesting efforts come from Cipiccia et. al.[2] and Peter et. al.[3] Both efforts propose leveraging Monte Carlo methods to create XPCI images which show very good agreement with experimental data. Cipiccia et. al. simulate Talbot interferometry, however only on a small-scale image with planar monochromatic waves over a relatively short propagation length still required simulating on the order of 10^9 particles at a processing time of approximately two hours. Peter et. al. also demonstrate Monte Carlo exploitation in a hybrid algorithm with somewhat similar performance limitations with respect to scale and propagation distance. Additionally, it is not entirely clear from both pieces of work how well these algorithms will scale computationally. Generally, Monte Carlo methods are challenging to run in most parallel environments while maintaining sufficient scalability. Since both groups modify traditional Monte Carlo methods, it is unclear if the general High Performance Computing approaches recommended in the scientific literature to improving/maintaining scalability across multiple compute nodes would be applicable.[12–14] Finally, it would be interesting to understand the computational performance of these approaches for larger detector areas, polychromatic sources, cone-beam geometries, and the addition of a g_0 grating at the source as these features likely increase the number of particles needed for a given simulation as well as increases the distance over which to propagate. Monte Carlo methods have much potential and future efforts will likely focus on feasibility studies for big-data applications.

3. APPROACH

The proposed method is inspired by the method put forward by Peterzol et. al.[1] with modifications to function at large-scale wtih respect to object space and detector size. The method proposed in this work attempts to simulate X-ray Talbot Interferometry by sequentially applying Fresnel-Kirchhoff Diffraction sequentially to 3 gratings (g_0, g_1, and g_2) and the object. In contrast to Peterzol et. al., this work will not represent the object space as a set of CAD models and will attempt to implement a sparse representation of a finely voxelized space. Although CAD model representation is clearly a more efficient implementation, it does not lend itself well to many applications of interest to industrial non-destructive evaluation and testing; such examples include simulated imaging applications of objects and/or gratings that exhibit slight defects, gradual interface transitions, and complex textures.

The first challenge realized in this approach is the required sampling rate along the ray path from the x-ray source to the detector plane. According to Peterzol et. al., the transmission function $t(x, y)$ must be sampled along a given ray path with a precision of less than a micron due to the high frequency oscillations of the propagator; this is further compounded in a grating-based system by the periods of each grating as well as by the phase-stepping of G_2 as the typical periods for relevant gratings is on the order of 2-4 microns. To compound the challenge, the sampling along the ray path must also be sufficiently small to allow for the simulation of phase-stepping where G_2 is translated one period and anywhere from 5 to 20 images are sampled within the length. The second challenge, as implied above, is the numerical stability of the algorithms related to the entire end-to-end simulation. If the first challenge forces a very high sampling rate over a significant distance, this creates a challenge in maintaining sufficient stability and accuracy for the complex algorithms related to the wavefront propagation.

Generally, computational complexity is not the biggest challenge in developing a big-data imaging system simulation. Instead, the biggest problems, as mentioned above, tend to be numerical stability as well as the movement of data at every stage of the simulation. The numerical stability element is of particular concern as the phase-contrast image formation process involves convolving an input function with a transfer function, which from a computational standpoint, the use of the Fourier transform (and its inverse) is essentially required in order to allow for the execution to occur efficiently on the processing architecture. Although the Discrete Fourier Transform algorithm is a very well studied algorithm on current processor and coprocessor architectures,[15, 16] it will have some level of not inconsequential numerical error in its results that will obscure the true results. For example, it is not unreasonable to try to represent a grating as some scaled sum of *rect* functions (either in 2D or 1D object space, amplitude, phase, or combination of both); unfortunately, the Fourier transform results in a sum of appropriately scaled *sinc* functions, each of which has infinite support. Therefore, the approximation is not only suffering from errors due to local finite sampling of the *rect* function, but also by potentially inadequate sampling in Fourier space. This is potentially exacerbated by size of the vectors or arrays; generally, the larger the vectors or arrays being transformed, the more significant the error.

To further confound the problem, the magnitude of the numerical values within the algorithm could also potentially introduce additional error due to arithmetic operation interaction between values with drastically disparate magnitudes. This could potentially be somewhat alleviated by performing phase and amplitude calculations separately within the simulation and then combining the results at the end as well as by designing the algorithms to minimize these types of interactions such as performing operations in log-space. This exploratory work will demonstrate numerical stability issues with a simplified example using "big-data" Talbot imaging and will discuss potential paths forward towards implementing BDXPCI.

4. TALBOT IMAGES

As a first step, a numerical simulation was developed to create a large Talbot carpet from a planar wave. The algorithm is fairly straightforward, requiring only an input signal, and applying it to to the free-space transfer function for a given propagation distance in Fourier space.[17] This simple environment provides us with the ability to isolate numerical noise due to the Fourier transform and it's inverse when operating on a single grating (i.e. a summation of complex scaled *rect* functions) as well as the option to consider "gratings" with larger periods to observe the numerical behaviour between openings.

For this work, two demonstrations will be presented. The first demonstration will present the differences in the output Talbot carpet when a input grating has a slight error contained within the imaginary component of the numerical representation; this will serve as a proxy for the estimation of the transmission function $t(x, y)$ when one must perform interpolation between voxel data as numerical interpolation will almost always introduce approximation errors. The second demonstration will present numerical behavior over several Talbot distances to approximately simulate the numerical behavior of the plane wave propagating over long distances as would be the case when one is simulating propagation from a g_0 grating to the imaging detector. Both demonstrations were implemented in Matlab version 8.4 (2014b).

For the first demonstration, a grating is sampled at 2^13 points with 40 samples per period with an aperture ratio of 3/40. The first grating will represent a pure π-phase grating where the input is:

$$\vec{f}(\vec{x}; p) = rect\left(\frac{\vec{x}}{p/2}\right) \otimes \sum_{n \in \left\{x_i \mid \frac{\vec{x}}{p} \in \mathbb{Z}\right\}} \delta\left(\vec{x} - n\right)$$

Where the sum of delta functions is called a comb function, $\vec{x}$ is discretized sampling position vector. The second grating will have a slight error introduced in the imaginary component.

$$\vec{f}_{err}(\vec{x}; p) = \begin{cases} \vec{f}(\vec{x}; p) + 10^{-16} j & \text{if } \vec{f}(\vec{x}; p) = -1 \\ \vec{f}(\vec{x}; p) & \text{otherwise} \end{cases}$$

. Where j is equal to $\sqrt{-1}$. Figure 1 shows a zoomed in absolute difference plot of pixel intensity along with colorbar to show the impact on the Talbot carpets when a small error is introduced into the input. As figure 1 demonstrates, a slight error of a mere 10^{-16} shows image deviation 16 orders-of-magnitude greater than the input error throughout the entire Talbot distance. Introducing the other gratings as well as the object will introduce more error as interpolation will be performed for every object in the field-of-view.

For the second demonstration, a grating is sampled at 2^13 at the same sampling pattern as above and sampled at the first 10 Talbot distances with a grating with no error present. This was done to demonstrate the impact propagation has on the phase over several Talbot distances. The sampling was increased so that some padding would occur on either side of the grating so that for at least shorter distances the DFT artifacts would not affect the numerical output. Figure 2 shows the phase at the first 10 Talbot distances. One should expect to see pi phase shifts at the apertures; however, the numerical simulation does not reflect such shifts, but instead shows a mixture of pi and $-pi$ shifts, even for early Talbot distances.

5. CONCLUSION

A brief literature search for numerical stability studies in the simulation of X-ray Phase Contrast Imaging yielded no results. In particular, there were no formal studies of numerical simulations of grating-based XPCI specifically. It is not entirely surprising as one can treat each grating in the imaging system as an imaged object in the field-of-view and one should still yield the correct images (to within some level of accuracy). Treating the gratings in the imaging system as pure phase gratings (i.e. no influence from amplitude), although potentially valuable, defeats the purpose of creating a simulation tool to help assist in system design as phase gratings are physically unrealisable.[18] However, even in the simplified example presented in this work, it is shown that even for pure-phase gratings, significant error is possible due to numerical inaccuracies when significant propagation distances are realized.

Although the implementation put forth by Peterzol et. al. is completely deterministic and noise-free (with respect to the system, not numerically), it is arguably the most viable approach to simulated BDXPCI as going to Monte Carlo-based methods (such as MCNP[19]) would likely be computationally prohibitive as the scale relevant to this work is too large to be done efficiently and would require significant time and computational resources that are not feasible.

The largest computational obstacle (which was not addressed in this position paper) lies in the interpolation steps when sampling the index-of-refraction along the ray path in object space. This is the same hurdle faced by every other ray-based X-ray image simulator and thus there exist many potential solutions algorithmically speaking.[11] Interpolation is a very data transfer and computationally intensive operation; parallel implementations are required in order to complete the calculations in a reasonable amount of time.[10] To further speed-up the task, one could also go to the massively multi-threaded environment of Graphics Processing Units (GPUs). GPUs however potentially bring up additional challenges in the efficiency of information transfer dependent upon algorithm design and implementation. Many big-data imaging algorithms implemented on a GPU exhibit irregular memory access patterns and can be extremely detrimental to performance.[10] Although GPUs will most likely be used for the full 3D-to-2D simulation, we forego it for now to ensure clarity in the algorithm's implementation.

This initial effort has helped confirm some of the early challenges identified by Peterzol et. al. as well as by Wolf et. al. The challenges include the burdensome computational expense as well as some numerical error sources. Further study will be pursued in implementing BDXPCI both accurately and efficiently for relevant applications for industrial non-destructive testing and evaluation. The impact of a successfully implemented BDXPCI simulation tool is potentially tremendous for the development and design of innovative designs to XPCI systems that seek to explore radiation energies that are not relevant to medical applications as well as for the development iterative reconstruction algorithms for XPCI computed tomography.

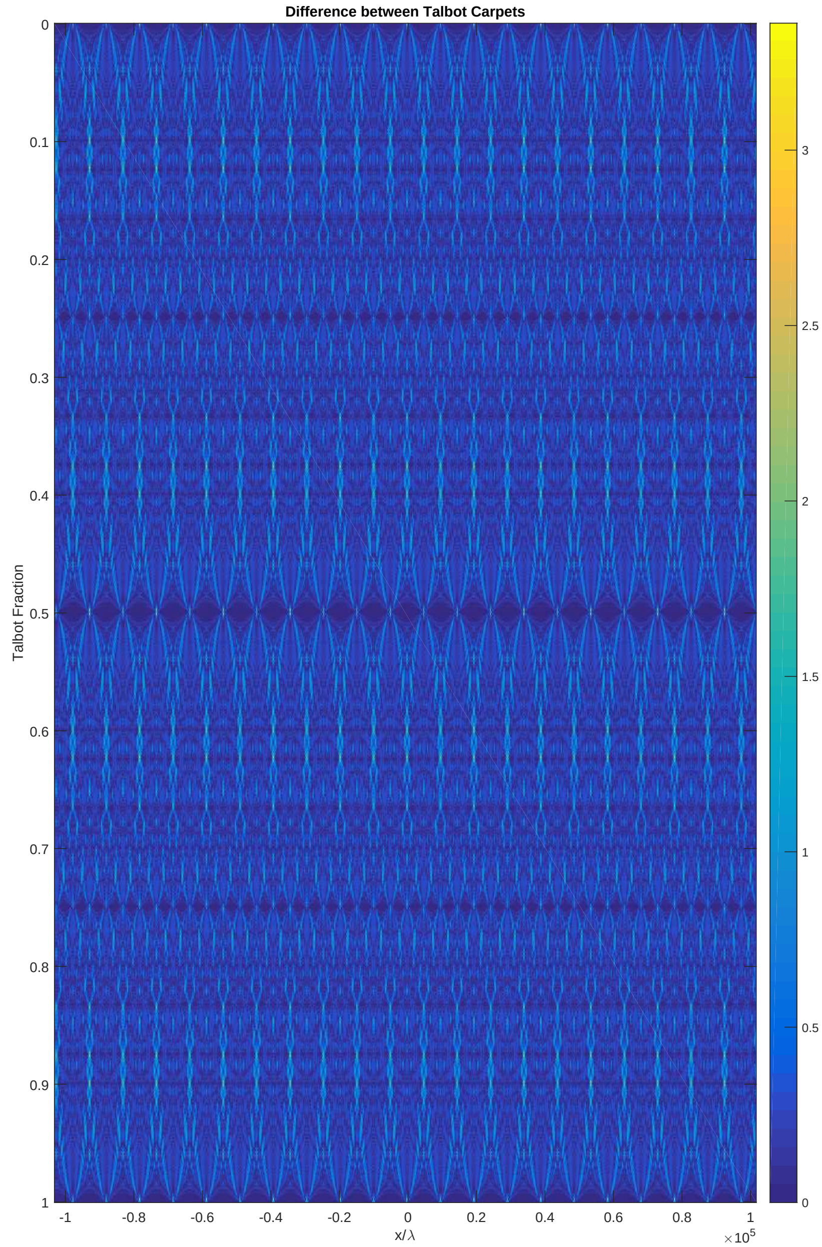

Figure 1. Difference in output Talbot carpet for slightly differing input gratings

6. ACKNOWLEDGEMENTS

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DEAC04-94AL85000.

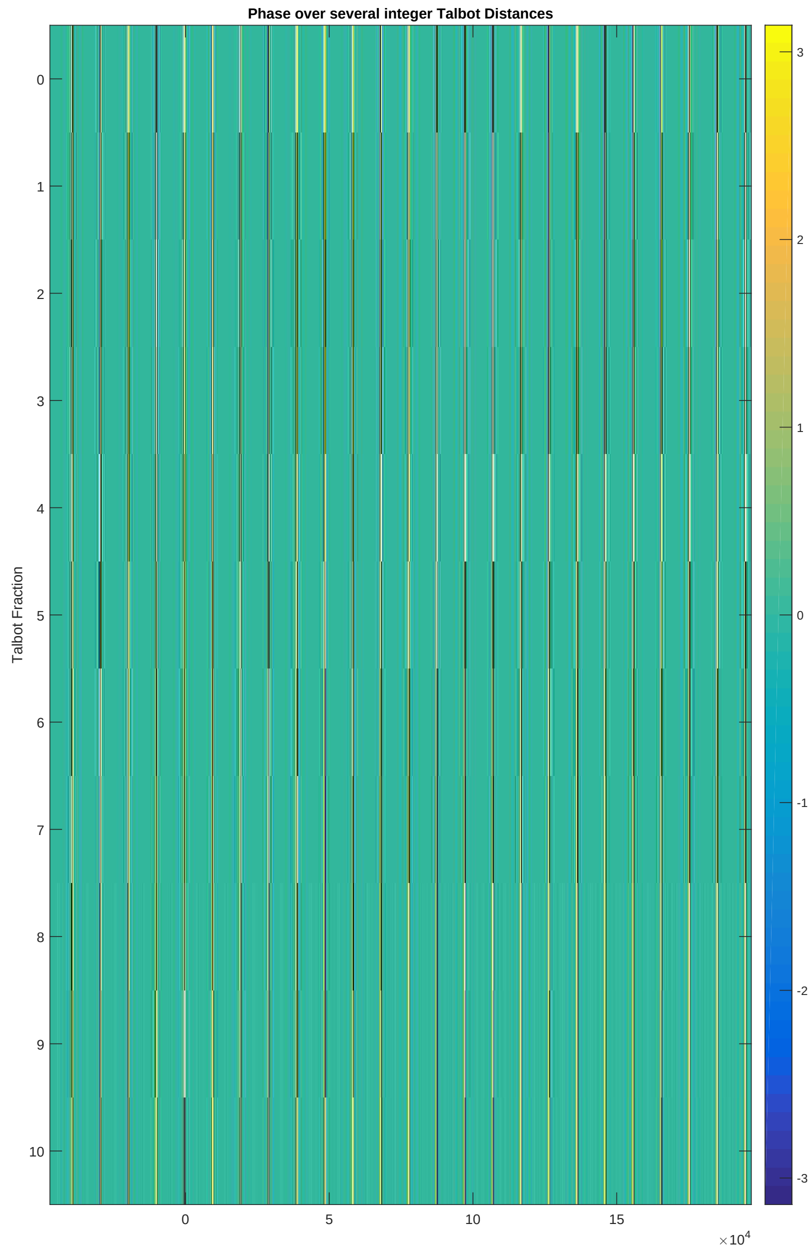

Figure 2. Simulated phase (zoomed in view) over the first 10 Talbot distances.

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