Advanced 3D Monte Carlo Algorithms for Biophotonic and Medical Applications

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This thesis is submitted in partial fulfilment for the degree of
PhD
at the
University of St Andrews

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Declaration

I, Lewis McMillan, hereby certify that this thesis, which is approximately ***** words in length, has been written by me, that it is the record of work carried out by me, or principally by myself in collaboration with others as acknowledged, and that it has not been submitted in any previous application for a higher degree.

I was admitted as a research student in September 2015 and as a candidate for the degree of PhD in September 2015; the higher study for which this is a record was carried out in the University of St Andrews between 2015 and 2019.

Date............................ Signature of candidate ....

I hereby certify that the candidate has fulfilled the conditions of the Resolution and Regulations appropriate for the degree of PhD in the University of St Andrews and that the candidate is qualified to submit this thesis in application for that degree.

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Abstract

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Acknowledgements

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3D Phase Tracking Monte Carlo Algorithm

1.1 Introduction

1.2 Theory

The Monte Carlo radiation transfer (MCRT) algorithm as described in **??**, must be adjusted so that wave phenomena such as interference and diffraction can be modelled. Modelling these wave behaviours allows us to model complex beams, where these phenomena are required to form the beam, e.g Bessel beams. As MCRT is a ballistic simulation of photon packets, meaning that the MCRT simulation presented thus far in this thesis only modelled the ballistic behaviour of photons. However for the work presented in this chapter, wave like behaviours is crucial to modelling the various experiments and phenomena.

In order to convert a ballistic simulation of photon packets into a ballistic/wave-like simulation, the complex phase of each photon packet is tracked. This is achieved, by simply tracking the complex phase of the photon as it propagates through a medium. Equation (1.1) shows how the phase is calculated.

$$\varphi = cos\left(\frac{2\pi l}{\lambda}\right) + i\ sin\left(\frac{2\pi l}{\lambda}\right) \tag{1.1}$$

Where φ $[-]$ is the phase of a photon packet, l $[m]$ is the distance the photons has travelled, and λ $[m]$ is the wavelength of the photon. Now we can calculate the phase of a photon at a position $\hat{p_o}$, if we know the distance it has travelled, and its original phase. To be able model the wave-like behaviour of photons, we let the photons packets interfere with one another in a volume or area element. We do not model the interference at just the points where photons packets cross one another as due to the ballistic nature of the MCRT simulation, this does not occur with enough frequency in order to give a good signal to noise ratio. The interference takes place in a volume element dV or area element dA instead. To calculate the interference from the phase, the phase if summed in each volume or area element and the absolute value taken, and then squared. Equation (1.2) shows the equation for interfernce for a volume element dV.

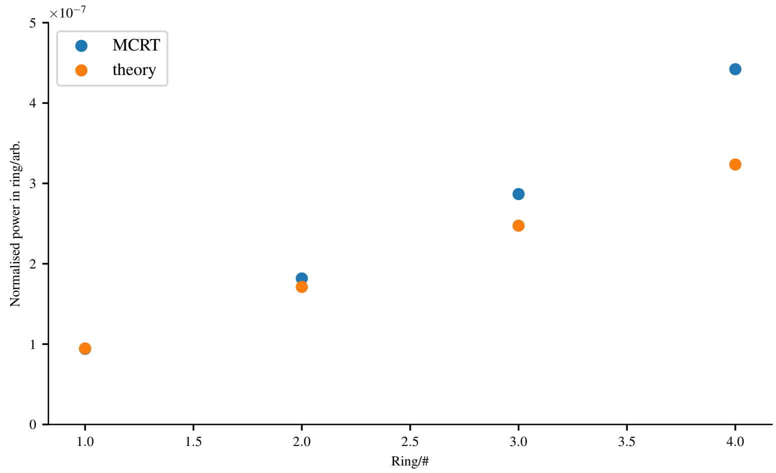

Figure 1.1: *Bessel beam power in each ring.*

$$I(\xi) = \left| \sum_{\xi} cos\left(\frac{2\pi d}{\lambda}\right) + i \sum_{\xi} sin\left(\frac{2\pi d}{\lambda}\right) \right|^2 , \quad \xi = (x, y, z) \tag{1.2}$$

Where:
l is the total distance travelled by a photon $[m]$;
λ is the wavelength of the photon $[m]$;
I is the intensity at the ξ^{th} cell [dunno];
and ξ is the x^{th}, y^{th}, z^{th} cell, volume dV.

As the MCRT simulation is now a quasi ballistic/wave simulation of photon behaviour, we compare our simulations to theoretical and experimental data to prove this model is accurate.

1.2.1 Validation of Phase Tracking Algorithm

The first test of our phase tracking algorithm, is to compare our simulation to a double slit experiment. The double slit experiment, is a simple experiment where monochromatic plane wave of light is incidence on two slits, and the interference pattern is observed on a screen a distance d away from the slits.

In this experiment blah bla ***

$$I(\theta) \propto cos^2\left(\frac{\pi d\ sin\theta}{\lambda}\right) sinc^2\left(\frac{\pi b\ sin\theta}{\lambda}\right) \tag{1.3}$$

Where the $sinc$ function is defined as $\frac{sin(x)}{x}$, for $x \neq 0$, b is the slit width, d is the slit separation and θ is the angular spacing of the fringes.

1.3 Bessel Beams

Bessel beams

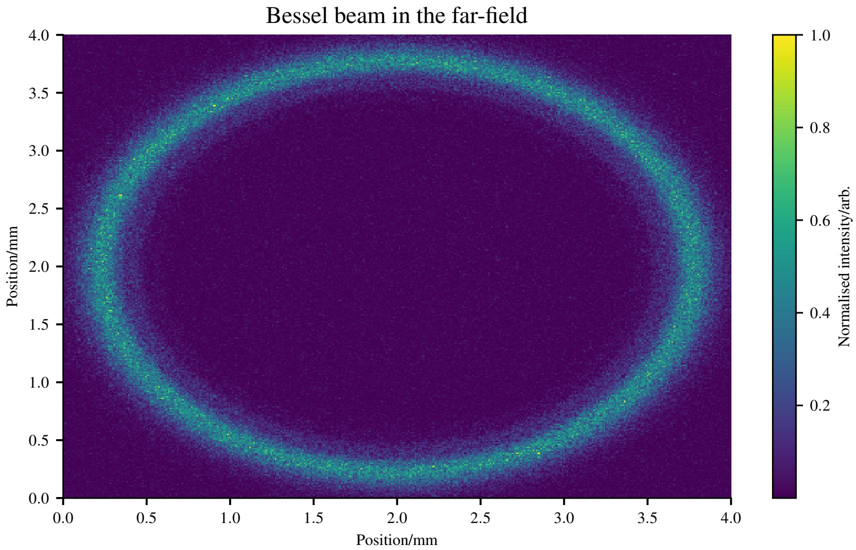

Figure 1.2: *Bessel beam in the far field.*

1.4 Gaussian Beams

1.5 Other Beams

Our technique outlined in the preceding sections, can also be applied to arbitrary non-diffracting or complex beams. The only requirements for our algorithm to be able to model a complex beam, is that there is some phase delay that can be modelled analytically*.

1.6 Discussion

a [1]

1.7 Conclusion

*It may be possible to model phase delays that are not analytical expressions. Simulating spatial light modulators may also be possible with our algorithm.

Bibliography

[1] Charles Mignon, Aura Higuera Rodriguez, Jonathan A Palero, Babu Varghese, and Martin Jurna. Fractional laser photothermolysis using bessel beams. *Biomedical optics express*, 7(12):4974–4981, 2016.