Advanced 3D Monte Carlo Algorithms for Biophotonic and Medical Applications

Lewis McMillan

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.

Date .... Signature of supervisor ....

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Abstract

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Acknowledgements

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Chapter 1

3D Phase Tracking Monte Carlo Algorithm

1.1 Introduction

Bessel beams have been the subject of intense research since their discovery in 1987 [1,2]. Durnin noticed that the blah blah. Bessel beams have since been used for blah blah They are really good and like are better than Gaussian beams allegedly.

This chapter examines how Bessel beams compare to other beam in a scattering medium. We investigate if the Bessel beams self-healing property has any effect in a turbid medium. We examine Bessel beams and the other beams by creating a novel Monte Carlo radiation transfer (MCRT) algorithm that allows the tracking of a photon as it propagates through a medium. The main focus of this chapter, is validation of our new novel technique, followed by using the new algorithm to compare Gaussian and Bessel beams, to see which one preforms better in a turbid medium. This chapter also extends out novel algorithm to other complex, diffraction less beams

1.2 Theory

The 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 interference for a volume element dV.

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

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. However before we validate our model we first introduce one further principle that is required for our model to work.

1.2.1 Huygens-Fresnel Principle

The Huygens-Fresnel principle is a method that is used to help mode the propagation of waves in the far-field limit and the near-field limit.

The Huygens-Fresnel principle: Every point point on a wavefront acts as a source of spherical wavelets, and that the sum of all the wavelets forms the wavefront. The principle is illustrated in **??**

1.2.2 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

From the scalar description of the electric component of the beam, we get:

$$E(r,z) = E_0\sqrt{\frac{2\pi kzw_0sin(\beta)}{z_{max}}}\ \exp^{\left(-\frac{z^2}{z_{max}^2}-\frac{i\pi}{4}\right)}\ J_0\left(krsin(\beta)\right)\ \exp^{(ikzcos(\beta))} \tag{1.4}$$

Where:
k is the wavevector, $k = \frac{2\pi}{\lambda}$ $[m]$;
z is the distance from the axicon tip $[m]$;
β is the angle the wavefront propagates at (see **??**) $[rad]$;
w_0 is the $\frac{1}{e^2}$ width of the input Gaussian beam $[m]$;
J_0 is the Bessel function of the first order;
r is radial distance from the optical axis $[m]$.

Equation (1.4) gives the electric field for a Bessel beam. The intensity can be calculated using:

$$I(r,z) = \frac{c\epsilon_0\left|E_0\right|^2}{2} \tag{1.5}$$

Using the definition total power transmitted by a beam as:

$$P = \frac{\pi I_0 w_0^2}{2} \tag{1.6}$$

Where I_0 is defined as on axis intensity of the incident Gaussian beam.

$$I_0 = \frac{c\epsilon_0 E_0^2}{2} \tag{1.7}$$

Substituting Eqs. (1.4), (1.6) and (1.7) into Eq. (1.5) yields:

$$I(r,z) = \frac{4k_r P}{w_0}\frac{z}{z_{max}} J_0^2\left(k_r\ r\right)\exp^{\left(-\frac{2z^2}{z_{max}^2}\right)} \tag{1.8}$$

Where:
k_r is the radial wavevector, $k_r = ksin(\beta)$;
P is the power of the incident Gaussian beam.

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*.

The first example of using our algorithm to model complex beams is to model a Laguerre-Gauss beam. A Laguerre-Gauss beam can be created by introducing a helical phase delay to a plane wave blah blah. ***put theory here + phase and interference patterns for all beams

Another example of our algorithms flexibility is that it can also model Hermite-Gauss beams, higher order Bessel beams and airy beams

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

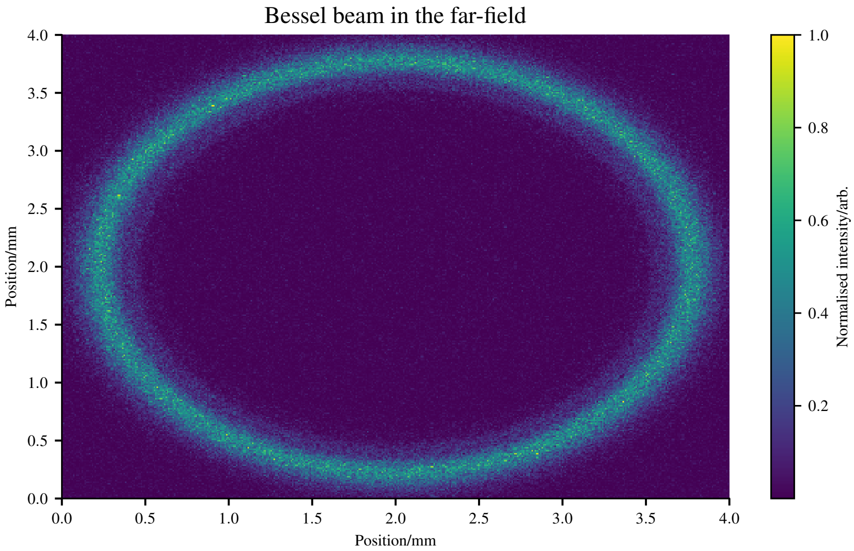

Figure 1.1: *Bessel beam in the far field.*

1.6 Discussion

a [3]

1.7 Conclusion

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