Investigating The Accuracy of Monte Carlo Simulation & Mie Theory, in The Context of Light Propagation in Whole Milk

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Research Final Project, Intermediate Computational Methods

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Abstract

Light propagation is one of the most vital things to understand in physics, whether that is through a single slit, multiple slits, media, or in the idea of its momentum. Light is a consistent player in the particle football game. Understanding how it interacts with matter, including ourselves, is one of the most vital things to grasp in terms of physical application. The goal of this specific study is to confirm our predictive model of how light propagates through a specific medium(milk), is accurate within a reasonable degree of error. This will be achieved by comparing our model experimentally through measuring distributions of intensity across the sample when exposed to a specific laser of x-wavelength. This model will focus mainly on Mie-scattering along with acknowledging experimental limitations due to Fresnel Reflection and possibly more intensive inelastic scattering. To provide the most accurate computational description, the size, shape, extinction coefficient, wavelength of the incoming light, and number of milk fat globules within the sample will all be vital players. For this specific model we will be focusing on wavelengths between 500nm and 700nm in order to maximize scattering while minimizing absorbtion and rayleigh scattering. The following variables are calculated using a combination of Mie-theory and Heynyey-Greensteins Phase function as a means of efficiency since our material can be treated as a homeogeneous spherical medium.

Introduction

Despite extensive research on photon transport like previous projects before including lights interaction in dense media, sunscreen purposed sprays and blood vessels.[3] [2][4] Accurately modeling the behavior of light in complex materials remains challenging due to factors such as anisotropic scattering, polarization effects, and possible interference. This study seeks to play the game of this gap by employing a Monte Carlo simulation to model the random walk of photons through various media, from controlled laboratory substances Starting with milk, to eventually bio-relevant tissues such as cataract-affected lenses in the eye. This model will be demonstrating an experiment in which light was passed through a cuvette then by comparing the electromagnetic intensity of each cuvette face, we aim to quantitatively assess the effective scattering characteristics of these media both in our model and in experiment. This work aims to deepen our understanding of photon to material interactions but also lays the groundwork for possibly new and insightful techniques in Ophthalmology. The following sections detail the methodology, results, and implications of our research, paving the way for future studies on complex light scattering in biological tissues and other applicable diseases.

Assumptions and Limitations

This model only looks at places where Mie scattering is dominant and absorbance index is minimal for cleaner experimental methodology, so for room temperature milk between the wavelengths of roughly between 500nm and 700nm, this model does not incorporate Rayleigh scattering of casein protein polymers within the milk.(Since it is not the dominant scattering effect at this wavelength.)

Experimental limitations include uncertainty in measurement due to fresnel reflection inside the cuvette material before or after interaction, which roughly is 4% of traveling photons. This experiment will only look at mediated whole milk with a x parts/drops milk to water ratio to demonstrate forward scattering effectively while balancing total incidents within material length for computational efficiency.
The computational model relies on a mixture of Mie theory computation from the classic book[1, 278-281] *Absorption and Scattering of Light by Small Particles* in which the original function was translated to Fortran by Bruce T. Draine then later into python by Clément Baruteau[8] from there we apply the Heynyey Greenstein Function, which is an approximation of the actual event interaction based on g(Which can be thought of similarly as the scattering crossection or $\cos\theta$ as a probability of potential theta,phi movements.) We are assuming the fat globules are homogeneous spheres in shape, meaning the interaction is simplified for Mie theory calculations. The experiment is using a sensitive photo-detector to measure intensity of light which may not absorb all wanted photons being emitted off of the surface of the cuvette. We get around this by looking at ratio distributions which is a safe claim however it is not an optimal proof.

Theory of light propagation in the context of the project

To start this off, one must pull the idea of light moving at a fixed speed inside of a material out of scope, and truly look microscopically at the interaction light begins to have with the components that make up specific materials macroscopically. In order to understand what allows us to make these assumptions of "fixed" speed, the underlying mathematics that builds these macroscopic interactions specifically in the context of milk will begin with the foundations in Mie theory,

Mie Theory

Mie Theory or Mie scattering is best described by the uses of maxwells equations how a EM plain wave interacts with a homogeneous sphere. For this specific investigation I looked into the usage of scattering extinction cross-sections,these specific cross sections can then be represented as coefficients for the specific interactions. The calculation of these coefficients, Q_a the absorption coefficient, Q_s the scattering coefficient, and Q_e the extinction coefficient. To find these values we do a series of summations in the context of spherical harmonics to easily find our coefficients.

$$Q_s = \frac{2}{k^2 r^2} \sum_{n=1}^{\infty} (2n+1)(|a_n^2| + |b_n^2|) \tag{1}$$

Where k is the spacial frequency and r is the radius of the particle and a and b are the contributions from the electric and magnetic multi-pole interactions.

$$Q_e = \frac{2}{k^2 a^2} \sum_{n=1}^{\infty} = (2n+1)\,\mathrm{Re}\,(a_n + b_n) \tag{2}$$

From the series we can then find the given coefficients of scattering and extinction for a single interaction to coefficients with a distance of 1 millimeter to then use in the step size calculation.

Afflicted Milk Composition

For this experiment I will only be looking at the fat globule interaction of light scattering in milk(correlating to Mie scattering and not Rayleigh scattering in casein polymers). The composition of milk fat globules is relatively homogeneous and spherical. Therefore an approximation for the fat globules composition is allowed with some respect to error for this given model.

Objective

The objective of this project was to demonstrate through computational modeling how light light scattering in turbid media(milk) could successfully be approximated using Monte-Carlo simulation and Mie-theory calculations. This model would then be compared experimentally to find whether or not the model in comparison to real world effects was a good fit.

Experimental Set-up

In the context of the experimental set-up for this project a 650nm ¿1mW laser was used and aligned with a plastic cuvette from there the sample cuvette was filled with water and milk was dropped and mixed thoroughly before measuring the intensity of each cuvette face with a photo-diode(s1723-05) that was connected to a power supply and voltmeter. More information can be found here
https://github.com/Hargis-Studies/Milk-Lab-Detailed-Procedure

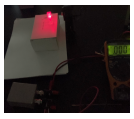

Figure 1: Experimental set-up

Methodology

To start us off I will be going through the methodology layer by layer in terms of this project. First starting with the most formulaic layers then diving deeper into the layered theory near the end. The first thing I will address is for this specific project due to lack of specialized equipment involving measuring the absorption index for the specifically used whole milk I will be pulling from a previous studies done by [7] and [6] for the range of absorption coefficients for raw milk to estimate my value of absorption.

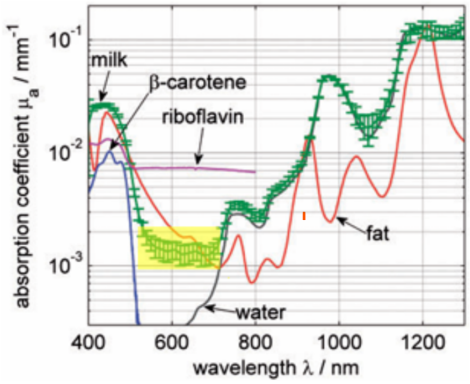

Figure 2: Absorption Coefficient by Wavelength, Figure 8.
Imaginary part of the refractive index (absorbance index)
for milk from 400–1300 nm. Data digitized and adapted from Stocker et al. (2016).

Moving on from absorption coefficients. In the context of predicting light scattering in milk there are a few things that we need to find. The step size, the allowed possible θ/ϕ of the scattering, the concentration of the milk, and the size of the viewed domain we want to look at. The specifics of these measurements can be determined through the following methods below.

Monte-Carlo

To explain Monte-Carlo in the most simplest form, one can describe it as randomness. Given a range of x number of space points, a point is picked. Then the process is repeated. In the context of this project we will be using the Beer Lambert law:

$$P = e^{-s\mu_t}$$

where μ_t is the extinction coefficient and s is the size of the step the light will take before it hits another milk particle. For classic monte-carlo simulation since we know P will give us a number between 0,and 1 we can use the idea of randomness, where we let p be some ϵ [0,1] then solve for the sampled step size.

$$p = e^{-\mu_t s} \rightarrow \frac{-\ln(p)}{\mu_t} = s$$

from there we now have a way to find how far the particle will travel before it's next collision.
From there we can involve our next element to find the θ of our given propagation. In the context of light propagation we can use the Henyey Greenstein Phase function[5]

$$P(\theta) = \frac{1}{4\pi}\left(\frac{1-g^2}{[1+g^2-2gcos(\theta)]^{3/2}}\right)$$

where g is an ϵ [-1,1] and dictates the direction of probabilistically allowed θ. We can use the same technique of assigning P as an ϵ [0,1] from there, with that element of p, given g(which will be derived in a moment) we can then solve for a θ. From there we have a θ and a step size. In the context of ϕ we have a evenly distributed θ between $[0, 2\pi]$ we are allowed to take this action through the idea of the interaction with the very sphere vs the EM field of the object. From there we have our ability to take the predicted direction

and size of step for the specific particle so we can start finding the interaction for any number of particles.
Finding g For calculating g theoretically we can use the following

$$g = \frac{2}{Q_{sca}} \sum_{n=1}^{\infty} \frac{n(n+2)}{n+1} \mathrm{Re}(a_n a_{n+1}^i + b_n b_{n+1}^i) + \frac{2n+1}{n(n+1)} \mathrm{Re}\left(a_n b_n^i\right)$$

Where a_n and b_n are the TE and TM components that are derived from the interaction of a plane wave with a homogeneous isotropic sphere, to solve for them we use a the Hankel and Hankel-Bessel functions ψ and ξ respectively.
Let x be the cross-sectional area of the particle over the wavelength of light

$$x = \frac{\pi r^2}{\lambda}$$

$$a_n = \frac{m\psi_n(mx)\psi_n'(x) - \psi_n(x)\psi_n'(mx)}{m\psi_n(mx)\xi_n'(x) - \xi_n(x)\psi_n'(mx)}$$

$$b_n = \frac{\psi_n(mx)\psi_n'(x) - m\psi_n(x)\psi_n'(mx)}{\psi_n(mx)\xi_n'(x) - m\xi_n(x)\psi_n'(mx)}$$

From there we can determine g,

once we have found g we then have everything we need to move our particle the way we would like to, the next steps would be to have a measurable way to compare to the experiment with the model. For this we looked at the change in intensity for each surface of the cuvette as the number of fat globules were increased, then compared with experimentation of the same situation to show a correlation.

Results & Data Analysis

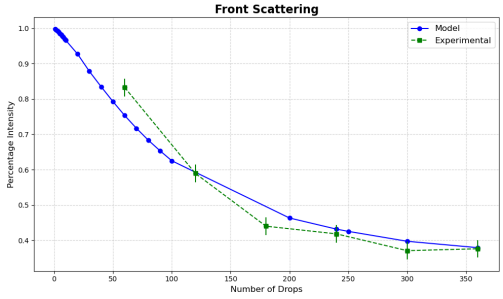

Figure 3: Foward Scattering Percentage as milk was added

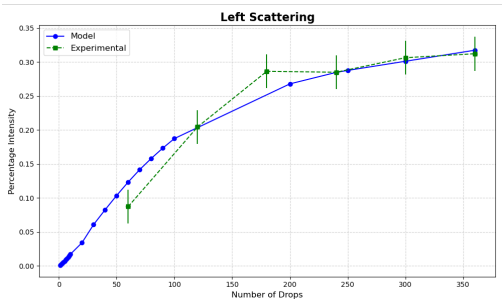

Figure 4: Left Scattering Percentage as milk was added

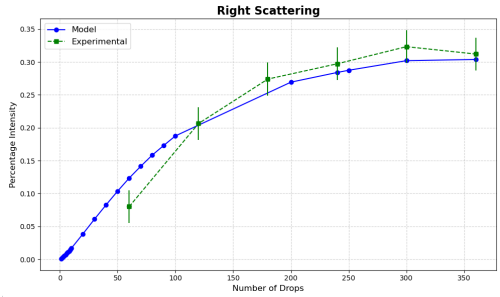

Figure 5: Right Scattering Percentage as milk was added

Error Analysis:

In our experiment we found the number of photons from a photo-diode using the formula

$$N = \frac{V\lambda}{hcRR_f}$$

where R is the photo-diode responsivity and R_f is the amplifier gain, from there we can calculate the uncertainty to be

$$\frac{\Delta N}{N} = \sqrt{\left(\frac{\Delta V}{V}\right) + \left(\frac{\Delta \lambda}{\lambda}\right) + \left(\frac{\Delta R}{R}\right) + \left(\frac{\Delta R_f}{R_f}\right)}$$

Which came out to be $\pm$ 7.82 %. In total 18 experimental points were collected to compare with the simulations expected results. Based on the given data with the highest general uncertainty between the computation to experiment was roughly 8% with most points falling into the 2.5% found error bar range. Given that, one would be able to say the following computational approach results in a relatively "good fitting model" to the prediction of light scattering in the attempted media for the specific light source.

Summary

This project investigated the accuracy of a Monte Carlo simulation coupled with Mie theory to model light scattering in whole milk—a turbid medium primarily influenced by fat globules. The simulation incorporated scattering and extinction coefficients derived from Mie theory and used the Henyey-Greenstein phase function to model angular scattering behavior.
Experimental validation involved measuring light intensity from a 650nm laser passing through a cuvette containing varying concentrations of milk, with results compared against the simulation's predictions. Despite experimental limitations, including Fresnel reflection losses and detector inefficiencies, the computational model showed relatively good agreement with observed data, typically within an 7.9% margin(matching our expected uncertainty) and often within a 2.5% error range. These findings support that the simulation approach is relatively "good" and suggest its potential for modeling photon transport in similarly complex biological materials, offering a strong foundation for future applications in fields like ophthalmology.

References

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