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A Dissertation Report on
Mie Scattering Phenomenon Modelling using DGTD method for Bio sensing Applications

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for the award of the degree

MASTER OF TECHNOLOGY

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By

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CERTIFICATE

Certified that the project work entitled "**Mie Scattering Phenomenon Modelling using DGTD method for Bio sensing Applications**" has been carried out by **Divya Shree S**, bearing USN: **1BY18SCS03**, a bonafide student of **B M S Institute of Technology and Management, Bengaluru** in partial fulfillment for the award of **Master of Technology** in **Computer Science and Engineering** of **Visvesvaraya Technological University, Belagavi** during the year 2019-2020. It is certified that all corrections/suggestions indicated for internal assessment have been incorporated in the report deposited in the departmental library. The project work report has been approved as it satisfies the academic requirement in respect of interim project work prescribed for the said degree.

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DECLARATION

I, Divya Shree S, student of fourth semester MTech, in the Department of Computer Science and Engineering, B M S Institute of Technology and Management, Bengaluru declare that the project work entitled Mie Scattering Phenomenon Modelling using DGTD method for Bio sensing Applications has been carried out by me and submitted in partial fulfillment of the course requirements for the award of degree in Master of Technology in Computer Science and Engineering of Visvesvaraya Technological University, Belagavi during the academic year 2019 - 2020. The matter embodied in this report has not been submitted to any other university or institution for the award of any other degree or diploma.

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ABSTRACT

In this project our Lab-on-a-Chip device sensor is implemented using DGTD technique of Mie Scattering phenomenon. Mie theory can be used to classify that scattered visible light from tissue differentiates the healthy cell and malignant cell nuclei and for optical analysis of haematology and its related diseases. This project work is the extended research work on previous work "FDTD Modelling of Mie Scattering Phenomenon using Gold Nano Particles for IoT based Bio-Sensing Applications".

Discontinuous Galerkin Time Domain (DGTD) method form a class of numerical methods for solving differential equations. It provides superior performance, independent of geometry complexity, within a design environment.

Total Field Scattered Field (TFSF) in DGTD can be of any arbitrary shape so scattering and absorption methods can be defined over a curved surface. The data extracted by the sensor device can later be pre-processed to extract essential insights about the user.

Lumerical FDTD is a component level simulation software which helps designers to predict light's behaviour with complex structures and systems.

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GLOSSORY

LOC	Lab on a Chip
FDTD	Finite Difference Time Domain
DGTD	Discontinuous Galerkin Time Domain
RBC	Red Blood Cells
RI	Refractive Index
API	Application Programming Interface
ODE	Ordinary Differential Equation
PDE	Partial Differential Equation
DAE	Differential Algebraic Equation
DDE	Delay Differential Equation
SDE	Stochastic Differential Equation

Chapter 1. Introduction

1.1 Background

The main objective behind this simulation work is to propose a non-invasive procedure for the detection of cancer and other malignant tumors. So, a nonlinear optical phenomenon such as Mie scattering is implemented for an arbitrary shaped geometric area and it is solved in Discontinuous Galerkin Time Domain method. Mie scattering suggests the electromagnetic scattering of light where the diameter of the particle is equal to the wavelength of light. There is no restriction with respect to the size of the particle and the solution converges for larger particles.

Mie scattering is classified into the following sub categories because of its non linear optical effect. They are Optical Kerr Effect, Stimulated Raman Scattering, Stimulated Brillouin Scattering. When a visible light is incident on a transparent medium, some part of light is scattered. The scattered light has same wavelength as that of incident light which is Rayleigh scattering. This Rayleigh scattered new light has wavelength shorter or longer wavelength than the excited light. This is defined by Raman scattering. In this Raman scattering of light other elementary parameters such as impurity, plasma, polaritons are studied.

On the other hand, if the scattered light is generated by the interaction of excitation field with acoustic parameters of liquid or solid, it is called Brillouin Scattering.

Light dissipation happening in the human tissues, for example, dermatology and hemtology properties are significant for some clinical trials. Refractive indices for dermatological and hematological applications for various frequencies of light is contemplated utilizing Discontinuous Galerkin Time Domain (DGTD) technique for Mie Scattering related photonic investigation and related sicknesses. These applications require various properties of the skin(epidermis) and haemoglobin, which assumes significance[1]. The refractive indices of hemoglobin in the visible light bandwidth is sensitive to the hemoglobin. Examination using optical and photonic means has significant clinical role[2].

Refractive Index of hemoglobin is a complex number with real and imaginary components [2]. Information regarding simulation is utilized for reenactment reason for hematology is alluded from [3]. The human blood for different refractive indices is tested at 11 unique frequencies which varies as low as 480 nm until 1550 nm at a temperature of $+24^0$ C [3]. Experimental reason requires that only the real part of the refractive index of hemoglobin was considered. Estimation was finished utilizing a refractometer at the frequencies ranging from as low as 480 nm all the way upto 1550 nano meters(nm) [3].

The reaction with respect to epidermis with regard to radiation of the light in the visible spectrum is critical to the dermatological applications including telemedicine [4]. The refractive index is a significant feature which is being considered. Refractive indices for various frequencies of light is considered wherein, light dispersing by organic cells is seen legitimately by employing Maxwell's equations. Dermatological information is alluded from [4]. Refractive index for human epidermis is an unpredictable having polarizations is s and r directions. In this study s polarization is considered for simulation of epidermis layer. Various frequencies considered from wavelength ranging from 325nm upto 1557 nm. Estimation regarding refractive index for epidermis at various frequencies are calculated using reflectometer [4].

Light dissipation from RBC cells and epidermis layer is calculated using FDTD and DGTD programming. Examination reveals the shape and volume, direction of a cell which impacts the forward dissipating of photons [1]. Techniques such as DGTD requires features such as spatial framework with respect to space and time prevents the optimal solution from divergence [5]. Simulation is carried out on a gold nano particle. This analysis is run for free space, hemoglobin and epidermis layer.

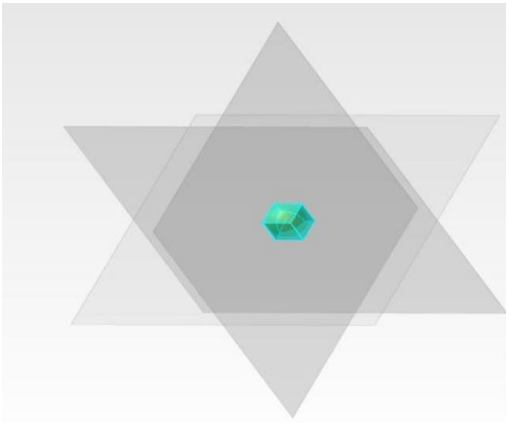

Figure 1. Vacuum as background simulation for gold sensor.

In Fig. 1, Gold sensor is placed at the centre for vacuum as the background simulation area.

1.2 Literature Survey

In this work done by Anders Karlsson, Jiangping He, Johannes Swartling, and Stefan Andersson-Engels [1] scattering of light in RBC is done using FDTD (Finite Difference Time Domain) method. Examination analysis explains that parameters such as dimension, magnitude, inclination of cells play a pivotal role in light dissipation.

Discontinuous Galerkin Time Domain method (DGTD) study is examined based on the experiment done on a fragment in vacuum in planar region. The work done by Frederick Ira Moxley III et al [5] discuss the required spatial gridding where size and time gives the non-diverging solution.

DGTD methods to solve the continuum differential equations promises the realization of parallel efficiency and scalability when going for petascale computations is discussed in the work done by Tomas Houba, Arnob Dasgupta, Shivasubramanian Gopalakrishnan, Ryan Gosse & Subrata Roy [6].

The electromagnetic scattering from nano structured particles is analysed using DGTD method. The transformed Maxwell's equations with periodic boundary conditions such as PEC and PMC, the DGTD method with FDTD Mie Scattering model is derived. The work is studied in [7].

DGTD methods proves to be stable and high order convergent in the work done by S. D. Gedney *et al*. [8]. For each and every parameter of Maxwell's equations a class of finite element methods that employ continuous basis and testing functions are discussed in this work. The hierarchical vector basis functions are used in this work done by Z. Ye and C. Wang [9]. The electric and magnetic fields are expanded to maintain high order efficiency using the DGTD method along with the parametric quantity for a 3-D implementation, reduced numerical dispersion error and the solution for Maxwell's curl equations [10].

In the work done in [11] enhanced optical radiation is induced from a single plasmonic nanoparticle. Mie scattering is analyzed with far field and near field in order to evolve non biopsy probs for confinement of light and utilization of living particles. The extent of immunoagglutination can be accurately measured without much visual disruption in the hemoglobin since Mie scattering is dependent on the angle and size of the cell [12].

The size of the cells and the nucleus contribute to the focusing effect and increase the intensity for single neuron stimulation. The neuron assists in the transfer of light to the target cell is discussed in the work [13].

The effects of cellular fine structure on light scattered from cells are studied by employing Finite Difference Time Domain Method (FDTD). In the work done in [14] diagnosis cellular fine structure for lymphocyte like cells and basophil like cells using the scattered light patterns.

The scattering cross section and the average cosine of the scattering angle are computed for cells as a function of volume fraction of melanin and mitochondria using FDTD for 3-D scattering patterns [15].

In the work done by Zhernovaya O, et al [2], the optical investigation of hemoglobin is done in the visible range of wavelength. Preventive medicine diagnosis and treatment, refractive index of hemoglobin concentration is considered since it is sensitive to the visible range. This study is referred in this simulation experiment.

Blood is a strongly scattering heterogenous medium [3]. RBC have large geometric size in the blood which determines the optical properties of the blood. The qualitative and quantitative information of the optical properties which is refractive index(RI) is particularly considered in this work.

Refractive index (RI) of the human skin is the important parameter to study the characterization of optical response of the skin [4]. The epidermis RI of human skin at different wavelengths of light 325 nm to 1557 nm is considered n this work.

1.3 Motivation

Main aim is to build point of care Lab-on-a-Chip sensing systems with high accuracy rate and low computation time. For many aspherical particles, Mie theory does not provide accurate results in much experimental geometry. By implementing DGTD, scattering and absorption methods can be defined over a curved surface.

1.4 Problem Statement

The Lab-on-a-Chip device sensor is to be implemented using Mie theory of electromagnetic light waves where Discontinuous Galerkin Time Domain (DGTD) technique is involved to study the far field phenomenon in the experimental grid.

1.5 Aim and Objective

➢ To simulate the Mie Scattering phenomenon using DGTD modelling

➢ To determine whether scattered light from tissue corresponds to healthy or cancerous cell nuclei

➢ To study the optical analysis of blood and blood related diseases

1.6 Scope

The scope of this project is to survey the related journals, transactions and to analyse the parameters involved in the simulation in the 3-D space for red blood cells, other tissues. Refractive index of blood and skin is studied as a function of wavelength.

1.7 Challenges

➢ For many aspherical particles, Mie theory does not provide accurate results in much experimental geometry. By implementing DGTD, scattering and absorption methods can be defined over a curved surface.

➢ Mie theory gives the solution only to nearly spherical object but not for any aspherical object and its orientation.

➢ Increased computation time.

1.8 Organization of the report

Chapter 1 mentions about the background research of this project work, literature survey done on this work, motivation for this work, problem statement, aim and objective for the project undertaken, scope of the project, challenges to be addressed.

Chapter 2 studies about the mathematical framework implemented in this project. The methodology of how the refractive index (RI) for a broad spectrum of visible light were calculated for Human blood and Human skin epidermis. Since the value of RI for skin and blood is a complex value, the experiment carried out to determine the values and the mathematical concept behind them are discussed in detail.

Since in this simulation work, the Mie scattering phenomenon is implemented in Space and time domain, the geometry to build the simulation mesh and the mathematical framework is studied in detail along with the introduction to Discontinuous Galerkin Time Domain (DGTD) method.

Chapter 3 discuss the system specifications, hardware and software requirements, introduction of the tools implemented in this work and their features.

Chapter 4 discuss the experimental procedure of the simulation of Human blood and epidermis layer as background simulation region with gold miniscule(nano) particle as a

sensor device. The raw data used for the experiment is mentioned in the discussion. Details have been provided as how the geometric mesh is constructed for the DGTD modelling.

Chapter 5 discuss about the Experimental analysis and Results. The plots obtained by this experimental work have been discussed in detail. How the radiation plots are scattered, their symmetry with respect to free space simulation, what they confer, are all provided in this section.

Chapter 6 deals with the challenges faced in this project, the limitations of this project, the challenges that were addressed in this work.

In Chapter 7 the conclusion of this project and the future work to be carried out or to be addressed is discussed in detail.

We have sections for the References used in this project, Sample Code programmed in Python for the experimental work, Snapshots of the simulation settings and papers that were published as a part of this research work are provided.

Chapter 2. Mathematical Fundamentals for the Simulation Work

Mathematical Framework Implemented in this Project

The accompanying numerical system and foundation are studied to execute the Mie scattering phenomenon along with DGTD. The Refractive Index (RI) as a function of differing wavelength of visible light is implemented since it explains that how living cells (hemoglobin and epidermis) interacts with the light dissipation [8-12].

The RI of Human blood and human skin (epidermis and dermis) consists of both real and imaginary component. n is the real part and it is the ratio of speed of light in vacuum and in the material. The equations 2.1 to 2.5 discussed in this work is used in calculated the RI of blood, human skin at different wavelengths of light. The test data provided in tables 4.2 and 4.3 are calculated using the equations 2.1 to 2.5.

$$n = c/v \tag{2.1}$$

Light attenuation is an imaginary component called k.

$$\bar{n} = n + ik \tag{2.2}$$

Tissues heterogeneity results in calculation of average RI which is N. RI of biological cells are calculated based on the classical theory of light dissemination [3].

$$n = 1 + 2\pi q^2 N(\omega_0^2 - \omega^2)/m(\omega_0^2 - \omega^2)^2 + \gamma^2\omega^2 \tag{2.3}$$

$$k=2\pi q^2 N\gamma\omega/m(\omega_0^2 - \omega^2) + \gamma^2\omega^2 \tag{2.4}$$

q = molecular charge

N = molecules per unit volume

m = mass of the molecule

ω = light frequency

ω_0 = molecular absorption band frequency

Υ = co-efficient of attenuation

Since epidermis and dermis layer are turbid in nature, calculating the RI is demanding. The perplexing RI of epidermis layer are dictated by non-straight relapse of R(θ) according to Fresnel conditions [4].

R^2 is the co-efficient of determination which is a consistent parameter when experimented and determined coherent reflectance curves are considered

$$R^2 = 1 - \sum_{i=1}^{N} (R_i - R_i)^2 / \sum_{i=1}^{N} (R_i - R)^2 \quad (2.5)$$

R_i and $\bar{R}_i$ = experimentally obtained and calculated reflectance at the i^{th} angle where incidence Θ_i

$\bar{R}$ = mean value of experimental reflectance over N with respect to Θ.

R^2 value lies as low as 0 and as high as 1, R^2 =1 for a perfect fit.

Discontinuous Galerkin Time Domain (DGTD) forms a class of numerical method to solve the Maxwell's differential equations using Finite element and Finite volume since our geometric mesh is an arbitrary shape. The equations which forms the basis of DGTD algorithm is discussed between the equations 2.6 to 2.8.

$$\frac{\partial \vec{D}}{\partial t} = \nabla \times \vec{H} \quad (2.6)$$

$$\frac{\partial \vec{H}}{\partial t} = -\frac{1}{\mu_0 \nabla} \times \vec{E} \quad (2.7)$$

$$\vec{D}\left(\vec{r}, \omega\right) = \varepsilon_0 \varepsilon_r \left(\vec{r}, \omega\right) \vec{E}\left(\vec{r}, \omega\right) \quad (2.8)$$

$\vec{E}$ = the electric field, $\vec{H}$ = magnetic field and $\vec{D}$ = displacement field. The simulation experiment is conducted with respect to space and time domain.

The Mie scattering phenomenon by a spherical particle is described by the set of equations given below as a solution to Maxwell's equations. Finite Difference Time Domain(FDTD) or Yee's method is a numerical technique which covers a wide range of frequencies in a single simulation to study the non linear optical phenomenon. The time dependent Maxwell's equations which are provided here from equations 2.9 to 2.19 are discretized using space and time partial derivatives. These equations are solved by first providing the vector components of electric field and the vector components of magnetic field are solved in the next instant for the same spatial volume.

FDTD equations are

Q_e = extinction co efficient.
Q_s = co efficient of scattering.
Q_a = co efficient of absorption
r = radius of gold sensor.
x = diffraction parameter.

$$Q_i = \sigma_i/\pi r^2 \quad (2.9)$$

$$\sigma_e = \sigma_s + \sigma_a \quad (2.10)$$

$$L = x + 4x^{1/3} + 2 \quad (2.11)$$

$$Q_s = 2/x^2 \sum_{1}^{\infty} (2L+1)(|a_L^2 + b_L^2|) \quad (2.12)$$

$$Q_e = 2/x^2 \sum_{1}^{\infty} (2L+1)\,\mathrm{Re}(a_L + b_L) \quad (2.13)$$

$$x = 2\pi r/\lambda \quad (2.14)$$

$$S_{L(z)} = \sqrt{\frac{\pi z}{2}} J_{L+\frac{1}{2}(Z)} \quad (2.15)$$

$$C_{L(z)} = \sqrt{\frac{\pi z}{2}} Y_{L+\frac{1}{2(Z)}} \quad (2.16)$$

$$z = x \quad (2.17)$$

$$I(\theta) = I_0\lambda^2/8\pi^2 r^2 (i_1(\theta) + i_2(\theta)) \quad (2.18)$$

$$P(\theta) = i_1(\theta) - i_2(\theta)/i_1(\theta) + i_2(\theta) \quad (2.19)$$

Chapter 3. Software Requirements

3.1 Introduction to Lumerical FDTD Simulation suite

Lumerical FDTD is a Multiphysics simulation suite for modeling nano scale devices. The Finite Difference Time Domain (FDTD) method is a reliable, powerful and scalable performance solver for a broad spectrum of bio medical devices. The interactive design environment provides for scripting capability, advanced post processing and optimization of the data.

The FDTD method is the state-of-the-art method to solve Maxwell's equations in complex geometries by providing both the time and space solution. The Maxwell's curl equations are solved for non-magnetic materials.

The main features of this lab suite are

- Device suite for physics phenomenon simulations such as Finite Difference Time Domain, Discontinous Galerkin Time Domain, etc
- Provides features to include automation APIs, to extract code from Matlab, etc
- System suite to for compilers, system library and to interconnect different circuits

3.2 Introduction to Wolfram Mathematica

Wolfram Mathematica is an advanced specialized registering framework utilized for most territories of specialized figuring, for example, neural systems, AI, image processing, geometry, information sciences, representation. The Wolfram Language is utilized as a programming language in Mathematica.

Features of Wolfram Mathematica

- Provides function library for mathematical elementary functions, Number theory function and combinatoric functions.

- Offers help for complex number, self-assertive exactness math, interim number-crunching, numbers with vulnerability blue-penciled information, worldly information, time arrangement, and unit-based information, and emblematic calculation
- Solvers for frameworks of conditions, diophantine conditions, common differential conditions (ODEs), non-straight fractional differential conditions (PDEs), differential arithmetical conditions (DAEs), deferred differential conditions (DDEs), stochastic differential conditions (SDEs), and recurrence relations
- Finite element analysis including 2D and 3D adaptive mesh generation

3.3 System Requirements Specification

3.3.1 Hardware Requirements

Windows 10, Intel Core i7 Processor, 16 GB RAM to run free space simulation in 3-D space coordinates.

To run simulations with Human Skin epidermis and Human Blood raw data, Dell Precision 5820 XCTO Tower Base Workstation with 32 GB RAM was used.

3.3.2 Operating System Requirements

Windows 10 Home, 64 – bit operating system.

3.3.3 Software Requirements

Lumerical FDTD is a simulator which is a Multiphysics suite built for the nsno scale device designers. It can be installed on Windows 10 with 64 – bit editions only.

For Wolfram Mathematica 12 the processor is to be Pentium dual core or higher,

Disk space of 19 GB, RAM atleast 4 GB.

Chapter 4. DGTD Modeling

4.1 Experiment Procedure

In this work, DGTD method is implemented since an unstructured mesh is used to model the geometry. The mesh is triangular in 2-D space and tetrahedral in 3-D. The simulation region such as human skin epidermis and human blood can be of any arbitrary shape. The accuracy of the DGTD calculation is calculated with both mesh and polynomial order.

To refine the mesh of the simulation region both surface and domain constraints are calculated for the geometry. Fig 4.1.1 represents the DGTD Mie Scattering experimental model with boundary conditions such as PMC and PEC.

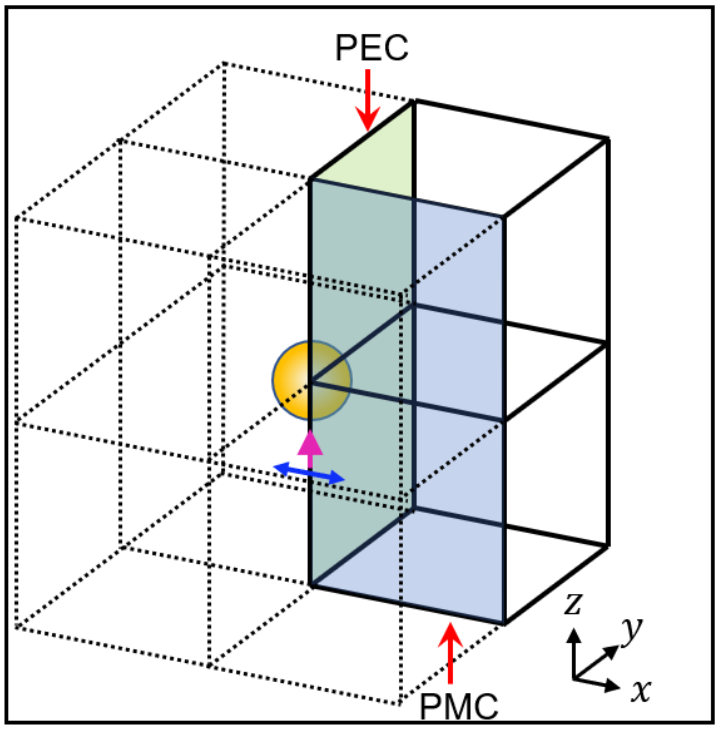

Figure 4.1.1 3-D space DGTD Mie Scattering model

DGTD for Mie theory is experimented utilizing FDTD Lumerical package. Au(gold) nano sensor of radii as small as 0.0003μm is utilized as a Lab-on-a-Chip device sensor. Perfect Electrical Conductor (PEC) and Perfect Magnetic Conductor (PMC) are defined boundary conditions simulation area. A Gaussian electromagnetic beam of light at various frequencies is used as a source which

varies as low as 320 nm to 1557 nm as the upper limit [3-4]. Gaussian beam is used source of light since it characterizes radiation spread a particular way with sufficiency characterized by its cross-area of a given guage. It gives a definite answer for Maxwell's conditions. Beam is incident along a line which is perpendicular to the direction of propagation heading and it is cut at the edges for the curve fitting [6].

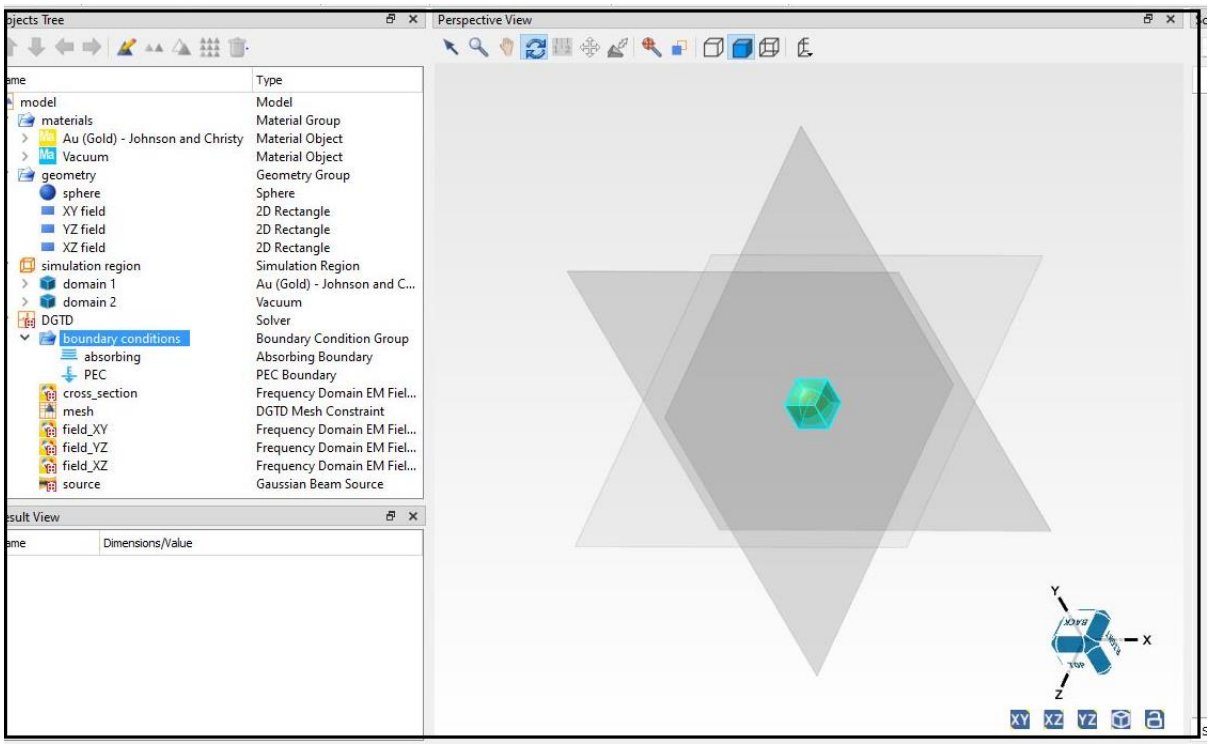

Figure 4.1.2 Simulation setting in the Lumerical Lab Suite

Fig 4.1 depicts the simulation settings in the Lumerical Lab Suite for the sensor device. The simulation is run in the vacuum, blood and epidermis layer of skin tissue.

4.2 Background Simulation Settings for Human blood

For human blood as background area, the simulation background area is set to be blood with geometry as shell where thickness is as low as 0.0004μm and the spatial settings are accomplished to build the experimental region. Fig 4.2 demonstates the 3-D simulation of a gold nano sensor with the experimental simulation area as blood. The gold nano sensor is appeared at the focal point of

the geometry, the circular beam of Gaussian light is around the nano sensor which assumes a significant job in the calculation of far field dissipating from experimental geometric area.

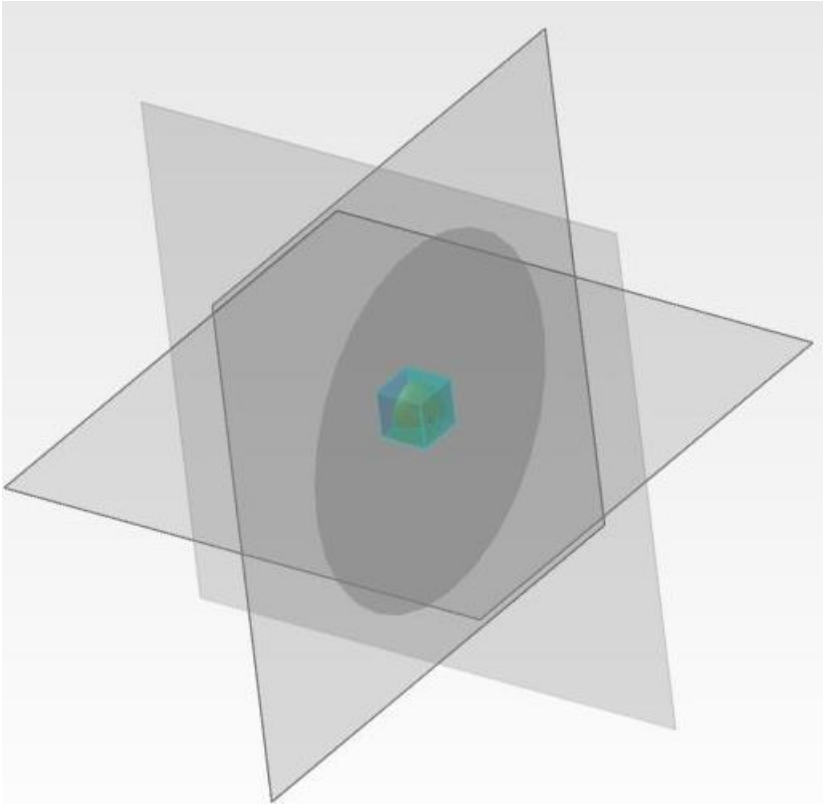

Figure 4.2.1 3-D simulation of a gold nano sensor with the simulation background as blood.

Wavelength (in nm)	**Refractive Index (real part)**
480	1.369
486	1.3686
546	1.3645
589	1.3635
644	1.3613
656	1.361
680	1.36
930	1.3561
1100	1.3537
1300	1.3497
1550	1.3456

Table 4.2 Test Data of Human Blood used for Simulation

Though RI is a complex value, only real value is considered for the simulation since building the geometry for human blood along with the sensor device takes

high computation time. With/without the imaginary part of the values is not making any significant difference in the simulation results. Table 4.2 represents the test data involved in simulation purpose. The test data is referred from work done by E.N. Lazareva et al. [3].

4.3 Simulation Settings for Human skin epidermis

The reaction with respect to epidermis with regard to radiation of the light in the visible spectrum is critical to the dermatological applications including telemedicine [4]. The refractive index is a significant feature which is being considered. Refractive indices for various frequencies of light is considered wherein, light dispersing by organic cells is seen legitimately by employing Maxwell's equations. Dermatological information is alluded from [4]. Refractive index for human epidermis is an unpredictable having polarizations is s and r directions. In this study s polarization is considered for simulation of epidermis layer. Various frequencies considered from wavelength ranging from 325nm upto 1557 nm. Estimation regarding refractive index for epidermis at various frequencies are calculated using reflectometer [4].The test data used for simulation purpose is referred from the work done by [4] which is provided below in the Table 4.3

Wavelength in nm	**RI of Human Skin epidermis with s polarization**
325	1.489
442	1.449
532	1.448
633	1.433
850	1.417
1064	1.432
1310	1.425
1557	1.404

Table 4.3. Test Data of Human Skin epidermis used for Simulation

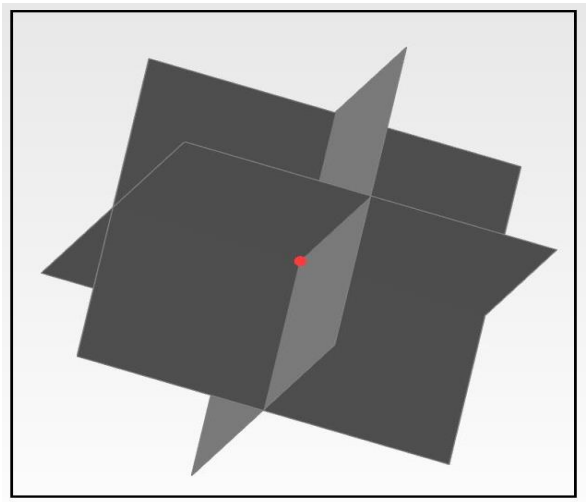

Figure 4.3.1. Human skin epidermis simulation model with gold nano sensor

Fig 4.3.1 represents the simulation model of Human skin epidermis with the gold sensor is shown as a red dot at centre of the simulation area. For the source Gaussian beam is used with s polarization values.

Chapter 5. Experimental Analysis and Results

The estimations of calculated dispersed field are far away from the scattered field which is radiation design. Dissipated far field is analysed against the experimental outcome [16].

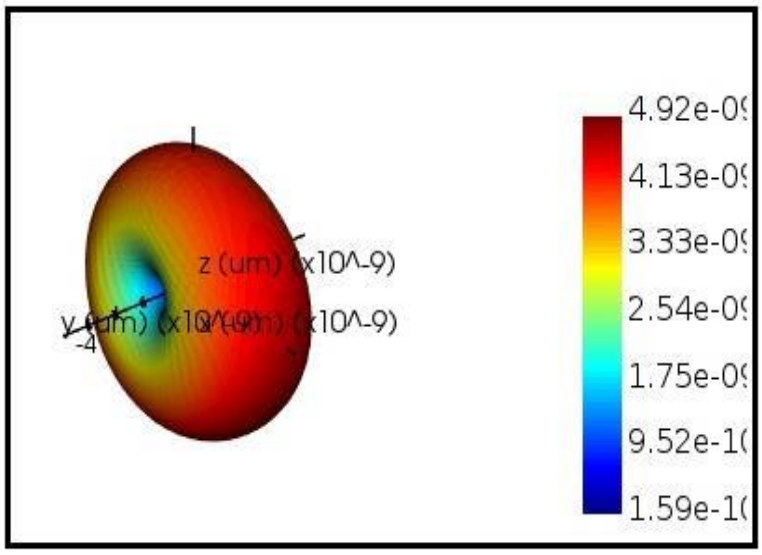

Figure 5.1 Electric field Far Field scattering with a broad-spectrum wavelength of light where blood is simulation background

Fig 5.1 represents far field plot dispersing in electric field with broad spectrum of frequencies of light where blood is background region. For this experiment the R.I of blood was referred the Table 4.3.

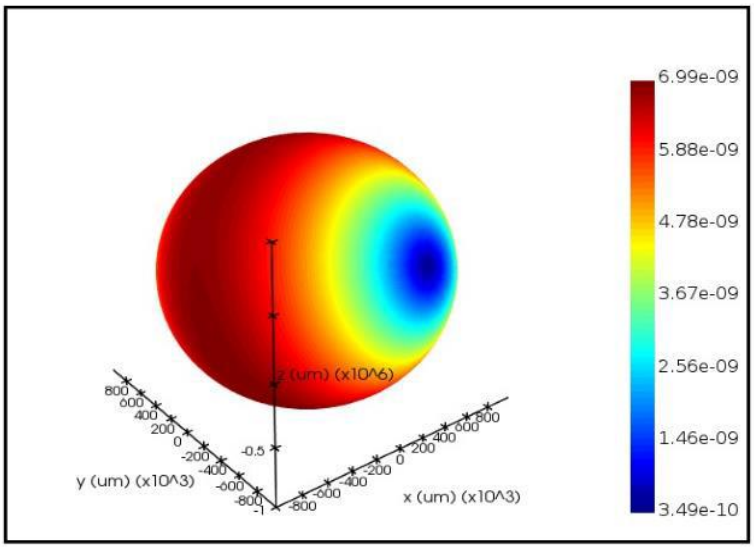

Figure 5.2 Far field surface plot where vacuum is simulation background.

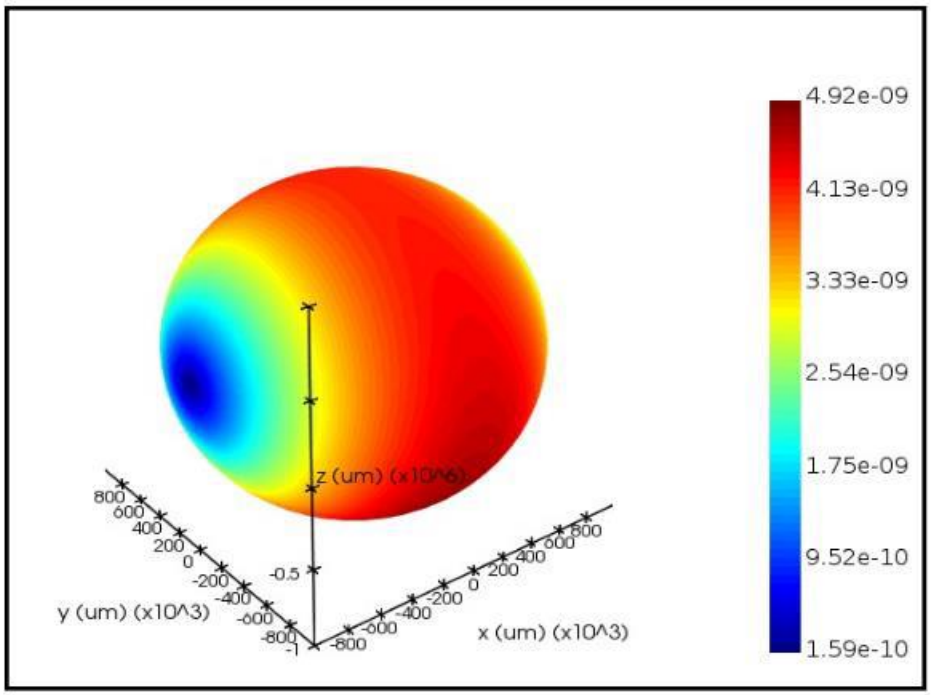

Figure 5.3 Far field surface plot
where is Blood is used as simulation background

Figures 5.2 and 5.3 speaks to far field surface plot in XYZ plane for vacuum, blood as experimental background individually. It is obvious from the plots spoken to by the figures 5.2 and 5.3 that when blood is taken as simulation area, far field electric field scattering is consistently scattered all through XYZ plane in correlation compared to the background taken in vacuum.

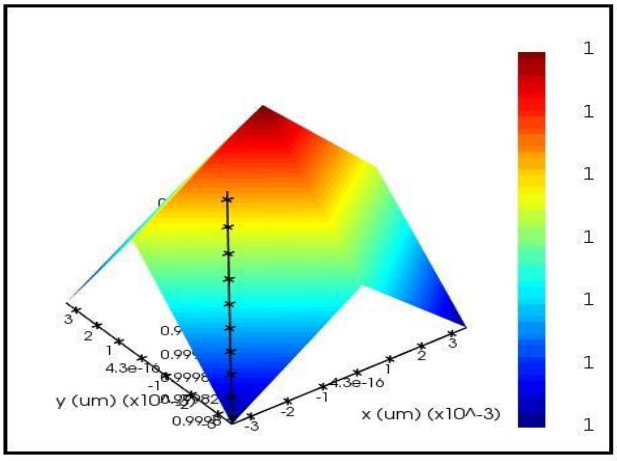

Figure 5.4 Surface plot of absorption in XYZ plane with epidermis as simulation background

Fig 5.4 explains the surface plot in electric field while proliferating through epidermis layer. Here distribution of absorption when the field proliferates through the human skin is studied. The result explains that the field intensity drops in an exponential scale.

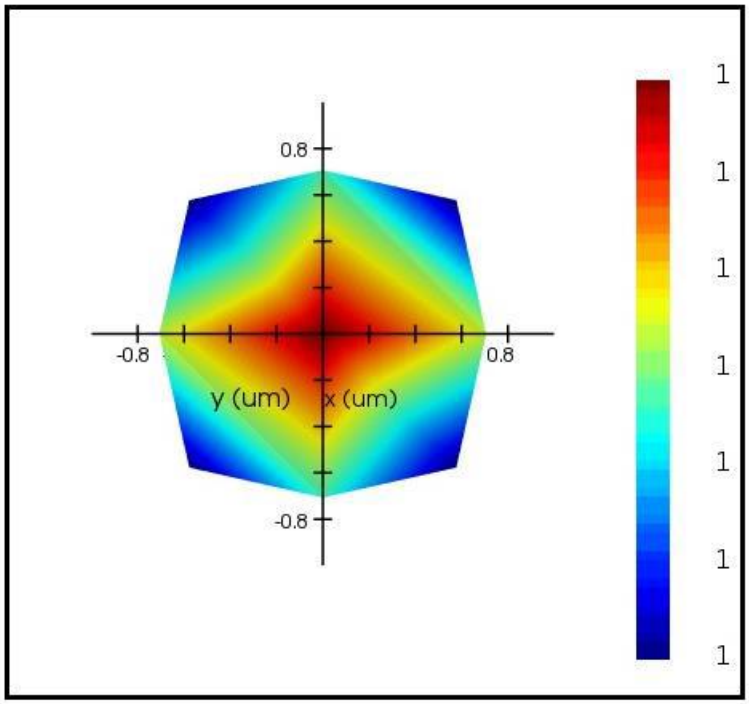

Figure 5.5. Surface radiation plot for Gaussian beam source for broad spectrum wavelength of light for epidermis layer

Fig 5.5 discuss the surface radiation plot in XYZ plane of electric field where Gaussian source for a broad spectrum of frequencies are studied in detail. The beam of light is made to pass through the epidermis layer. As found in the fig 5.4, as the field transmits through the epidermis for about 0.6μm, there is an exponential drop in the field.

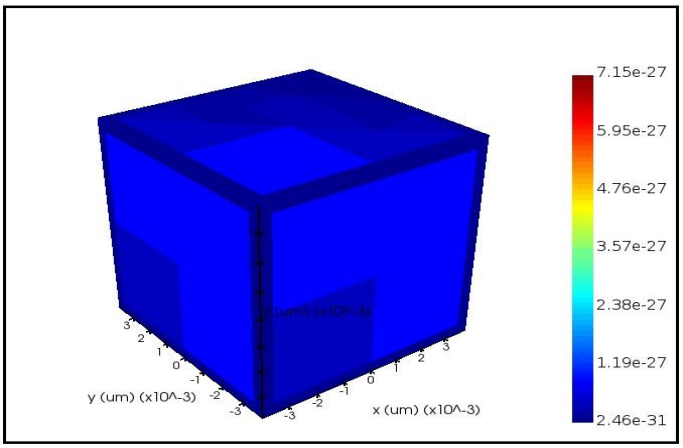

Figure 5.6. Grid volume for Human Skin epidermis

Since the simulation is run on the raw data of human blood and epidermis, the geometric mesh is a custom non uniform grid. Fig 5.6 represents the grid volume for human skin epidermis at different energy of wavelengths of light. The simulation is run in 3-D space at different simulation background, the space vectors are set in position in X, Y and Z axes. The simulation time is set to auto shut off mode which means the simulation will end automatically when most of the energy has left the simulation volume. For some results the divergence is analysed at the end of the simulation when the total energy of the simulation volume is greater than the maximum energy injected into the simulation area.

Chapter 6. Challenges

Mie Scattering provides an accurate solution to Maxwell's equations for spherical and nearly spherical particles which can be used extensively in biological applications. As a result, prediction of electromagnetic scattering based on spheres can yields exact results in determining the classification of scattering in biological beings such as cell nuclei in healthy and malignant cells.

Despite its applicability Mie theory does not provide much results in the experimental geometry and does not provide any direct information about the orientation of aspherical object.

To overcome these challenges Discontinuous Galerkin Time Domain (DGTD) model is implemented on the Mie theory instead of Finite Difference Time Domain (FDTD). The main advantages of implementing DGTD were

1. The mesh of any geometry could be constructed to the simulation area
2. The performance of the simulation results is controlled with polynomial order of the mesh
3. Boundary conditions such as PEC (Perfect Electric Conductor) and PMC (Perfect Magnetic Conductor) is a controlling parameter of the simulation

Though the results were promising, the following were the limitations

1. The simulation for raw human data (hemoglobin and epidermal tissue), the computation time is too high.
2. The simulation is stable only for nano scale devices. (Lesser the dimension of the sensor device and the simulation area, results are more accurate)
3. Optimizing the data results in loss of sensitivity.
4. The simulation for actual Human skin dermis on a nano scale is more unstable.
5. For the devices smaller than nano scale, the visualization of the geometry, boundary conditions and mesh are challenging.

Chapter 7. Conclusion

In this simulation work, our Lab-on-a-Chip device sensor is implemented using DGTD technique of Mie Scattering phenomenon. Gold particle of nano size acts as a sensor on the device. Simulation and analysis results of gold nano particles are obtained using Discontinuous Galerkin Time Domain (DGTD) method.

DGTD method form a class of numerical methods for solving differential equations. It provides superior performance, independent of geometry complexity, within a design environment.

Mie theory can be used to determine whether the light scattered from tissue can be analysed to classify the healthy cell and malignant cell nuclei and for optical analysis of haematology and its related diseases.

Future Work

In this work Mie scattering phenomenon is implemented as Lab-on- a-Chip nano sensor utilizing DGTD strategy. The light is engendering through epidermis layer and blood for a broad spectrum of visible light. Such sensors whenever manufactured can be utilized as a cutting-edge nano photonic bio sensing device for early diagnosis of terminal diseases, for example, skin malignant growth and different other neurotic conditions [16].

In order to fine tune the model, RI is not a fool proof method. The model has to be focused more towards the reflectance from blood cells and absorption towards other cancerous or pre-cancerous cells apart from RI of blood and human skin epidermis. More stress to be laid out towards the simulation of human skin dermis layer since the simulation is more unstable when RI is used as a function of wavelength.

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APPENDICES

APPENDIX A – Sample Snapshots

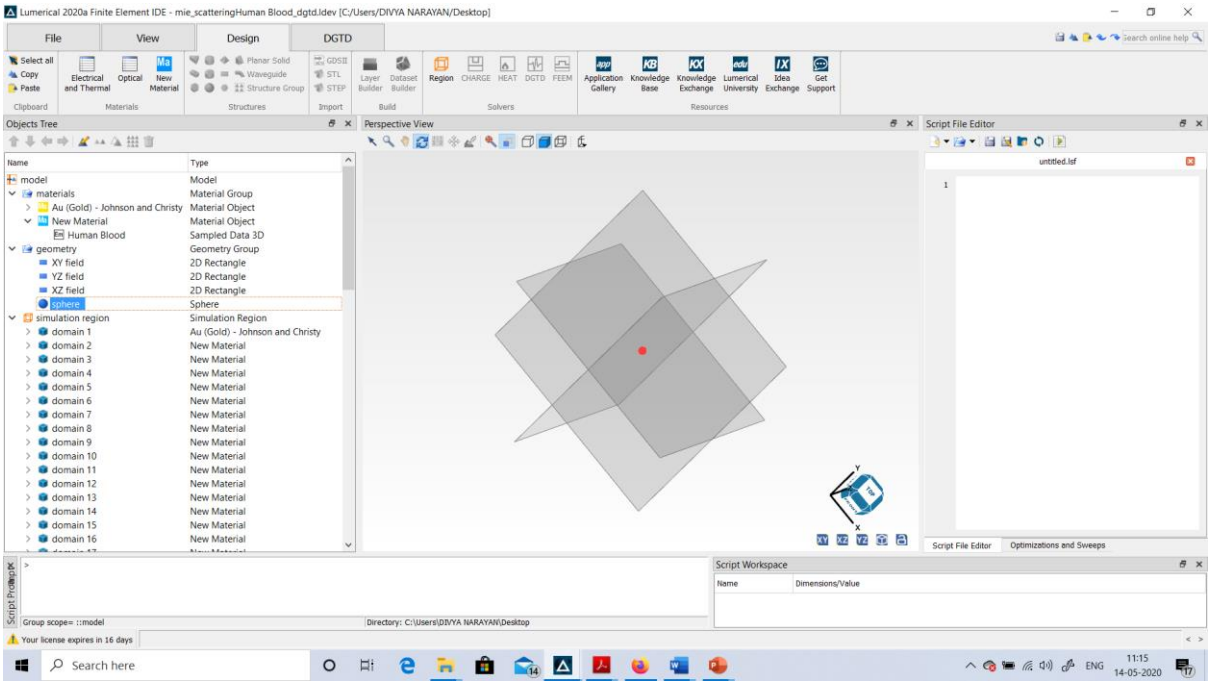

Figure B1 represents the Blood as simulation region with gold nano sensor at the centre (red dot) in Lumerical lab suite

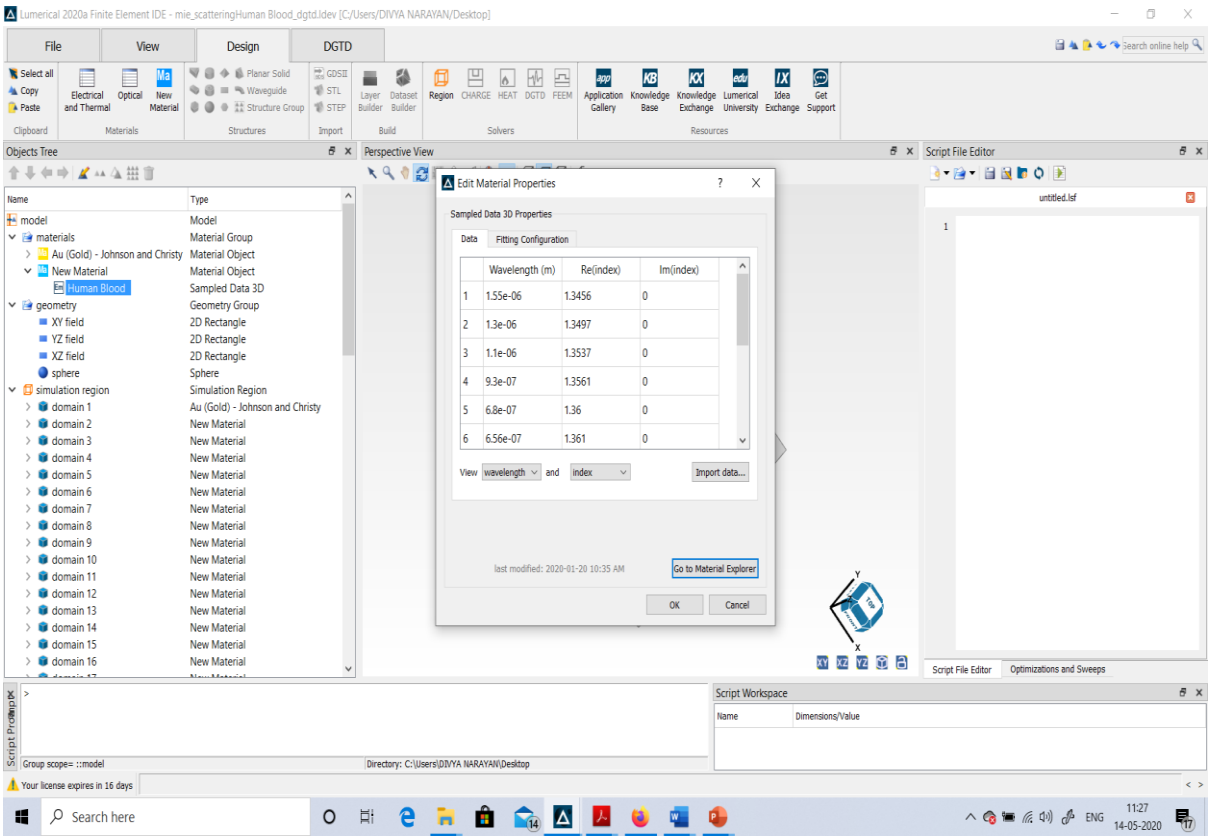

Figure B2 represents the Refractive Index of Human Blood at different wavelengths. Refractive Index of Human Blood is a complex value with both real and imaginary parts.

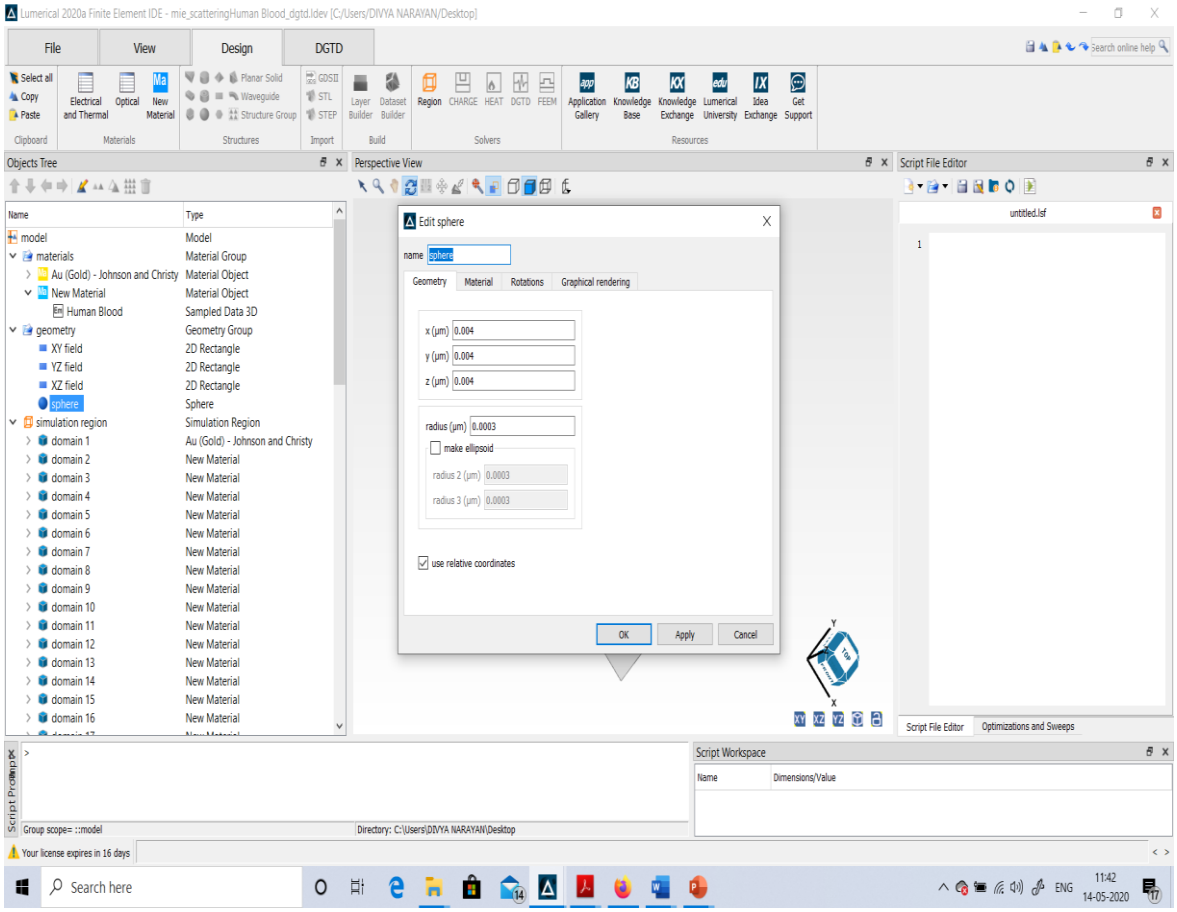

Figure B3 represents the geometrical dimensions of the gold nano sensor. The dimension remains the same for different simulation regions such as Human blood and Human skin epidermis.

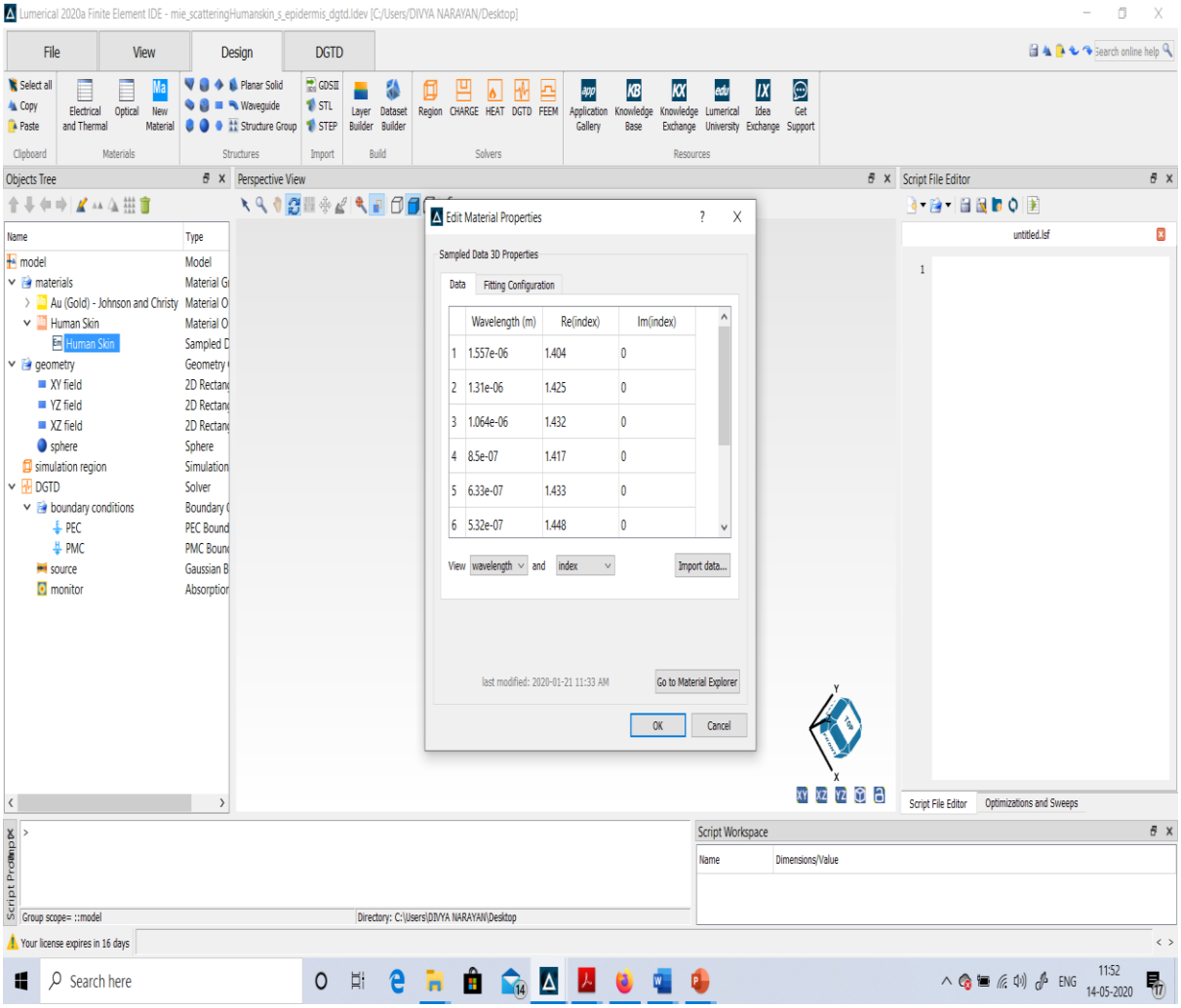

Figure B4 represents the Refractive Index of Human skin epidermis at different wavelengths. Refractive Index of Human skin epidermis is a complex value with both real and imaginary parts.

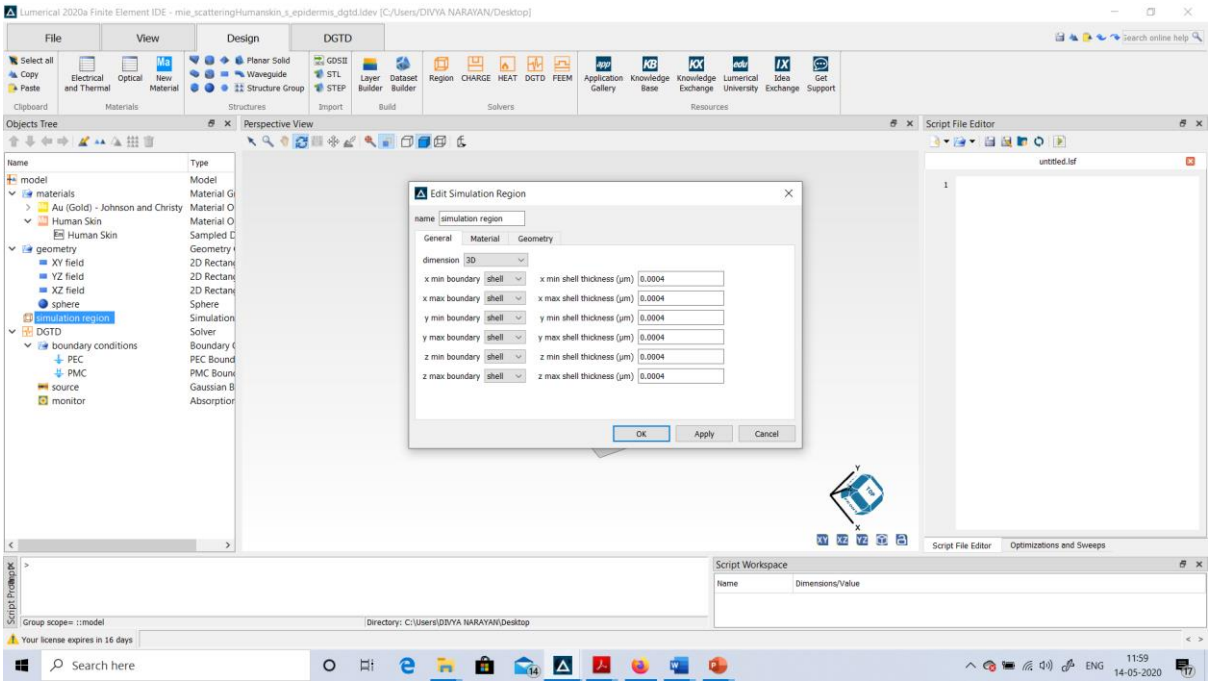

Figure B5 represents the Human skin simulation background geometric dimensions in 3D space

APPENDIX B – Papers

The following were the list of papers that were published as an outcome of this project.

1. Divya Shree S., Bharathi Malakareddy A., Kavya Uralakatte P., Bina Rajan, and Narayan K., "DGTD modeling of Mie scattering phenomenon of gold nano particles for biosensing applications," Proc. SPIE 11362, Clinical Biophotonics, 113620B (1 April 2020); doi: https://doi.org/10.1117/12.2555036

2. Divya Shree S, M. Shwetha, K. Narayan, “Modeling of Mie Scattering using Gold Nano Particles for Bio-Sensing Applications”, Presented as Poster at IEEE WARP 2019, held at IIT Guwahati between 13-14th December 2019

3. M. Venkatesha,Divya Shree .S, B. M. Chaya, K. Narayan, “Design and Analysis of Optical Wavelength Division Demultiplexer (OWDM) using Photonic Crystal”, Presented as Poster at IEEE WARP 2019, held at IIT Guwahati between 13-14th December 2019

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