RES-MATCH Fall’2024 - FINAL REPORT

Higher-Accuracy Calculations for Light Propagation Modeling

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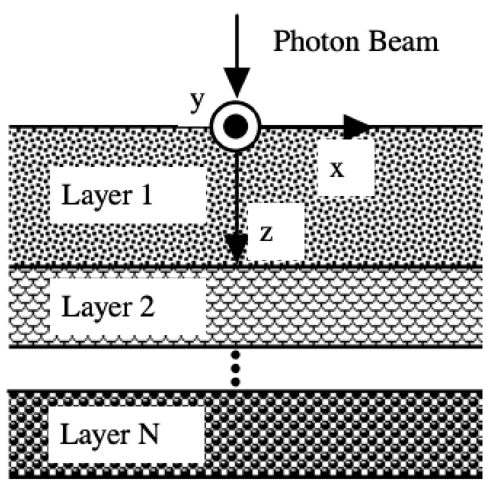
I. Introduction:

This research aims to enhance the accuracy of Light Propagation Modeling by extending the IIT CODES framework, which leverages distributed computation and is built on the CODES/ROSS platform. Previously, the IIT-CODES framework focused on simulating light propagation in a homogeneous infinite medium, where the material or tissue possesses uniform optical properties throughout the entire domain. The goal was to improve photon trajectory simulations by incorporating multi-layered media, allowing for more realistic modeling of light-tissue interactions.

II. Methods:

We implemented the Monte Carlo Modeling for Multi-Layered Media(MCML) in Python to simulate photon transport through multi-layered tissues and integrated into the IIT-CODES framework. The implementation tracks photon interactions across layers with varying optical properties such as scattering, absorption, refractive index, and anisotropy factor.



X - The horizontal position in the tissue layer (across the surface).
Y - The horizontal position in the tissue layer, perpendicular to the x-axis
Z - The depth or vertical position, representing how far the photon travels into the tissue.

By incorporating multi-layered tissue structures, our approach improves the simulation of photon behavior in complex biological media, where each layer has distinct optical characteristics. Each tissue layer is defined by specific scattering, absorption, refractive index, and anisotropy factor, allowing for accurate modeling of light propagation in heterogeneous environments. The model simulates photon interactions within each layer, accounting for both scattering and absorption, while also considering reflection and refraction at layer boundaries. These boundary transitions are governed by Fresnel's equations, ensuring precise handling of refractive index variations at layer interfaces.

Sample input for 2 layers:

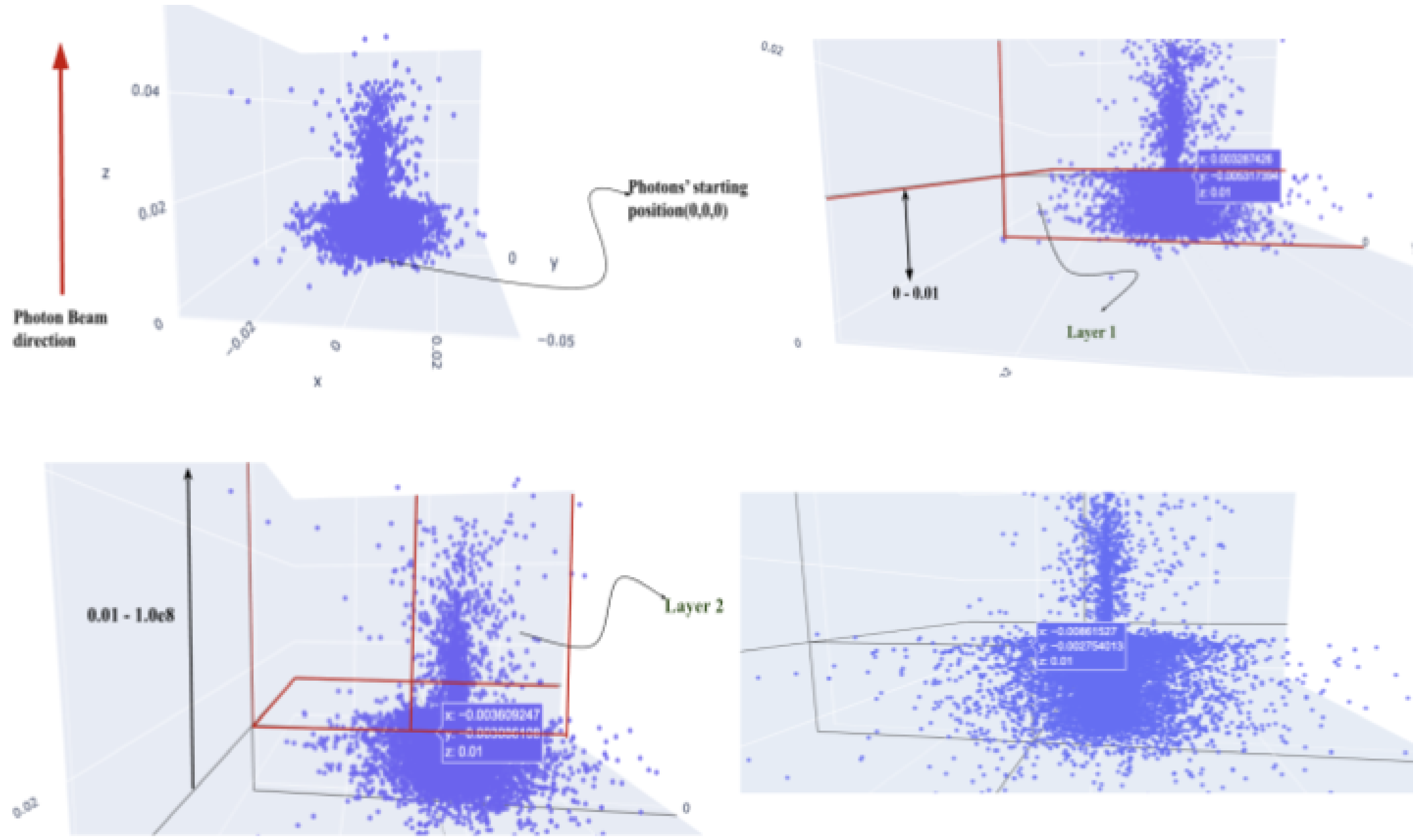
```
layer_params = {
"num_layers": 2,
"layerspecs": [
    {"z0": 0.0, "z1": 0.01, "n": 1.3, "mua": 20, "mus": 200, "g": 0.7, "cos_crit0": 0.0,
      "cos_crit1": 0.0},
    {"z0": 0.01, "z1": 1.0e8, "n": 1.4, "mua": 10, "mus": 200, "g": 0.9, "cos_crit0":
      0.0, "cos_crit1": 0.0}
 ] }
```

Parameter Representation:

1. **Z0** - Lower boundary of the layer. [Unit cm]
2. **Z1** - Upper boundary of the layer. [Unit cm]
   Eg: **Layer 1:** Ranges from **0.0 to 0.01**
   Layer 2: Ranges from **0.01 to 1.0e8(1*10^8)**
3. **N** - Refractive index of the layer.[Unit ratio]
   Eg: **Layer 1:** 1.3
   Layer 2: 1.4
4. **mua** - Absorption rate of the layer. [Unit cm^{-1}]
   Eg: **Layer 1:** 20
   Layer 2: 10
5. **mus** - Scattering rate of the layer. [Unit cm^{-1}]
   Eg: **Layer 1:** 200
   Layer 2: 200
6. **g** - Anisotrophy factor
   Eg: **Layer 1:** 0.7
   Layer 2: 0.9
7. **Cos_crit0** and **cos_crit1** are the cosine values of the **critical angles** for total internal reflection at the interfaces between tissue layers.
   - **cos_crit0**: The cosine of the critical angle at the boundary where a photon transitions from a given layer to the layer above.

- **cos_crit1**: The cosine of the critical angle at the boundary where a photon transitions from a given layer to the layer below.

III. Results: (Simulations with two layers)



The 3D visualizations of photon simulations reveal the following conclusions:

1. **Energy Distribution:** Photon concentration is higher in Layer-1, due to its greater absorption (20 vs. 10 in Layer-2). This is crucial for medical simulations, like laser treatments, where energy deposition varies by tissue depth.
2. **Depth of Penetration:** The higher absorption rate in Layer-1 (20) absorbs photons quickly, limiting their depth. Layer-2, with a lower absorption rate (10), allows photons to travel deeper before losing intensity.
3. **Photon Trajectories:** Layer-1's lower refractive index (1.3) causes photons to scatter more frequently, reducing penetration. Layer-2's higher refractive index (1.4) allows photons to bend and penetrate deeper into the tissue.
4. **Depth and Intensity:** In Layer-1, high absorption causes a rapid intensity drop, limiting photon survival. In Layer-2, lower absorption allows photons to reach deeper areas with a more gradual intensity decrease.

IV. Discussion:

This project has successfully enhanced the accuracy of light propagation modeling, enabling the simulation of photon trajectory paths across a variety of media, not just biological tissues. By tuning key parameters such as the absorption coefficient (μa), scattering coefficient (μs), and refractive index (n), the model can be adapted to simulate light interactions in a wide range of materials. For instance, the absorption coefficient allows for the simulation of materials like skin, bone, or water, which absorb light at different rates. The scattering coefficient provides flexibility in modeling both highly scattering tissues like muscle and fat, as well as more transparent materials like water or glass. Additionally, the refractive index can be adjusted to account for denser or optically complex materials, like glass or skin, as well as transparent environments like air. This versatility extends the model's applicability to various fields.

V. Conclusion:

In conclusion, this project made significant strides in advancing light propagation simulations by integrating the Monte Carlo Modeling for Multi-Layered Media (MCML) method with the IIT-CODES framework. This integration enabled more precise modeling of light interactions across multi-layered tissues. The combination of MCML and distributed computation through IIT-CODES improved accuracy, performance, and scalability, making it possible to simulate complex, heterogeneous media with greater efficiency. This work opens up new possibilities for applications in medical imaging, therapeutic treatments, and material science, showcasing the potential of blending of distributed modeling with multi-layered simulations to enhance light propagation simulations across various fields.

VI. Overall Impression:

Participating in RES-MATCH project and collaborating with Dr. Nik Sultana was an incredibly rewarding experience. The integration of Monte Carlo Modeling for Multi-Layered Media (MCML) within the IIT-CODES framework gave me valuable hands-on experience in distributed computing, computational modeling, and light propagation simulations. The program's flexible structure and the exceptional support from coordinators fostered a seamless and productive research journey. As RES-MATCH continues to grow, introducing scholarships for students which would enable students to engage in pioneering research, gaining hands-on experience and making valuable contributions to advanced scientific projects.