Monte Carlo Simulation for Light Transport in Multilayer Tissue with Embedded Object in Standard C

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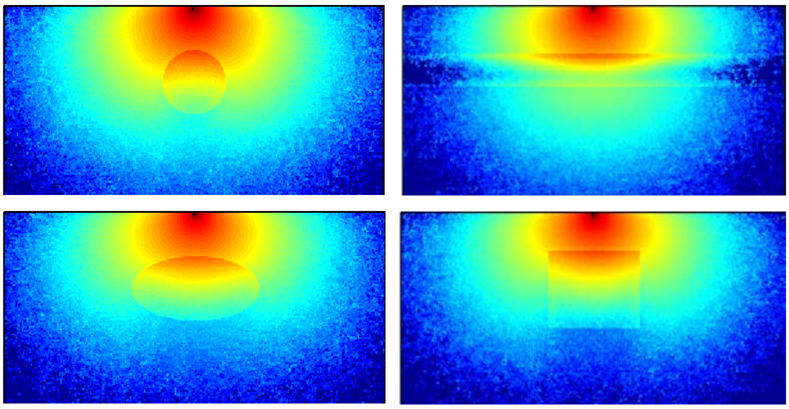

Abstract

Monte Carlo Modeling of steady-state Light Transport in Multilayered Tissues (MCML) by Dr. Lihong Wang and Dr. Steven Jacques is a tool used to simulate the light transport in biological tissues. It can provide diffuse reflectance, diffuse transmittance and absorbance in a multi-layered tissue structure. It can be used to obtain the absorbance of light inside tissue as well, which is useful in many applications such as photoacoustic imaging, photodynamic therapy, diffuse optical tomography etc. The simulation is statistical and hence requires large number of photons to be tracked to reduce variation. Since photon is treated as a particle, the phase and polarization is ignored. The aim of MCML is to look at radiant energy distribution in a turbid medium where phase and polarization is quickly randomized and hardly have any role to play in the optical output. Currently MCML simulations exist for infant brain, surficial blood vessels, etc. Modifications of basic MCML are time-resolved MCML, GPU speeded-up MCML and Mesh-based MCML. We have worked on a modified MCML to incorporate spherical, cylindrical, ellipsoidal, or cuboidal inclusion inside the turbid medium to mimic sentinel lymph node (SLN) structure, tumor, cells, blood clots, blood vessels, etc. Position and dimension of the object is taken from the user through input file. Refractive index mismatch between the embedded object and the surrounding layer is taken into account. Absorption within object is recorded and normalized by the number of photons to be displayed in the output file.

Table of Contents

1. Introduction

Here we assume that the user is well versed with the original MCML code. If not, we recommend them to first go through the original MCML code and relevant support document to understand how the Monte Carlo modelling is done for light transport in multi-layered tissues. The original MCML codes with support files are available on Dr. Lihong Wang's website (http://oilab.seas.wustl.edu/mc.html).

We have modified the original MCML to handle an embedded object (EO) which has refractive-index mismatched boundary with respect to the surrounding layer. For simulation, object of any size can be embedded in any layers (Fig. 1). Light is launched from the origin. Weight dropped by photons in the embedded object is accumulated till all the input photons are traced. Then the total weight dropped by the photons in the sphere is normalized by the number of photons. At present four types of object can be embedded: spherical, cylindrical, ellipsoid, and cuboidal.

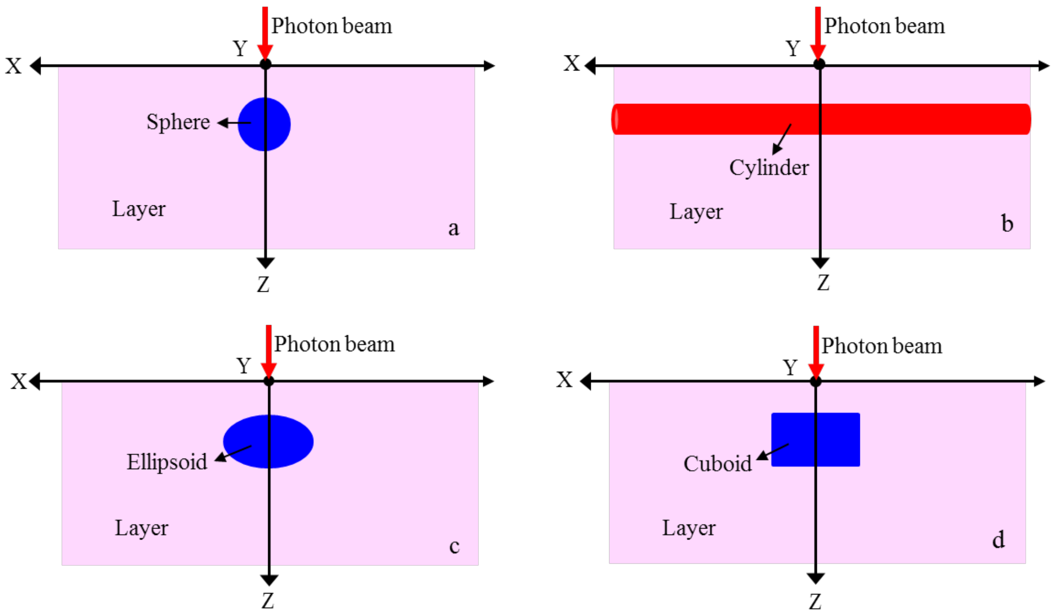

Figure 1: Schematic representation of the embedded objects in Cartesian co-ordinate system. Y-axis points inwards.

2. Input templates

a. Input template for sphere

```
####
# Template of input files for Monte Carlo simulation
# for turbid media with embedded object (MCML_EO).
# Anything in a line after "#" is ignored as comments.
# Space lines are also ignored.
# Lengths are in cm, mua and mus are in 1/cm.
####

1.0                               # file version
1                                 # number of runs

objTemp2.mco     A                # output filename, ASCII/Binary
100000                            # No. of photons
30E-4 50E-4                       # dz, dr
5     2     3                     # No. of dz, dr & da.

1                                 # No. of layers
1                                 # Object code: 0)No embedded object
                                  # 1)Sphere 2)Cylinder 3)Ellipsoid
                                  # 4)Cuboid
1                                 # Object layer
# n   mua     mus   g   d         # One line for each layer
1.0                               # n for launch medium.
1.4  0.2525   254  0.9 30         # layer 1
1.0                               # n for medium below.

1.35  2.10   773  0.9             # Object properties
1.5                               # Object depth (upto center)
0.5                               # Object dimensions
```

b. Input template for cylinder

```
####
# Template of input files for Monte Carlo simulation
# for turbid media with embedded object (MCML_EO).
# Anything in a line after "#" is ignored as comments.
# Space lines are also ignored.
# Lengths are in cm, mua and mus are in 1/cm.
####

1.0                               # file version
1                                 # number of runs

objTemp2.mco     A                # output filename, ASCII/Binary
100000                            # No. of photons
30E-4 50E-4                       # dz, dr
5     2     3                     # No. of dz, dr & da.

1                                 # No. of layers
2                                 # Object code: 0)No embedded object
                                  # 1)Sphere 2)Cylinder 3)Ellipsoid
                                  # 4)Cuboid
1                                 # Object layer
# n    mua      mus    g   d      # One line for each layer
1.0                               # n for launch medium.
1.4  0.2525   254  0.9 30         # layer 1
1.0                               # n for medium below.

1.35  2.10   773  0.9             # Object properties
1.5                               # Object depth (upto center)
0.5                               # Object dimensions
```

c. Input template for ellipsoid

```
####
# Template of input files for Monte Carlo simulation
# for turbid media with embedded object (MCML_EO).
# Anything in a line after "#" is ignored as comments.
# Space lines are also ignored.
# Lengths are in cm, mua and mus are in 1/cm.
####

1.0                             # file version
1                               # number of runs

objTemp3.mco     A              # output filename, ASCII/Binary
100000                               # No. of photons
30E-4 50E-4                     # dz, dr
5     2     3                              # No. of dz, dr & da.

1                               # No. of layers
3                               # Object code: 0)No embedded object
                                # 1)Sphere 2)Cylinder 3)Ellipsoid
                                # 4)Cuboid
1                               # Object layer
# n    mua    mus    g    d     # One line for each layer
1.0                             # n for launch medium.
1.4  0.2525 254  0.9  30        # layer 1
1.0                             # n for medium below.

1.3  1.7049    180  0.9         # Object properties
1.5                             # Object depth (upto center)
1.0   0.8 0.5                   # Object dimensions
```

d. Input template for cuboid

```
####
# Template of input files for Monte Carlo simulation
# for turbid media with embedded object (MCML_EO).
# Anything in a line after "#" is ignored as comments.
# Space lines are also ignored.
# Lengths are in cm, mua and mus are in 1/cm.
####

1.0                                 # file version
1                                   # number of runs

objTemp4.mco     A                  # output filename, ASCII/Binary
100000                              # No. of photons
30E-4 50E-4                         # dz, dr
5     2     3                       # No. of dz, dr & da.

1                                   # No. of layers
4                                   # Object code: 0)No embedded object
                                    # 1)Sphere 2)Cylinder 3)Ellipsoid
                                    # 4)Cuboid
1                                   # Object layer
# n    mua    mus    g    d         # One line for each layer
1.3                                 # n for launch medium.
1.4  0.2525 254  0.9  30            # layer 1
1.0                                 # n for medium below.

1.3  1.7049   180  0.9              # Object properties
1.5                                 # Object depth (upto center)
0.5   0.8 1.0                       # Object dimensions
```

e. Input template with no embedded object (original MCML)

```
####
# Template of input files for Monte Carlo simulation
# for turbid media with embedded object (MCML_EO).
# Anything in a line after "#" is ignored as comments.
# Space lines are also ignored.
# Lengths are in cm, mua and mus are in 1/cm.
####

1.0                            # file version
1                              # number of runs

objTemp0.mco     A             # output filename, ASCII/Binary
100000                         # No. of photons
30E-4 50E-4                    # dz, dr
5     2     3                  # No. of dz, dr & da.

1                              # No. of layers
0                              # Object code: 0)No embedded object
                               # 1)Sphere 2)Cylinder 3)Ellipsoid
                               # 4)Cuboid
1                              # Object layer
# n   mua   mus   g   d        # One line for each layer
1.3                            # n for launch medium.
1.4  0.2525 254  0.9  30       # layer 1
1.0                            # n for medium below.
```

Number of layers is followed is by the object code which ranges from 0 to 4.

0. No embedded object (only the layer geometry)
1. Sphere
2. Cylinder (x-axis aligned)
3. Ellipsoid (axis aligned)
4. Cuboid. (planes parallel to axis)

Object code is followed by layer in which the object is present. This value can range from 0 to the number of layers. 0 implies the absence of object. Object's optical properties follow the layer properties. Refractive index of object with respect to the surrounding medium, absorption coefficient μ_a and scattering coefficient μ_s and scattering anisotropy g determine the path taken by the photon within the object. Depth of the object (from the origin to the centre of the object) in cm is given. Next are the dimensions of the object.

Table 1 gives the list of the dimensions to be given.

Object code	**Embedded object**	**Dimensions as input (cm)**
0	-	-
1	Sphere	Radius
2	Cylinder	Radius
3	Ellipsoid	Radius in x, y and z axis
4	Cuboid	Length (x-axis), width (y-axis), height (z-axis)

3. Changes in code files

Object code, dimension and location of embedded object is read from the input file. Photon structure when launched is initialized with a pointer to indicate if the photon is within the object. When the photon is not in the layer of EO then hop, drop and spin is same as original MCML. When the photon is in the layer of EO, boundary check with respect to object is performed in hop function apart from check for boundary above and below. If the photon does not cross over the object boundary drop and spin are done with the optical properties of that layer. If the photon is in the object the optical properties of object are used for hop, drop and spin in the object. Drop within the object is scored in an array and then normalized. Figure 2 is the flow chart of MCML_EO. In case the user wants to run the original MCML without any embedded object he needs to set the object code 0.

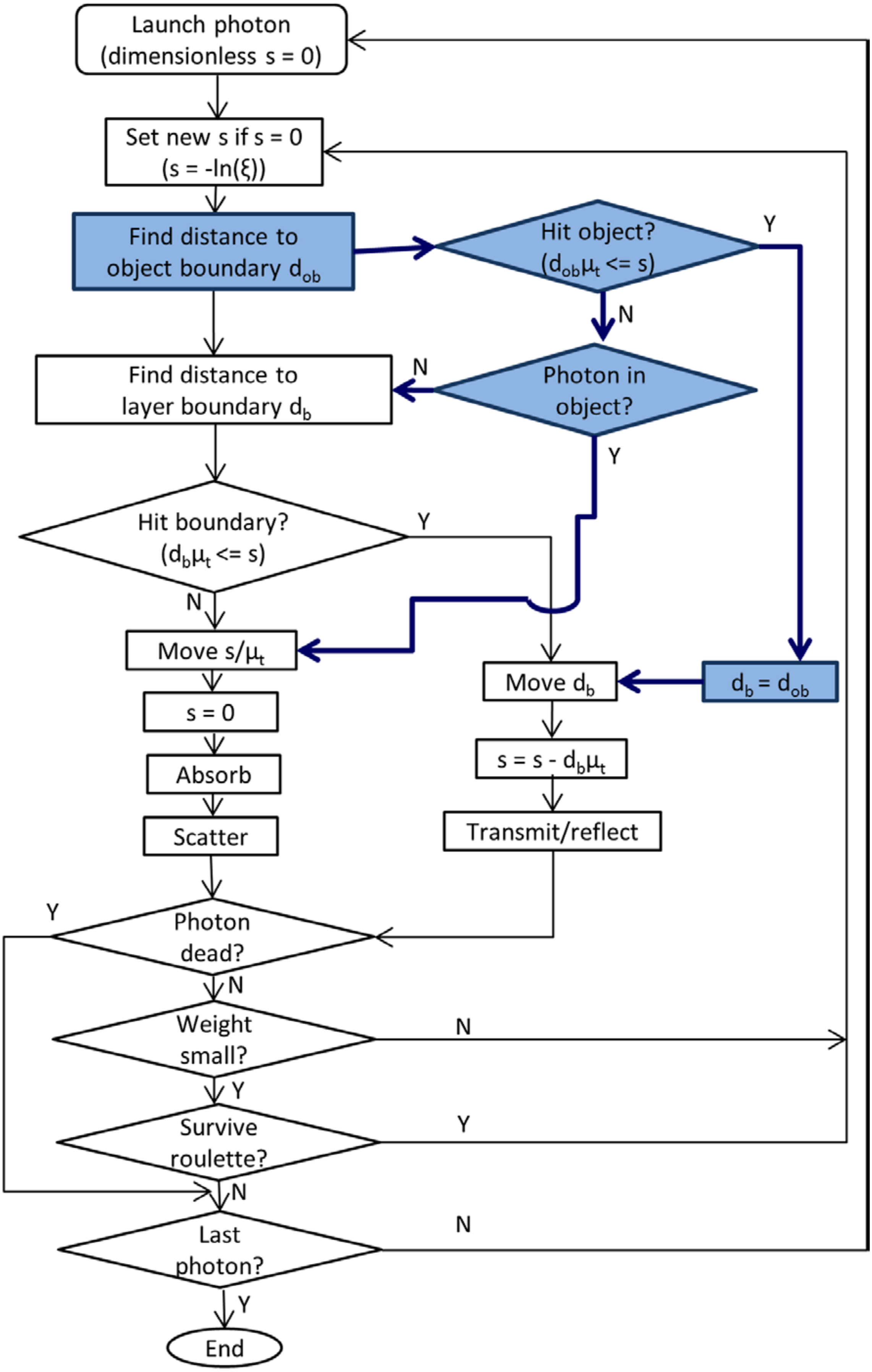

Figure 2: Flow chart for Monte Carlo simulation of Multi-layered tissue with Embedded Object

a. Changes in MCML.H
    i. Structure for optical properties and location of object.
    ii. To read object properties from input file in input structure.
    iii. Add a variable for absorbance within object in output structure.

b. Changes in MCMLMAIN.C
    i. Check input pointer, if the object is present. If the object is present, include inObj variable in Photon_ pointer when the photon is launched.

c. Changes in MCMLIO.C
    i. Function Readparm was updated to read object properties.
    ii. Absorbance within object is scaled by number of photons
    iii. Display the absorbance within object in output file after absorbance in layers.
    iv. Computation of planes for cuboid object.

d. Changes in MCMLGO.C
    i. Function HopDropSpinInTissueObj is reprogrammed to check boundaries of object.
    ii. Function HitObj finds the distance between a photons current location to the sphere surface.
    iii. Function CrossOrNotObj checks if the photon is transmitted or reflected at the boundary of the object and surrounding layer. Change in the direction cosines is computed in local Cartesian co-ordinate system.
    iv. Function DropObj drops weight within the object into an accumulative array.
    v. When the photon is in object function StepSizeInObject generates the step size with μ_t of the object.

None of the functions in file MCMLNR.C was changed.

4. Output template

```
InParm                     # Input parameters. cm is used.
objTemp1.mco     A         # output file name, ASCII.
100000                     # No. of photons
0.003 0.005                # dz, dr [cm]
5     2     3              # No. of dz, dr, da.

1                               # Number of layers
1                               # Embedded object code
1                               # Layer of object
#n    mua     mus g     d       # One line for each layer
1                               # n for medium above
1.4   0.2525 254 0.9   30       # layer 1
1                               # n for medium below

1.3   1.7049     180   0.9      # Object properties
1.5                             # Sphere depth

0.5                             # Sphere radius (cr)


RAT #Reflectance, absorption, transmission.
0.0277778       #Specular reflectance [-]
0.600708        #Diffuse reflectance [-]
0.371515        #Absorbed fraction [-]
0               #Transmittance [-]

A_l #Absorption as a function of layers. [-]
      0.3715
Absorption in object. [-]
    0.001928
```

The first few lines of the output is shown above. Output of the code, absorption within the object is printed between "*A_l #Absorption as a function of layers*" and "*A_z #A[0], [1],..A[nz-1]. [1/cm]*".

5. Bibliography

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