Monte Carlo simulation for time domain optical coherence tomography for embedded objects with improved importance sampling

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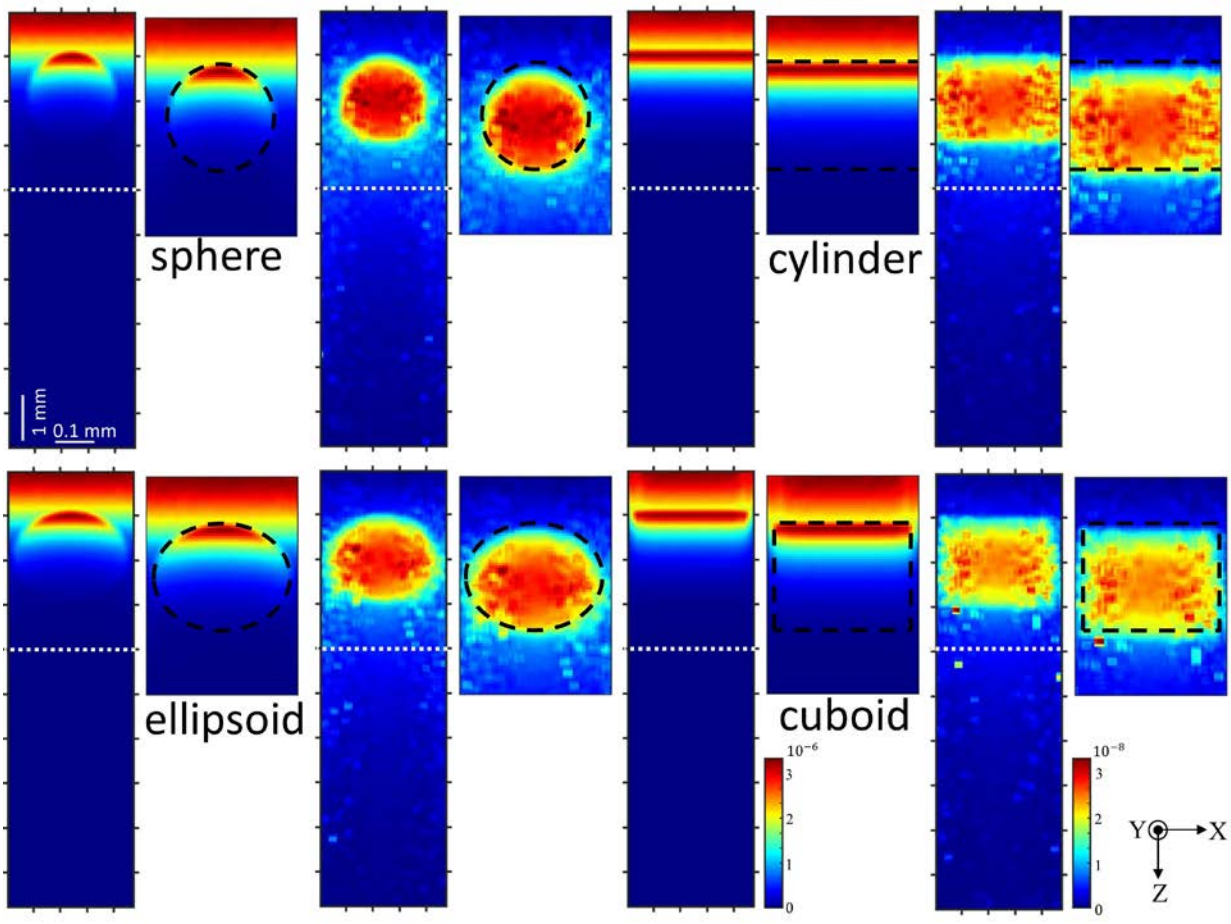

Abstract

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. MCML was modified to handle embedded objects (MCEO) such as sphere, cylinder, ellipsoid and cuboid. Absorption of light in the embedded object given in MCEO is inadequate for simulation of optical coherence tomography (OCT) which requires computation of class I and class II photons. Improved importance sampling is used in the current work to reduce the computational time of the simulation of OCT for embedded objects (MCEO-OCT). Class I and class II photons are recorded for the given collecting fiber properties which are collecting diameter and collecting angle. The OCT signal and noise also depend on the coherence length of the input laser source. The simulations here are for a source of pencil beam. B-scan imaging can also be done using this code. Class I and class II photons collected for B-scan are recorded as a matrix dimension of tracking depth and lateral scan length. Output file contains class I and class II photons of A-line scan and B-scan.

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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). Familiarizing with MCL-EO, MCML for embedded objects is an added advantage.

We have modified the original MCML-EO to handle an optical coherence tomography which requires computation of class I and class II photons, based on the optical properties of the simulation medium, geometry of collecting fiber and coherence length of input source. For simulation, object of any size can be embedded in any layers (Fig. 1). Light is launched from the center of collecting fiber tip. Photons are tracked till they die either due to negligible weight or by escaping from the simulation medium. If a photon is tracked escapes from the launch surface then it is checked if it satisfices the condition of collecting optics. On meeting the conditions of collecting optics, based on the depth reached by the photon it is either recorded as class I or class II photons in the respective grid of depth and lateral dimension.

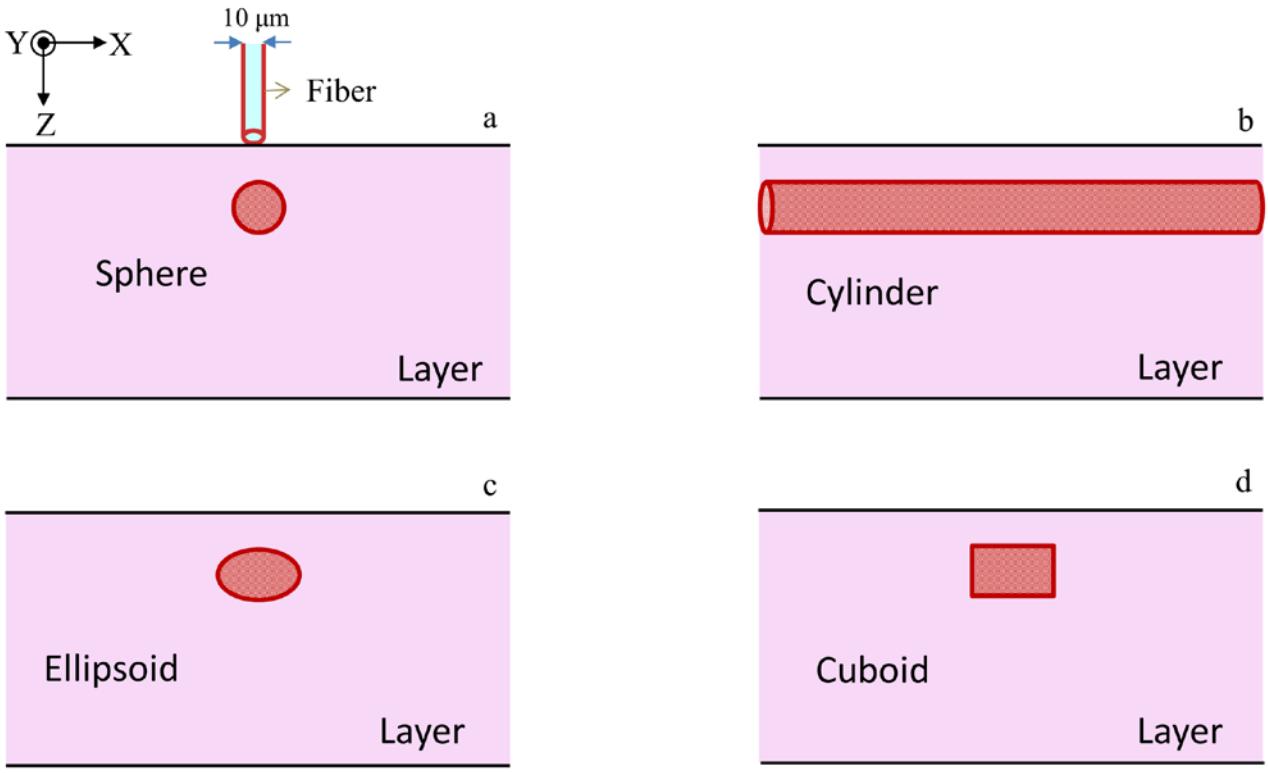

Figure 1: Schematic representation of the embedded objects in Cartesian co-ordinate system. Y-axis points inwards.

2. Input templates

a. Input template for layers

```
####
# Template of input files for Monte Carlo simulation of
# optical coherence tomography for layers (MCML-OCT).
# 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.
# Object codes 0. No embedded object 1. Sphere; 2. Cylinder;
#                       3. Ellipsoid; 4. Cuboid.
####

1.0                                     # file version
1                                       # number of runs

objTemp0.mco  A             # output filename, ASCII/Binary
10000000                            # No. of photons
5E-4   50E-4                        # dz, dr
201    2      3                     # No. of dz, dr & da.

15E-4  5.0           0.0010              # coherence length,detector receive angle
in degree,collecting radius
-0.015 0.015  10                        # x_start, x_end & # scans

11                                  # No. of layers
0                                   # Object code [0)No embedded object
       #1)Sphere 2)Cylinder 3)Ellipsoid 4)Cuboid]

# n    mua    mus    g      d             # One line for each layer
1.0                                     # n for medium above.
1.0    1.5    60     0.90   0.0200        # layer 1
1.0    3      120    0.90   0.0015        # layer 2
1.0    1.5    60     0.90   0.0150        # layer 3
1.0    3      120    0.90   0.0030        # layer 4
1.0    1.5    60     0.90   0.0250        # layer 5
1.0    3      120    0.90   0.0015        # layer 6
1.0    1.5    60     0.90   0.0100        # layer 7
1.0    3      120    0.90   0.0015        # layer 8
1.0    1.5    60     0.90   0.0125        # layer 9
1.0    3      120    0.90   0.0015        # layer 10
1.0    1.5    60     0.90   0.0085        # layer 11
1.0                                     # n for medium below.
```

b. Input template for sphere

```
####
# Template of input files for Monte Carlo simulation of
# optical coherence tomography with embedded sphere (MCES_OCT).
# 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.
# Object codes 0. No embedded object 1. Sphere; 2. Cylinder;
#                      3. Ellipsoid; 4. Cuboid.
####

1.0                                    # file version
1                                      # number of runs


objTemp1.mco A            # output filename, ASCII/Binary
500000000                       # No. of photons
0.0005 50E-4              # dz, dr
201   2     3                 # No. of dz, dr & da.
15E-4  5.0          0.001       ## coherence length,detector receive angle
in degree,collecting radius
-0.015 0.015  50          ## x_start, x_end & # scans

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.
1.0  1.5   60  0.9 0.1          # layer 1
1.0                                    # n for medium below.

1.0  3   120  0.9        ## Object properties
0.02                            ## Object depth (upto center)
0.01                            ## Object dimensions
```

c. Input template for cylinder

```
####
# Template of input files for Monte Carlo simulation of
# optical coherence tomography with embedded cylinder (MCEC_OCT).
# 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.
# Object codes 0. No embedded object 1. Sphere; 2. Cylinder;
#                   3. Ellipsoid; 4. Cuboid.
####

1.0                              # file version
1                                # number of runs


objTemp2.mco    A          # output filename, ASCII/Binary
10000000                   # No. of photons
0.0005     50E-4           # dz, dr
201   2     3               # No. of dz, dr & da.
15E-4 5.0        0.001     ## coherence length,detector receive
angle in degree,collecting radius
-0.015     0.015 50        ## x_start, x_end & # scans

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.
1.0  1.5   60  0.9    0.1        # layer 1
1.0                              # n for medium below.

1.0  3   120  0.9          ## Object properties
0.02                             # Object depth (upto center)
0.01                       # Object dimensions
```

d. Input template for ellipsoid

```
####
# Template of input files for Monte Carlo simulation
# for turbid media with embedded sphere (MCML_ES).
# 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.
# Object codes 0. No embedded object 1. Sphere; 2. Cylinder;
#                       3. Ellipsoid; 4. Cuboid.
####

1.0                                     # file version
1                                       # number of runs

objTemp3.mco  A             # output filename, ASCII/Binary
100000                      # No. of photons
0.0005 50E-4                # dz, dr
201    2      3                 # No. of dz, dr & da.
15E-4  5.0           0.001        ## coherence length,detector receive angle in
degree,collecting radius
-0.015 0.015  50            ## x_start, x_end & # scans

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.
1.0  1.5   60  0.9   30     # layer 1
1.0                                           # n for medium below.

1.0  3   120  0.9           # Object properties
0.02                                    # Object depth (upto center)
0.013  0.008 0.01                       # Object dimensions
```

e. Input template for cuboid

```
####
# Template of input files for Monte Carlo simulation
# for turbid media with embedded sphere (MCML_ES).
# 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.
# Object codes 0. No embedded object 1. Sphere; 2. Cylinder;
#                       3. Ellipsoid; 4. Cuboid.
####

1.0                                     # file version
1                                       # number of runs


objTemp4.mco  A                         # output filename, ASCII/Binary
10000000                                # No. of photons
0.0005 50E-4                # dz, dr
201    2      3                         # No. of dz, dr & da.
15E-4  5.0           0.001              ## coherence length,detector receive angle in
degree,collecting radius
-0.015 0.015  50            ## x_start, x_end & # scans

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
1.0                                     # n for launch medium.
1.0  1.5   60  0.9   0.1           # layer 1
1.0                                     # n for medium below.

1.0  3   120  0.9           ## Object properties
0.2                                     # Object depth (upto center)
0.026  0.015  0.02                      # Object dimensions
```

Number of dz, dr and da is followed by the coherence length, receiving angle of collecting fiber, and radius of collecting fiber. 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

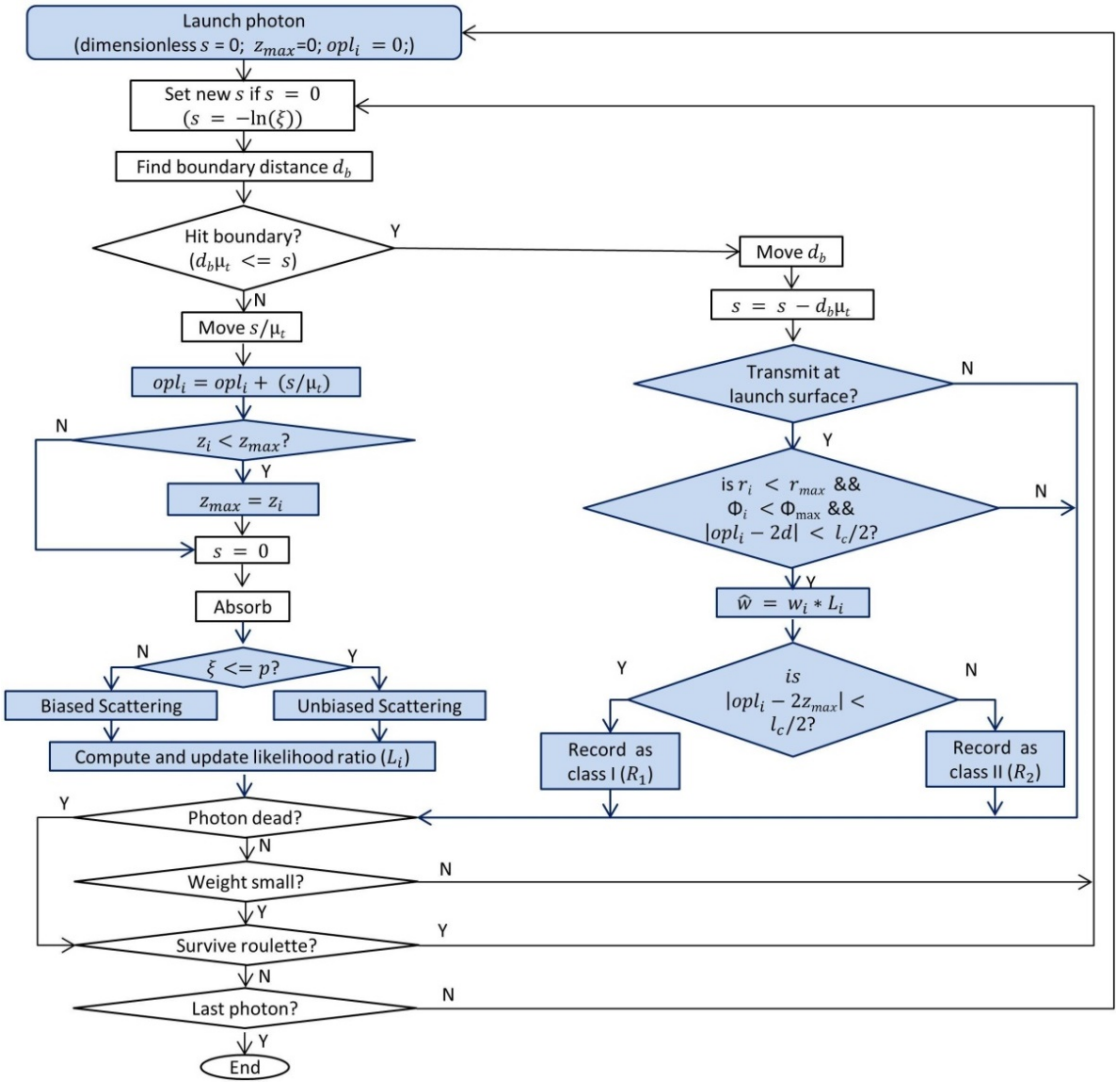

Figure 2: Flow chart for Monte Carlo simulation of Multi-layered tissue with Embedded Object for Optical Coherence Tomography

Object code, dimension and location of embedded object is read from the input file. Properties of light source and collecting fiber are also given in the input file. Photon structure when launched is initialized with a pointer to indicate if the photon is within the object. The maximum depth reached by the photon, biasing factor based on the biased and unbiased scattering and the optical path length travelled by the photon is also computed. For better understanding of the algorithm please refer to the references. When the photon is not in the layer of EO then hop, drop and spin is performed. Decision is made on whether the current scattering is biased or unbiased scattering. Unbiased scattering is the Henyey Greenstein function as in MCML, unbiased scattering is given improved importance sampling. 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 MCEO-OCT. In case the user wants to run the MCML for class I and class II photons of OCT without any embedded object one needs to set the object code 0.

a. Changes in MCML.H
   I. *Photon_Struct* to include maximum depth reached by the photon, bias factor, optical path length, pointer for first biased scattering and the launch location for b-scan.
   II. *Input_Struct* for lateral step size during b-scan, number of scan, start and end points of b-scan, launch counter, coherence length, radius of collecting fiber, collecting angle, probability of biasing factor and biasing coefficient.
   III. *Output_Struct* for A-line class I and class II photons, b-scan class I and class II photons.

b. Changes in MCMLMAIN.C
   I. In function *DoOneRun*, LaunchPhoton function is replaced with LaunchPhotonObj.

c. Changes in MCMLIO.C
   I. Updated *ShowVersion*.
   II. Included the function *ReadLC_CA_CD* to read coherence length, detection angle and radius of collecting fiber. Also initialize bias coefficient and bias factor to 0.925 and 0.5, respectively.
   III. New function *ReadXStr_XEnd_numOfScan* to read start, end and number of scans in b-scan.
   IV. Modified *ReadParam* to include *ReadLC_CA_CD* and *ReadXStr_XEnd_numOfScan.*
   V. Memory for B-scan class I and class II photons, A-line class I and class II is allotted in the function *InitOutputData.*
   VI. Memory allotted to A-line and B-scan class I and class II photon is released in *FreeData*.
   VII. A-line scans are normalized by # photons in *ScaleRdTt*.
   VIII. Updated *WriteVersion.*
   IX. Updated *WriteInParam* to print the details of collection fiber and input source.
   X. *WriteRd_z1_bs* and *WriteRd_z2_bs* prints class I and class II photons in the output file.
   XI. A-line class I and class II photons are printed by *WriteRd_z.*
   XII. Functions *WriteRd_z1_bs* and *WriteRd_z2_bs* are called by *WriteResult.*

d. Changes in MCMLGO.C

   I. *LaunchPhotonObj* is modified to initialize maximum depth reached by the photon, optical path length, bias factor and first_bias_scatter.
   II. Included *SpinTheta_forA* to compute biased scatter angle.
   III. *RecordR* is modified to record a-lines and b-scans.
   IV. *HopDropSpinInTissueObj* is modified to call *SpinBiased.*

V. *SpinBiased* is a new function added to handle the biased scattering for the modified importance sampling.

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

4. Output template for sphere

```
A1        # Version number of the file format.
####
# Data categories include:
# InParm, RAT
# A_l, Absorbance in EO, A_z, Rd_r, Rd_a, Tt_r, Tt_a,
# A_rz, Rd_ra, Tt_ra
# Rd_z1, Rd_z2, Rd_z1_bscan, Rd_z2_bscan
####
# User time: 20 sec =0.01 hr.Simulation time of this run.
InParm                        # Input parameters. cm is used.
objTemp1.mco        A                  # output file name, ASCII.
100000.000000                          # No. of photons
0.0005    0.005               # dz, dr [cm]
201       2         3         # No. of dz, dr, da.

0.001500  0.001000  5.000000  # coherence length, collecting radius in cm, detector receive
angle in degree,.
-0.015000 0.015000  50        # x_start, x_end in [cm] and no. of scans

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         1.5       60        0.9       0.1       # layer 1
1                                                 # n for medium below

1         3         120       0.9                                                 #
Object properties
0.02                                                      # Sphere depth
0.01                                              # Sphere radius (cr)


RAT #Reflectance, absorption, transmission.
0                   #Specular reflectance [-]
43.8873             #Diffuse reflectance [-]
5.00924             #Absorbed fraction [-]
1.10343             #Transmittance [-]

A_l #Absorption as a function of layers. [-]
       5.009
Absorption in object. [-]
       1.427
 A_z #A[0], [1],..A[nz-1]. [1/cm]
...
Rd_r #Rd[0], [1],..Rd[nr-1]. [1/cm2]
 ...
Rd_a #Rd[0], [1],..Rd[na-1]. [sr-1]
 ...
Rd_z1 #Rd[0], [1],..Rd[nz-1]. [1/(cm)]
...
Rd_z2 #Rd[0], [1],..Rd[nz-1]. [1/(cm)]
...
# Rd_z1_bs[depth][scan].
# Rd[0][0], [0][1],..[0][ns-1]
# Rd[1][0], [1][1],..[1][ns-1]
# ...
# Rd[nz-1][0], [nz-1][1],..[nz-1][ns-1]
Rd_z1_bs
201        50
 ...

# Rd_z2_bs[depth][scan].
# Rd[0][0], [0][1],..[0][ns-1]
# Rd[1][0], [1][1],..[1][ns-1]
# ...
# Rd[nz-1][0], [nz-1][1],..[nz-1][ns-1]
Rd_z2_bs
201        50
 ...

Tt_r #Tt[0], [1],..Tt[nr-1]. [1/cm2]
 ...

Tt_a #Tt[0], [1],..Tt[na-1]. [sr-1]
 ...

# A[r][z]. [1/cm3]
# A[0][0], [0][1],..[0][nz-1]
# A[1][0], [1][1],..[1][nz-1]
# ...
# A[nr-1][0], [nr-1][1],..[nr-1][nz-1]
A_rz
 ...
# Rd[r][angle]. [1/(cm2sr)].
# Rd[0][0], [0][1],..[0][na-1]
# Rd[1][0], [1][1],..[1][na-1]
# ...
# Rd[nr-1][0], [nr-1][1],..[nr-1][na-1]
Rd_ra
 ...
# Tt[r][angle]. [1/(cm2sr)].
# Tt[0][0], [0][1],..[0][na-1]
# Tt[1][0], [1][1],..[1][na-1]
# ...
# Tt[nr-1][0], [nr-1][1],..[nr-1][na-1]
Tt_ra
 ...
```

5. Bibliography

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