Code manual

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LIBRARIES

import numpy as np import multiprocessing as mp from multiprocessing import Queue, cpu_count import matplotlib.pyplot as plt import time import os

Simulation files:

Parameter	meaning	symbol	unit	Data from	Data to	To know
wavelengt h	all wavelength data for this program					
Model_inp ut	some parameters of the simulated tissue model					
Mua_wate r	the optical absorption properties (μ _a cm ⁻¹) of water	μ _a	Cm ⁻¹	0.000266 8	0.04337 6	
Mua_oxy	the optical absorption properties (µ _a cm ⁻¹) of oxygenated whole blood	μ _a	Cm ⁻¹			150 g hemoglobin/liter or 2.33x10 ⁻³ M From https://omlc.org/software/mc/mcxyz/index.html
Mua_mela nin	the optical absorption properties (µ _a cm ⁻¹) ofinterior of typical cutaneous melanosome	μ _a	Cm ⁻¹			

Initial parameters:

WEIGHT:

WEIGHT = 1e-4 # critical weight for roulette

CHANCE = 0.1 # Chance of roulette survival

PARTIALREFLECTION = 0 # 1=split photon, 0=statistical reflection.

COSZERO = 1.0 - 1.0e-12 # cosine of about 1e-6 rad COS90D = 1.0e-6 # cosine of about 1.57 - 1e-6 rad

path = os.path.dirname(__file__)

Table 5.1. Important constants in the program mcml.

Constants	File	Value	Meaning			
WEIGHT	mcml.h	1×10 ⁻⁴	threshold weight			
CHANCE	mcml.h	0.1	chance of surviving a roulette			
STRLEN	mcml.h	256	string length			
COSZERO	mcmlgo.c $1-1\times10^{-12}$ cosine of ~ 0		cosine of ~ 0			
cos90D mcmlgo.c		1×10 ⁻⁶	cosine of ~ 90°			
THINKCPROFILER	mcmlmain.c	1/0	switch for THINK C profiler on Macintosh			
gnuce memlmain.c 1/0 s		switch for GNU C compiler				
STANDARDTEST	mcmlgo.c	1/0	switch for fixed sequence of random numbers			
PARTIAL- mcmlgo.c		1/0	switch for partial internal reflection at boundary			

The parameters that are needed to describe a layer of tissue are grouped into one

structure:

```
typedef struct {
  double z0, z1;
  double n;
    double mua;
  double mua;
  double mus;
  double mus;
  double g;
  /* scattering coefficient. [1/cm] */
  double cos_crit0, cos_crit1;
} LayerStruct;
```

For both air and water, a moderate scattering coefficient is specified so that the photon steps through the tissue, but the value of g is set to 1.0 so there is not photon deflection. Also a very very low absorption coefficient is specified (eg., $\mu_a = 0.0001 \text{ cm}^{-1}$ for air, or the absorption of water at the chosen wavelength). Hence, the photon will step through air or water, and deposit a very small amount of photon weight in the voxels, thereby specifying its pathlength spent in the air or water. But the energy lost in the air is negligible, so it does not significantly influence the distribution of light. The absorption in water depends on the chosen wavelength. At the end of the program (discussed in How to use mcxy.c, below), the fluence rate ϕ is calculated by dividing the deposited energy by the very small μ_a which recovers the ϕ in the air and water.

MEDIUM CLASSE

Medium:

```
n - refractive index
mua - absorption coefficient. [1/cm]
mus - scattering coefficient. [1/cm]
g - anisotropy
```

MEDIUMS and default parameters

All made from:

- oxygenated whole blood (150 g hemoglobin/liter or 2.33x10⁻³ M)
- deoxygenated whole blood
- water
- interior of typical cutaneous melanosome
- fat

Medium	Biological name	Refractive index n	Attenuation coefficitn <u>mua</u>	Scattering coefficient mus	g	Cb	Cwater	Cmel	thickness
Air	Air	1	0		1				
Tissue 1	epidermis	1.5	((0.1-(0.3e-4*wavelength))+1.25 *Rayleigh)*(1- Cwater)+Cwater*water	1000	0.86				20e-4
Tissue 2	dermis	1.34	(Cmel*melanin+(1- Cmel)*Rayleigh)*(1- Cwater)+Cwater*water	450.0	0.8				80e-4
Tissue 3		1.4	((1- S)*gamma*Cb*deoxy)+(S*gamma*C b*oxy)+((1- gamma*Cb)*Cwater*water)+((1- gamma*Cb)*(1-Cwater)*Rayleigh)	300	0.9	0.04	0.5		150e-4
Tissue 4		1.39	((1- S)*gamma*Cb*deoxy)+(S*gamma*C b*oxy)+((1- gamma*Cb)*Cwater*water)+((1- gamma*Cb)*(1-Cwater)*Rayleigh)	350	0.95				80e-4
Tissue 5		1.4	((1- S)*gamma*Cb*deoxy)+(S*gamma*C b*oxy)+((1- gamma*Cb)*Cwater*water)+((1- gamma*Cb)*(1-Cwater)*Rayleigh)	250	0.8				1500e-4

Tissue 6	1.38	((1- S)*gamma*Cb*deoxy)+(S*gamma*C b*oxy)+((1- gamma*Cb)*Cwater*water)+((1- gamma*Cb)*(1-Cwater)*Rayleigh)	300	0.95	80e-4
Tissue 7	1.44	((1- S)*gamma*Cb*deoxy)+(S*gamma*C b*oxy)+((1- gamma*Cb)*Cwater*water)+((1- gamma*Cb)*(1-Cwater)*Rayleigh)	50	0.75	6000e-4

- B = blood volume fraction
- S = oxygen saturation of hemoglobin
- W = water volume fraction
- M = melanosome volume fraction
- F = fat volume fraction
- $\mu_{s.500\text{nm}}$ ' = reduced scattering coeff. at 500 nm [cm⁻¹]
- f = fraction of scattering at 500 nm due to Rayleigh scattering
- 1-f = fraction of scattering at 500 nm due to Mie scattering
- b_{mie} = scattering power for Mie scattering

$$\mu_{\text{s}}\text{'} = \mu_{\text{s}.500\text{nm}}\text{'} \left(f_{Rayleigh}(\lambda/500\text{nm})^{-4} + f_{Mie}(\lambda/500\text{nm})^{-bMie}\right)$$

- $\mu_{s.500nm}'$ = reduced scattering coeff. at 500 nm
- $f_{Rayleigh}$ = fraction of Rayleigh scattering at 500 nm
- f_{Mie} = fraction of Mie scattering at 500 nm
- $\lambda = \text{wavelength [nm]}$
- b_{Mie} = scattering power of Mie scattering

The melanin content is described by the volume fraction (M_f) of a standard cutaneous melanosome in the epidermis. The absorption coefficient of the interior of a melanosome was estimated by the threshold pulsed laser radiant exposure required to explode a cutaneous melanosome:

From < https://omlc.org/news/feb15/generic_optics/index.html>

$$\mu_{a.melanosome} = (679 \text{ cm}^{-1}) \left(\frac{\lambda}{500nm}\right)^{-3.33}$$

stratum corneum boundary

With a starting photon weight W of 1, every time a photon packet interacts with a bin it loses part of its weight and then gets scattered in a direction determined by the anisotropy factor and scattering coefficient. At the end of the simulation, all diffusely scattered photons locating at the incident side (z<0) were added up to give a diffuse reflectance spectrum. </br>

Table 6.6. The optical properties of the three-layer tissue.

Layer		Absorption Coeff. (cm ⁻¹)	Scattering Coeff. (cm ⁻¹)	Anisotropy Factor g	Thickness (cm)	
1	1.37	1	100	0.9	0.1	
2	1.37	1	10	0	0.1	
3	1.37	2	10	0.7	0.2	

MODEL SIMULATION CLASS

Wth - play roulette if photon weight < Wth

dz - z grid separation [cm]

dr - r grid separation [cm]

da - alpha grid separation [radian]

nz - array range 0..nz-1

nr - array range 0..nr-1

na - array range 0..na-1

layerObj - medium layer structure class instance

FUNCTIONS TO EXPLAIN

np.genfromtxt:

np.power

MIGHT BE NEEDED MODIFICATION

Line 740:

This program can only be produced to 8 core operations. If you want to expand more core operations, please add the following code such as:
Increase the number of cores in order below m8.start()
if c.get(8):
boundary = c[8]
q9 = Queue()
m9 = mp.Process(target=job, args=(q9,model,N,boundary))
m9.start()
And so on...

```
cpu_number = int(cpu_number)
            elif cpu_number>cpu_count():
                cpu_number = cpu_count()
                cpu_number = 1
            tStart = time.time()
736
            model = PhotonModel()
            c = \{\}
            # This program can only be produced to 8 core operations. If you w
            # Increase the number of cores in order below m8.start()
             # if c.get(8):
             # q9 = Queue()
             # m9 = mp.Process(target=job, args=(q9,model,N,boundary))
             # m9.start()
            for i in range(0,cpu_number):
               c[i] = [int(0+i*316/cpu_number), int((i+1)*316/cpu_number)]
            if c.get(0):
                boundary = c[0]
                q1 = Queue()
                m1 = mp.Process(target=job, args=(q1,model,N,boundary))
                m1.start()
            if c.get(1):
                houndary - c[1]
```

Line 785:

This program can only be produced to 8 core operations. If you want to expand more core operations, please add the following code such as:

Increase the number of cores in sequence below R.append(q8.get())

if c.get(8):

m9.join()

R.append(q9.get())

And so on...

```
m6.start()
               if c.get(6):
                   boundary = c[6]
                   q7 = Queue()
                   m7 = mp.Process(target=job, args=(q7,model,N,boundary))
                   m7.start()
               if c.get(7):
                   boundary = c[7]
                   q8 = Queue()
                   m8 = mp.Process(target=job, args=(q8,model,N,boundary))
                   m8.start()
               print('Currently using %d cores in the operation'%(i+1))
               # This program can only be produced to 8 core operations. If you w
                # Increase the number of cores in sequence below R.append(q8.get(
                # if c.get(8):
                # m9.join()
               # R.append(q9.get())
  790
               R = []
               if c.get(0):
                   m1.join()
                   R.append(q1.get())
               if c.get(1):
function tissue = makeTissueList(nm)
%function tissueProps = makeTissueList(nm)
% Returns the tissue optical properties at the wavelength nm:
%
    tissueProps = [mua; mus; g]';
%
    global tissuenames(i).s
% Uses
%
    SpectralLIB.mat
%% Load spectral library
load spectralLIB.mat
% muadeoxy 701x1
                           5608 double
% muamel
              701x1
                          5608 double
             701x1
                          5608 double
% muaoxy
% muawater 701x1
                           5608 double
% musp
            701x1
                         5608 double
% nmLIB
            701x1
                         5608 double
MU(:,1) = interp1(nmLIB,muaoxy,nm);
MU(:,2) = interp1(nmLIB,muadeoxy,nm);
MU(:,3) = interp1(nmLIB,muawater,nm);
MU(:,4) = interp1(nmLIB,muamel,nm);
LOADED = 1;
%% Create tissueList
j=1;
tissue(j).name = 'air';
tissue(j).mua = 0.0001; % Negligible absorption yet still tracks,
tissue(j).mus = 1.0; % but take steps in air
tissue(j).g = 1.0; % and don't scatter.
j=2;
tissue(j).name = 'water';
tissue(j).mua = MU(3);
tissue(j).mus = 10; % Take steps in water,
tissue(j).g = 1.0; % but don't scatter.
j=3;
tissue(j).name = 'blood';
В
   = 1.00;
S
    = 0.75;
W
     = 0.95;
M
    = 0:
musp500 = 10;
```

```
fray = 0.0;
bmie = 1.0;
gg = 0.90;
musp = musp500*(fray*(nm/500).^-4 + (1-fray)*(nm/500).^-bmie);
X = [B*S B*(1-S) W M]';
tissue(j).mua = MU*X;
tissue(j).mus = musp/(1-gg);
tissue(j).g = gg;
j = 4;
tissue(j).name = 'dermis';
B = 0.002;
S = 0.67;
W = 0.65;
M = 0;
musp500 = 42.4;
fray = 0.62;
bmie = 1.0;
gg = 0.90;
musp = musp500*(fray*(nm/500).^-4 + (1-fray)*(nm/500).^-bmie);
X = [B*S B*(1-S) W M]';
tissue(j).mua = MU*X;
tissue(j).mus = musp/(1-gg);
tissue(j).g = gg;
j=5;
tissue(j).name = 'epidermis';
B = 0;
S = 0.75;
W = 0.75;
M = 0.03;
musp500 = 40;
fray = 0.0;
bmie = 1.0;
gg = 0.90;
musp = musp500*(fray*(nm/500).^-4 + (1-fray)*(nm/500).^-bmie);
X = [B*S B*(1-S) W M]';
tissue(j).mua = MU*X;
tissue(j).mus = musp/(1-gg);
tissue(j).g = gg;
j=6;
tissue(j).name = 'skull';
B = 0.0005;
S = 0.75;
W = 0.35;
M = 0;
musp500 = 30;
fray = 0.0;
bmie = 1.0;
gg = 0.90;
musp = musp500*(fray*(nm/500).^-4 + (1-fray)*(nm/500).^-bmie);
X = [B*S B*(1-S) W M]';
tissue(j).mua = MU*X;
tissue(j).mus = musp/(1-gg);
tissue(j).g = gg;
j=7;
tissue(j).name = 'gray matter';
B = 0.01;
S = 0.75;
W = 0.75;
M = 0;
musp500 = 20;
fray = 0.2;
```

```
bmie = 1.0;
gg = 0.90;
musp = musp500*(fray*(nm/500).^-4 + (1-fray)*(nm/500).^-bmie);
X = [B*S B*(1-S) W M]';
tissue(j).mua = MU*X;
tissue(j).mus = musp/(1-gg);
tissue(j).g = gg;
j=8;
tissue(j).name = 'white matter';
B = 0.01;
S = 0.75;
W = 0.75;
M = 0;
musp500 = 20;
fray = 0.2;
bmie = 1.0;
gg = 0.90;
musp = musp500*(fray*(nm/500).^-4 + (1-fray)*(nm/500).^-bmie);
X = [B*S B*(1-S) W M]';
tissue(j).mua = MU*X;
tissue(j).mus = musp/(1-gg);
tissue(j).g = gg;
j=9;
tissue(j).name = 'standard tissue';
tissue(j).mua = 1;
tissue(j).mus = 100;
tissue(j).g = 0.90;
disp(sprintf('---- tissueList ------ \tmua \tmus \tg \tmusp'))
for i=1:length(tissue)
  disp(sprintf('\%d\t\%15s\t\%0.4f\t\%0.1f\t\%0.3f\t\%0.1f',...
    i,tissue(i).name, tissue(i).mua,tissue(i).mus,tissue(i).g,...
    tissue(i).mus*(1-tissue(i).g)))
end
disp('')
```