Rayleigh Scattering

21777

1a.

This question involved implementing two separate methods that draw random numbers, between 0 and π, from a probability distribution of

$$P(\theta) = \frac{3}{8}(1 + cos^2\theta)sin\theta, \qquad (1)$$

where θ is random value between 0 and π taken from a flat probability distribution. The first method implemented was a rejection method. This involves generating two random numbers from a flat probability distribution. The first, x_0, between 0 and π and the second, y_0, between 0 and $1/\sqrt{6}$, the maximum value of equation 1 in the desired range. If $y_0 < P(x_0)$ then the point is accepted, otherwise it is rejected.

The second method chosen was a cumulative function approach. A normalised probability distribution will have an area of 1, therefore the integral of the distribution will be 1 in the desired range. The method works by finding the integral of the distribution and generating a random number between 0 and 1, equivalent to generating a random area of the desired probability distribution. Using the integral, the value of θ that corresponds to this area is found. Parts of the probability distribution that are more probable will have larger areas and therefore theta values in these regions are more likely to be chosen. This involved implementing the equation

$$P_{cum}(\theta) = \int_0^\theta P(\theta')\,d\theta' \qquad (2)$$

$$\Rightarrow \int_0^\theta \frac{3}{8}(1 + cos^2\theta')sin\theta' d\theta' = A \Rightarrow [-\frac{1}{8}cos^3\theta' - \frac{3}{8}cos\theta']_0^\theta = A, \qquad (3)$$

where A is random number between 0 and 1 taken from a flat distribution.

$$\Rightarrow cos^3\theta + 3cos\theta + 8A - 4 = 0 \qquad (4)$$

This cubic equation was then solved using the cubic formula [1] that requires the equation to be in the form $x^3 + ax^2 + bx + c = 0$. Firstly,

$$p = b - \frac{a^2}{3} \text{ and } q = \frac{2a^3}{27} - \frac{ab}{3} + c \qquad (5)(6)$$

The discriminant,

$$\Delta = \frac{q^2}{4} + \frac{p^3}{27} = \frac{c^2}{4} + \frac{b^3}{27} = \frac{c^2}{4} + 1, \qquad (7)$$

is always positive and therefore the cubic has only one real solution given by,

$$cos\theta = (-\frac{q}{2} + \sqrt{\Delta})^{1/3} + (-\frac{q}{2} - \sqrt{\Delta})^{1/3} \qquad (8)$$

Equation 9 was then used to find the resulting values of θ for each random area generated.

The two methods were tested using 1,000,000 values of θ where each value was put into one of 20 bins. Figure 1 shows the output of the program comparing these two methods. Both produce almost identical probabilities in each bin, as expected. The main difference between the two is their efficiencies, the efficiency is defined as the percentage probability that any given point will be accepted into the distribution. The efficiency of the discard method was maximised by forcing y_0 to be between 0 and the maximum value of equation 1, any larger value would cause a higher discard probability. The efficiency for any discard method is directly related to the area that the distribution covers beneath a horizontal line at the maximum of the function, here the efficiency of the discard method was 77.92%. This highlights a clear advantage of the cumulative function approach as every input point is converted to an output value that belongs to the desired distribution, an efficiency of 100%.

Bin No.	Bin Prob. Discard	Bin Prob. Cumulative
1	0.009109	0.009159
2	0.026576	0.026496
3	0.041124	0.041664
4	0.052774	0.053194
5	0.060097	0.060240
6	0.063912	0.063222
7	0.064085	0.063483
8	0.062491	0.062079
9	0.060219	0.060491
10	0.059218	0.059154
11	0.058780	0.059202
12	0.060247	0.060510
13	0.062503	0.062595
14	0.064266	0.064181
15	0.063160	0.063983
16	0.060030	0.059560
17	0.053528	0.053368
18	0.042020	0.041676
19	0.026689	0.026681
20	0.009171	0.009062

Number of points used in Discard: 779195
Discard Efficiency: 77.92%
Number of points used in Cumulative: 1000000
Cumulative Efficiency: 100.00%

Figure 1. the program output for 1,000,000 runs of a discard method and a cumulative function method for producing random numbers with a distribution of $P(\theta) = \frac{3}{8}(1 + cos^2\theta)sin\theta$ where the values produced are stored in 20 bins.

1b.

This question involved simulating the isotropic scattering motion of photons through a slab of atmosphere, which runs from $Z_{min} = 0$ to $Z_{max} = 2$ with infinite x and y axes, and recording the theta angle with which they exit the top of the slab. The recorded angles were placed into 20 bins each $1/20^{th}$ of 2π (the number of steradians in a hemisphere), the angle of each bin was calculated using the equation

$$\frac{\pi}{10} = \int_0^{2\pi}\int_{\theta_1}^{\theta_2} sin\theta d\theta d\phi = 2\pi[-cos\theta]_{\theta_1}^{\theta_2} \Rightarrow \frac{1}{20} = cos\theta_1 - cos\theta_2 \quad (9)$$

where θ_1 is the lower bound of the bin and θ_2 is the upper bound.

Each new scattering position was generated in spherical polar coordinates and then converted into Cartesian coordinates. The polar coordinates were generated randomly; the phi coordinate was taken from a flat distribution between 0 and 2π. The distance coordinate, τ, was taken from an exponential decay probability distribution implemented using the cumulative function method

$$P(\tau) = e^{-\tau} \Rightarrow \int_0^{\tau} e^{-\tau'}d\tau' = A \Rightarrow [-e^{-\tau'}]_0^{\tau} = A \Rightarrow e^{-\tau} = 1 - A \Rightarrow \tau = -\ln(1 - A) \quad (10)$$

The distance of movement was then calculated using the equation

$$L = \frac{\tau}{\tau_{max}} Z_{max}, \quad (11)$$

where L is the distance the photon moves and τ_{max} is a parameter dictated by the makeup of the atmosphere. Finally, the theta coordinate was taken from a normalised $sin\theta$ ditribution. This distribution comes from the fact that the scattering takes place around a unit sphere. There is only one possible position for the particle to be scattered directly upwards or downwards but many ways for it to be scattered with $\theta = \pi/2$. This was again implemented using the cumulative function approach

$$P(\theta) = \frac{1}{2}sin\theta \Rightarrow \frac{1}{2}\int_0^{\theta} sin\theta' d\theta' = A \Rightarrow [-cos\theta']_0^{\theta} = 2A \Rightarrow \theta = \arccos(1 - 2A) \quad (12)$$

The particles were initiated at the origin and sent directly upwards, they were continually scattered within the atmospheric slab until they were absorbed (this program does not allow absorption but includes the functionality for later exploration), they escaped via the bottom of the slab (here they are not detected and the photon counter is decreased by one) or they escaped via the top of the slab (here they are detected and their theta angle of exit is binned).

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Isotropic Scattering
Tau: 10.00 Zmin: 0.00 Zmax: 2.00
Bin No.   Central Bin Angle   Normalised Energy      Error
1            0.158780            0.120549           0.000347
2            0.384294            0.110751           0.000333
3            0.502919            0.101834           0.000319
4            0.599156            0.092666           0.000304
5            0.683118            0.083932           0.000290
6            0.759067            0.076178           0.000276
7            0.829305            0.068568           0.000262
8            0.895254            0.060513           0.000246
9            0.957864            0.053630           0.000232
10           1.017815            0.046903           0.000217
11           1.075614            0.040376           0.000201
12           1.131655            0.034623           0.000186
13           1.186252            0.029119           0.000171
14           1.239664            0.023911           0.000155
15           1.292110            0.018745           0.000137
16           1.343777            0.014668           0.000121
17           1.394833            0.010664           0.000103
18           1.445428            0.007318           0.000086
19           1.495702            0.003907           0.000063
20           1.545786            0.001145           0.000034
Percentage of photons absorbed: 0.00%
Average Magnitude X: 0.982416 Y: 0.983264
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Figure 2. the program output for the simulation of 1,000,000 photons through a slab of atmosphere with $Z_{min} = 0$, $Z_{max} = 2$ and $\tau_{max} = 10$. The output shows the results for the binned theta values that escape through the top of the slab with the normalised energy per bin and the associated error.

Figure 2 shows the results for a simulation with 1,00,000 photons. Each photon was initiated with the same energy and hence the number of detected photons per bin is directly proportional to the energy. In addition to the normalised energy and error per bin it also displays the percentage of photons absorbed (0% here as the simulation did not allow for absorption) and the average magnitude of the x and y coordinates when the photons escape out of the top of the slab. The angle-energy distribution is what you would expect from this simulation. When moving a given distance, L, the smallest theta values ($\theta = 0$ corresponds to vertical motion) travel a further distance towards the Z_{max} boundary and are therefore more likely to cross over the boundary.

One issue that occurs with the program is that roughly 0.003% of the photons manage to escape with $\theta > \pi/2$, this should not be possible as it indicates they cross it travelling backwards. A check was put in place to detect and omit these from the results.

1c.

This question involved a similar simulation to the previous section however it now describes Rayleigh scattering. The probability distribution of the theta values now follows equation 1, implemented using the cumulative function method described in section 1a. This value of theta is no longer taken down from the z axis but is instead taken from a new Z axis which is in the direction of motion of the photon. This means that points generated in the new frame of reference need to be transformed into the original frame so that the position and direction of the photon is known. This was accomplished using proper Euler angles and a rotation matrix.

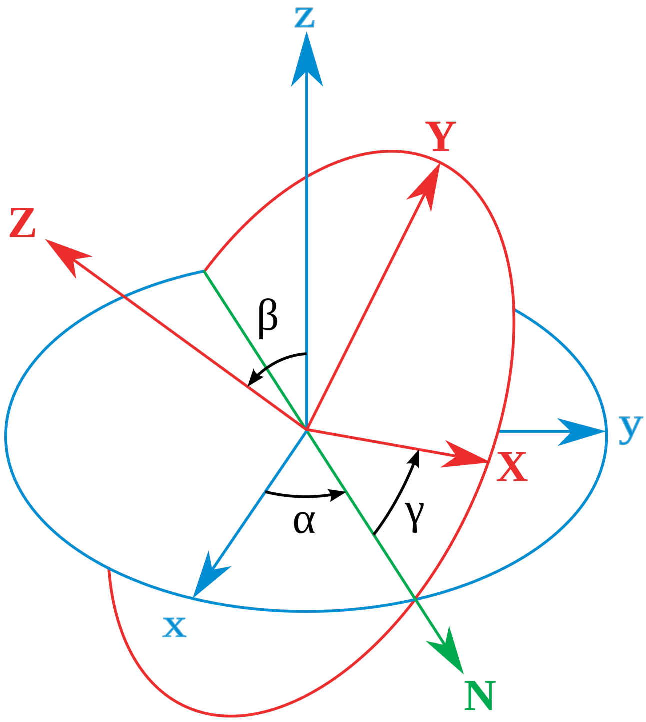

Figure 3. diagram showing the Euler angles between two sets of coordinate systems. $(\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{z})$ represents the original frame of motion and $(\boldsymbol{X}, \boldsymbol{Y}, \boldsymbol{Z})$ represents the new frame where $\boldsymbol{Z}$ is the direction of motion of the photon. $\boldsymbol{N}$ is a vector produced by $\boldsymbol{z}\times\boldsymbol{Z}$, β is the angle between $\boldsymbol{z}$ and $\boldsymbol{Z}$, α is the angle between $\boldsymbol{x}$ and $\boldsymbol{N}$ and γ is the angle between $\boldsymbol{N}$ and $\boldsymbol{X}$.

Figure 3 shows a diagram of two different coordinate systems: $(\boldsymbol{x}, \boldsymbol{y}, \boldsymbol{z})$ represents the original frame of motion and $(\boldsymbol{X}, \boldsymbol{Y}, \boldsymbol{Z})$ represents the new frame where $\boldsymbol{Z}$ is the direction of motion of the photon. The Euler angles α and β can be found by taking the dot product between the appropriate axes. γ is always set to 0, this is because the angle phi is taken around the $\boldsymbol{Z}$ axis and is taken from a flat probability distribution between 0 and 2π. This means that every angle of phi is equally likely and so the orientation of the $\boldsymbol{X}, \boldsymbol{Y}$ plane is arbitrary. The direction vector, $\boldsymbol{Z}$, of the photon at each point is found by subtracting the two previous position vectors of the photon, this then allows $\boldsymbol{N}$ to be calculated and subsequently α and β.

These values are used in the equation

$$\frac{1}{cos^2\alpha cos^2\beta+sin^2\alpha+sin\alpha cos\alpha sin\beta}\begin{bmatrix} cos\alpha cos\beta & -sin\alpha & cos\alpha sin\beta \\ sin\alpha cos\beta & cos\alpha & sin\alpha sin\beta \\ -sin\beta & 0 & cos\beta \end{bmatrix}\begin{bmatrix} X \\ Y \\ Z \end{bmatrix} = \begin{bmatrix} x \\ y \\ z \end{bmatrix} \tag{13}$$

using the inverse of the rotation matrix from [2]. The coordinates found are used to update the position of the photon and to calculate the theta value which are again binned on escape from the top of the slab.

The simulation was repeated twice with 1,000,000 photons, one with $\tau_{max} = 10.0$ to simulate the scattering of blue light and one with $\tau_{max} = 0.1$ to simulate the scattering of other colours.

Rayleigh Scattering
Tau: 10.00 Zmin: 0.00 Zmax: 2.00

Bin No.	Central Bin Angle	Normalised Energy	Error
1	0.158780	0.635282	0.000797
2	0.384294	0.042226	0.000205
3	0.502919	0.032165	0.000179
4	0.599156	0.026625	0.000163
5	0.683118	0.023355	0.000153
6	0.759067	0.021376	0.000146
7	0.829305	0.019697	0.000140
8	0.895254	0.018266	0.000135
9	0.957864	0.017164	0.000131
10	1.017815	0.016431	0.000128
11	1.075614	0.015809	0.000126
12	1.131655	0.015464	0.000124
13	1.186252	0.015159	0.000123
14	1.239664	0.014511	0.000120
15	1.292110	0.014578	0.000121
16	1.343777	0.014471	0.000120
17	1.394833	0.014291	0.000120
18	1.445428	0.014349	0.000120
19	1.495702	0.014299	0.000120
20	1.545786	0.014482	0.000120

Percentage of photons absorbed: 0.00%
Average Magnitude X: 17.514851 Y: 15.944120

Rayleigh Scattering
Tau: 0.10 Zmin: 0.00 Zmax: 2.00

Bin No.	Central Bin Angle	Normalised Energy	Error
1	0.158780	0.200601	0.000448
2	0.384294	0.068083	0.000261
3	0.502919	0.063749	0.000252
4	0.599156	0.060532	0.000246
5	0.683118	0.055353	0.000235
6	0.759067	0.053443	0.000231
7	0.829305	0.048810	0.000221
8	0.895254	0.047240	0.000217
9	0.957864	0.045433	0.000213
10	1.017815	0.043192	0.000208
11	1.075614	0.041337	0.000203
12	1.131655	0.039773	0.000199
13	1.186252	0.038527	0.000196
14	1.239664	0.035647	0.000189
15	1.292110	0.034385	0.000185
16	1.343777	0.032269	0.000180
17	1.394833	0.029886	0.000173
18	1.445428	0.026927	0.000164
19	1.495702	0.022981	0.000152
20	1.545786	0.011832	0.000109

Percentage of photons absorbed: 0.00%
Average Magnitude X: 1.990568 Y: 2.084560

Figure 4. the program output for two simulations of 1,000,000 photons through a slab of atmosphere with $Z_{min} = 0$, $Z_{max} = 2$ for $\tau_{max} = 10$ and $\tau_{max} = 0.1$. The output shows the results for the binned theta values that escape through the top of the slab with the normalised energy per bin and the associated error and the average magnitude of the x and y coordinates at the point where the photon crosses the upper boundary.

Figure 4 shows the results for these two simulations. The most noticeable difference is the average distance away from the origin that the particles cross the Z_{max} boundary. The blue photons cross at a significantly larger distance from the origin which could explain the reason that the sky is dominated by blue photons when looking far away from the Sun. The angle-energy distributions both follow a similar pattern, both with a greater proportion of photons in the first angular bin that isotropic scattering, then a large drop and then a slow decrease of energy per bin. The blue photons are more directed at the observer with 63.5% of the photons crossing with a theta in the first angular bin, compared with 20.1% for other colours. This does not follow the angular distribution you would expect to prove that blue light dominates when not staring at the source. This could be due to a mistake in the theory behind calculating the values of theta after the change in the frame of reference, further investigation would be required to find the source of this error.

References

[1] *Solving Cubic Equations* (Maths Extenstion, accessed 18 March 2019); http://www2.trinity.unimelb.edu.au/~rbroekst/MathX/Cubic%20Formula.pdf
[2] Evans P R 2001 *Biological Crystallography* Rotations and Rotation Matrices