1 The RTE

Let $I(r, \hat{s})$ be the specific intensity, where

$$r = \begin{pmatrix} x \\ y \\ z \end{pmatrix}, \quad \hat{s} = \begin{pmatrix} s_x \\ s_y \\ s_z \end{pmatrix}. \quad (1)$$

We consider a Monte Carlo simulation corresponding to the following RTE [1, 2].

$$\hat{s} \cdot \nabla I(r, \hat{s}) + \mu_t I(r, \hat{s}) = \mu_s \int_{S^2} A(\hat{s} \cdot \hat{s}') I(r, \hat{s}') d\hat{s}' + S(r, \hat{s}). \quad (2)$$

2 Monte Carlo Simulation

1. Launch a photon or a photon packet Suppose the source $S$ is placed at the origin and photons are emitted in the direction of the positive $z$-axis. Particles propagate at every Monte Carlo time $t$. The initial conditions are given by

$$r(t = 0) = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \quad \hat{s}(t = 0) = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}. \quad (3)$$

2. Distance Then, we follow the path of a photon until it has an interaction. The distance $\Delta r$ obeys

$$p(\Delta r) = \mu_t e^{-\mu_t \Delta r}. \quad (4)$$
Let $\xi \in [0, 1]$ be a uniform random variable. By the inverse transform sampling, $\Delta r$ is given by

$$\xi = \int_0^{\Delta r} p(\Delta r')d\Delta r' = 1 - e^{-\mu_s \Delta r}. \quad (5)$$

That is,

$$\Delta r = -\frac{\ln(1 - \xi)}{\mu_t}. \quad (6)$$

Since $1 - \xi \in [0, 1]$, we further obtain

$$\Delta r = -\frac{\ln \xi}{\mu_t}. \quad (7)$$

Then, the change in position coordinates are updated as

$$\begin{cases} x' = x + s_x \Delta r, \\ y' = y + s_y \Delta r, \\ z' = z + s_z \Delta r. \end{cases} \quad (8)$$

3. **Scattered or absorbed** We produce another uniform random variable $\xi \in [0, 1]$. If $\xi < \mu_a/\mu_t$, absorption occurs. Otherwise the photon is scattered.

4. **Scattering** A particle changes its direction from $\hat{s}$ to $\hat{s}'$ by each scattering. Let $\theta$ be the angle between $\hat{s}$ and $\hat{s}'$. The Henyey-Greenstein phase function is written as

$$A(\cos \theta) = \frac{1 - g^2}{2(1 + g^2 - 2g \cos \theta)^{3/2}}. \quad (9)$$

Since $A \in [0, 1]$, we can give $\cos \theta$ as

$$\cos \theta = \begin{cases} \frac{1}{2g} \left[ 1 + g^2 - \left( \frac{1 - g^2}{1 - 2g} \right)^2 \right], & g > 0, \\ 2\xi - 1, & g = 0, \end{cases} \quad (10)$$

where $\xi \in [0, 1]$ is a uniform random variable. By producing another $\xi$, we give the azimuthal angle $\varphi$ as

$$\varphi = 2\pi \xi. \quad (11)$$
Thus, \( \hat{s}' \) are calculated as

\[
\begin{align*}
\hat{s}'_x &= \frac{\sin \theta}{\sqrt{1 - s_z^2}} (s_x s_z \cos \varphi - s_y \sin \varphi) + s_x \cos \theta, \\
\hat{s}'_y &= \frac{\sin \theta}{\sqrt{1 - s_z^2}} (s_y s_z \cos \varphi + s_x \sin \varphi) + s_y \cos \theta, \\
\hat{s}'_z &= -\sin \theta \cos \varphi \sqrt{1 - s_z^2} + s_z \cos \theta.
\end{align*}
\]  

(12)

Note that we can calculate \( \hat{s}' \) as follows when \( |s_z| \) is close to 1 (for example, when \( |s_z| > 0.99999 \)).

\[
\begin{align*}
\hat{s}'_x &= \sin \theta \cos \varphi, \\
\hat{s}'_y &= \sin \theta \sin \varphi, \\
\hat{s}'_z &= \text{sgn}(s_z) \cos \theta,
\end{align*}
\]  

(13)

where \( \text{sgn}(s_z) = 1 \) for \( s_z > 0 \) and \( \text{sgn}(s_z) = -1 \) for \( s_z < 0 \).

5. **Inner loop**  Repeat Steps 2 through 4 until the photon is absorbed or is no longer capable of affecting the answer to any appreciable extent.

6. **Outer loop**  Repeat the whole process from Step 1 as many times as necessary to achieve the accuracy needed for the solution.

7. **Average from all the histories**

References
