Appendix A

P_N Approximation Method

I follow the P_N approximation to reduce the general transport equation to a diffusion equation. The method is simply to expand all angular dependent quantities in a spherical harmonic series and truncate the series at the N^{th} moment [54, 55, 56]. I first review the method for the photon transport equation and then apply it to the correlation transport equation.

A.1 Photon Transport Equation

The linear transport equation for photons propagating in media that scatter and absorb photons is [54, 55, 56]

$$\frac{1}{v}\frac{\partial L(\mathbf{r},\hat{\Omega},t)}{\partial t} + \nabla \cdot L(\mathbf{r},\hat{\Omega},t)\hat{\Omega} + \mu_t L(\mathbf{r},\hat{\Omega},t) = \mu_s \int L(\mathbf{r},\hat{\Omega}',t) f(\hat{\Omega},\hat{\Omega}') \mathrm{d}\hat{\Omega}' + S(\mathbf{r},\hat{\Omega},t) \ . \tag{A.1}$$

This equation is described in detail in section 2.1. $L(\mathbf{r},\hat{\Omega},t)$ is the radiance at position $\mathbf{r}$, traveling in direction $\hat{\Omega}$, at time t, with units of W m^{-2} sr^{-1} (sr=steradian=unit solid angle). The normalized phase function is $f(\hat{\Omega},\hat{\Omega}')$ which represents the probability of scattering into an angle $\hat{\Omega}'$ from angle $\hat{\Omega}$. v is the speed of light in the medium and $\mu_t = \mu_s + \mu_a$ is the transport coefficient where μ_s is the scattering coefficient and μ_a is the absorption coefficient. $S(\mathbf{r},\hat{\Omega},t)$ is the spatial and angular distribution of the source with units of W m^{-3} sr^{-1}. The photon fluence is given by

$$\Phi(\mathbf{r},t) = \int d\hat{\Omega} L(\mathbf{r},\hat{\Omega},t) \ , \tag{A.2}$$

while the photon flux, or current density, is given by

$$\mathbf{J}(\mathbf{r},t) = \int d\hat{\Omega} L(\mathbf{r},\hat{\Omega},t)\hat{\Omega} \ . \tag{A.3}$$

Both the fluence and the flux have units of W m^{-2}.

Within the P_N approximation the radiance and source distribution are expanded as

$$L(\mathbf{r},\hat{\Omega},t) = \sum_{l=0}^{N} \sum_{m=-l}^{l} \phi_{l,m}(\mathbf{r},t) Y_{l,m}(\hat{\Omega}) \ , \tag{A.4}$$

and

$$S(\mathbf{r},\hat{\Omega},t) = \sum_{l=0}^{N} \sum_{m=-l}^{l} q_{l,m}(\mathbf{r},t) Y_{l,m}(\hat{\Omega}) \ . \tag{A.5}$$

The photon fluence $\Phi(\mathbf{r},t)$ is given by $\phi_{0,0}$ (see eq. (A.19)) and the components of the flux $\mathbf{J}(\mathbf{r},t)$ are given by $\phi_{1,m}$ (see eq. (A.20)). The $q_{l,m}(\mathbf{r},t)$ are the amplitudes of the different angular moments of the source at position $\mathbf{r}$ and time t.

For the phase function, we make the reasonable assumption that the probability amplitude is only dependent on the change in direction of the photon and thus

$$\begin{aligned} f(\hat{\Omega}\cdot\hat{\Omega}') &= \sum_{l=0}^{\infty} \frac{2l+1}{4\pi} g_l P_l(\hat{\Omega}\cdot\hat{\Omega}') \\ &= \sum_{l=0}^{\infty} \sum_{m=-l}^{l} g_l Y^*_{l,m}(\hat{\Omega}') Y_{l,m}(\hat{\Omega}) \ , \end{aligned} \tag{A.6}$$

where $P_l(x)$ is a Legendre Polynomial and the second line is obtained using the angular addition rule [63]. The phase function is normalized and therefore $g_0 = 1$.

Substituting these expansions into the photon transport equation, eq. (A.1), we obtain

$$\begin{aligned} &\sum_{l=0}^{N} \sum_{m=-l}^{l} \Bigg[\left[\frac{1}{v}\frac{\partial}{\partial t} + \hat{\Omega}\cdot\nabla + \mu_t \right] \phi_{l,m}(\mathbf{r},t) Y_{l,m}(\hat{\Omega}) - q_{l,m} Y_{l,m}(\hat{\Omega}) \\ &- \mu_s \int d\hat{\Omega}' \phi_{l,m}(\mathbf{r},t) Y_{l,m}(\hat{\Omega}') \sum_{l'=0}^{\infty} \sum_{m'=-l}^{l} g_{l'} Y^*_{l',m'}(\hat{\Omega}') Y_{l',m'}(\hat{\Omega}) \Bigg] = 0 \ . \end{aligned} \tag{A.7}$$

Here $\mu_t = \mu_s + \mu_a$ is the transport coefficient. The integral over $\hat{\Omega}'$ is calculated using the orthogonality relation for the spherical harmonics, i.e.

$$\int \mathrm{d}\hat{\Omega} Y_{l,m}(\hat{\Omega}) Y^*_{l',m'}(\hat{\Omega}) = \delta_{l,l'}\delta_{m,m'} \ . \tag{A.8}$$

The transport equation then becomes

$$\sum_{l=0}^{N}\sum_{m=-l}^{l}\left[\left[\frac{1}{v}\frac{\partial}{\partial t} + \hat{\Omega}\cdot\nabla + \mu_t^{(l)}\right]\phi_{l,m}(\mathbf{r},t) - q_{l,m}\right] Y_{l,m}(\hat{\Omega}) = 0 \ , \tag{A.9}$$

where $\mu_t^{(l)} = \mu_s(1-g_l) + \mu_a$ is the reduced transport coefficient.

Next, we multiply eq. (A.9) by $Y^*_{\alpha,\beta}(\hat{\Omega})$ and integrate over $\hat{\Omega}$. We can use the orthogonality relation for spherical harmonics (eq. (A.8)) on all the terms except the term with $\hat{\Omega}\cdot\nabla\phi_{l,m}(\mathbf{r},t)$. The result is

$$\frac{1}{v}\frac{\partial}{\partial t}\phi_{\alpha,\beta} + \mu_t^{(\alpha)}\phi_{\alpha,\beta} + \sum_{l=0}^{N}\sum_{m=-l}^{l}\int \mathrm{d}\hat{\Omega} \ \ \hat{\Omega}\cdot\nabla\phi_{l,m} Y_{l,m}(\hat{\Omega}) Y^*_{\alpha,\beta}(\hat{\Omega}) = q_{\alpha,\beta} \ . \tag{A.10}$$

The $\mathbf{r}$ and t dependence of $\phi_{l,m}$, and $q_{l,m}$ is assumed.

We now focus on the remaining integral. First take the dot product between $\hat{\Omega}$ and the gradient operator so that we have the components $\hat{\Omega}_x\frac{\partial}{\partial x}$, $\hat{\Omega}_y\frac{\partial}{\partial y}$, and $\hat{\Omega}_z\frac{\partial}{\partial z}$. The components of $\hat{\Omega}Y_{l,m}(\hat{\Omega})$ can be written in terms of spherical harmonics, specifically

$$\begin{aligned}
\hat{\Omega}_x Y^*_{\alpha,\beta}(\hat{\Omega}) &= \sin\theta\cos\phi Y^*_{\alpha,\beta}(\hat{\Omega}) \\
&= -\frac{1}{2}\left[\frac{(\alpha+\beta+1)(\alpha+\beta+2)}{(2\alpha+1)(2\alpha+3)}\right]^{1/2} Y^*_{\alpha+1,\beta+1}(\hat{\Omega}) \\
&\quad +\frac{1}{2}\left[\frac{(\alpha-\beta)(\alpha-\beta-1)}{(2\alpha-1)(2\alpha+1)}\right]^{1/2} Y^*_{\alpha-1,\beta+1}(\hat{\Omega}) \\
&\quad +\frac{1}{2}\left[\frac{(\alpha-\beta+1)(\alpha-\beta+2)}{(2\alpha+1)(2\alpha+3)}\right]^{1/2} Y^*_{\alpha+1,\beta-1}(\hat{\Omega}) \\
&\quad -\frac{1}{2}\left[\frac{(\alpha+\beta)(\alpha+\beta-1)}{(2\alpha-1)(2\alpha+1)}\right]^{1/2} Y^*_{\alpha-1,\beta-1}(\hat{\Omega}) \ , \qquad (A.11) \\
\hat{\Omega}_y Y^*_{\alpha,\beta}(\hat{\Omega}) &= \sin\theta\sin\phi Y^*_{\alpha,\beta}(\hat{\Omega}) \\
&= \frac{1}{2i}\left[\frac{(\alpha+\beta+1)(\alpha+\beta+2)}{(2\alpha+1)(2\alpha+3)}\right]^{1/2} Y^*_{\alpha+1,\beta+1}(\hat{\Omega})
\end{aligned}$$

$$
\begin{aligned}
& -\frac{1}{2i}\left[\frac{(\alpha-\beta)(\alpha-\beta-1)}{(2\alpha-1)(2\alpha+1)}\right]^{1/2} Y^*_{\alpha-1,\beta+1}(\hat{\Omega}) \\
& +\frac{1}{2i}\left[\frac{(\alpha-\beta+1)(\alpha-\beta+2)}{(2\alpha+1)(2\alpha+3)}\right]^{1/2} Y^*_{\alpha+1,\beta-1}(\hat{\Omega}) \\
& -\frac{1}{2i}\left[\frac{(\alpha+\beta)(\alpha+\beta-1)}{(2\alpha-1)(2\alpha+1)}\right]^{1/2} Y^*_{\alpha-1,\beta-1}(\hat{\Omega}) \,, \qquad \text{(A.12)}
\end{aligned}
$$

$$
\begin{aligned}
\hat{\Omega}_z Y^*_{\alpha,\beta}(\hat{\Omega}) &= \cos\theta Y^*_{\alpha,\beta}(\hat{\Omega}) \\
&= +\left[\frac{(\alpha-\beta+1)(\alpha+\beta+1)}{(2\alpha+1)(2\alpha+3)}\right]^{1/2} Y^*_{\alpha+1,\beta}(\hat{\Omega}) \\
&\quad +\left[\frac{(\alpha-\beta)(\alpha+\beta)}{(2\alpha-1)(2\alpha+1)}\right]^{1/2} Y^*_{\alpha-1,\beta}(\hat{\Omega}) \,. \qquad \text{(A.13)}
\end{aligned}
$$

$\hat{\Omega}$ is the direction of the photon where θ and ϕ are respectively the polar and azimuthal angles of the photon direction. These equations are derived with the help of the recurrence relations for associated Legendre polynomials using the Condon-Shortley phase convention. Refer to section 12.9 of Arfken [147] for more details. The book by Rose entitled *Elementary Theory on Angular Momentum* is also helpful [148].

Upon substituting eqs. (A.11)-(A.13) into eq. (A.10) the integral of three spherical harmonics becomes an integral of two spherical harmonics which is easily calculated using the orthogonality relation eq. (A.8). After straight-forward algebra the transport equation finally becomes

$$
\begin{aligned}
\frac{1}{v}\frac{\partial}{\partial t}\phi_{\alpha,\beta} + \mu_t^{(\alpha)}\phi_{\alpha,\beta} \;&-\; \frac{1}{2}\sqrt{\frac{(\alpha+\beta+2)(\alpha+\beta+1)}{(2\alpha+1)(2\alpha+3)}}\left(\frac{\partial}{\partial x}+i\frac{\partial}{\partial y}\right)\phi_{\alpha+1,\beta+1} \\
&+\; \frac{1}{2}\sqrt{\frac{(\alpha-\beta-1)(\alpha-\beta)}{(2\alpha+1)(2\alpha-1)}}\left(\frac{\partial}{\partial x}+i\frac{\partial}{\partial y}\right)\phi_{\alpha-1,\beta+1} \\
&+\; \frac{1}{2}\sqrt{\frac{(\alpha-\beta+1)(\alpha-\beta+2)}{(2\alpha+1)(2\alpha+3)}}\left(\frac{\partial}{\partial x}-i\frac{\partial}{\partial y}\right)\phi_{\alpha+1,\beta-1} \\
&-\; \frac{1}{2}\sqrt{\frac{(\alpha+\beta)(\alpha+\beta-1)}{(2\alpha+1)(2\alpha-1)}}\left(\frac{\partial}{\partial x}-i\frac{\partial}{\partial y}\right)\phi_{\alpha-1,\beta-1} \\
&+\; \sqrt{\frac{(\alpha+\beta+1)(\alpha-\beta+1)}{(2\alpha+1)(2\alpha+3)}}\frac{\partial}{\partial z}\phi_{\alpha+1,\beta}
\end{aligned}
$$

$$+ \quad \sqrt{\frac{(\alpha+\beta)(\alpha-\beta)}{(2\alpha+1)(2\alpha-1)}} \frac{\partial}{\partial z}\phi_{\alpha-1,\beta} = q_{\alpha,\beta} \ . \tag{A.14}$$

This is a coupled set of linear differential equations for $\phi_{\alpha,\beta}$. The P_N approximation is obtained by neglecting all $\phi_{\alpha,\beta}$ and g_α for $\alpha > N$.

A.1.1 P_1 and Diffusion Approximation

Within the P_1 approximation, the $\alpha = 0$ equation gives

$$\frac{1}{v}\frac{\partial}{\partial t}\phi_{0,0}+\mu_a\phi_{0,0}+\frac{1}{2}\sqrt{\frac{2}{3}}\left[\frac{\partial}{\partial x}-i\frac{\partial}{\partial y}\right]\phi_{1,-1}-\frac{1}{2}\sqrt{\frac{2}{3}}\left[\frac{\partial}{\partial x}+i\frac{\partial}{\partial y}\right]\phi_{1,1}+\sqrt{\frac{1}{3}}\frac{\partial}{\partial z}\phi_{1,0} = q_{0,0} \ , \tag{A.15}$$

and the $\alpha = 1$ equations give

$$\begin{aligned}
\frac{1}{v}\frac{\partial}{\partial t}\phi_{\mathbf{1,0}} + \mu_t^{(1)}\phi_{\mathbf{1,0}} + \sqrt{\frac{1}{3}}\frac{\partial}{\partial z}\phi_{0,0} &= q_{1,0} \ , &\text{(A.16)}\\
\frac{1}{v}\frac{\partial}{\partial t}\phi_{\mathbf{1,1}} + \mu_t^{(1)}\phi_{\mathbf{1,1}} - \frac{1}{2}\sqrt{\frac{2}{3}}\left[\frac{\partial}{\partial x}-i\frac{\partial}{\partial y}\right]\phi_{0,0} &= q_{1,1} \ , &\text{(A.17)}\\
\frac{1}{v}\frac{\partial}{\partial t}\phi_{\mathbf{1,-1}} + \mu_t^{(1)}\phi_{\mathbf{1,-1}} + \frac{1}{2}\sqrt{\frac{2}{3}}\left[\frac{\partial}{\partial x}+i\frac{\partial}{\partial y}\right]\phi_{0,0} &= q_{1,-1} \ . &\text{(A.18)}
\end{aligned}$$

We now transform $\phi_{0,0}$ and the $\phi_{1,m}$'s in eqs. (A.15)-(A.18) into the fluence $\Phi(\mathbf{r},t)$ and net flux $\mathbf{J}(\mathbf{r},t)$. The fluence is

$$\Phi(\mathbf{r},t) = \int \mathrm{d}\hat{\Omega} L(\mathbf{r},\hat{\Omega},t) = \sum_{l=0}^{\infty}\sum_{m=-l}^{l} \phi_{l,m}\int \mathrm{d}\hat{\Omega} Y_{l,m}(\hat{\Omega}) = \sqrt{4\pi} \quad \phi_{0,0} \ . \tag{A.19}$$

The $\phi_{1,m}$'s can be gathered in appropriate linear combinations to give the components of the net flux $\mathbf{J}$. The appropriate linear combinations are obtained from the definition of the net flux (recall eq. (A.3)). They are

$$\begin{aligned}
\mathbf{J}(\mathbf{r},t) &= \int \mathrm{d}\hat{\Omega} L(\mathbf{r},\hat{\Omega},t)\hat{\Omega}\\
&= \sum_{l=0}^{\infty}\sum_{m=-l}^{l} \phi_{l,m}\int \mathrm{d}\hat{\Omega}\left[\sin\theta\cos\phi\hat{x}+\sin\theta\sin\phi\hat{y}+\cos\theta\hat{z}\right]Y_{l,m}(\hat{\Omega})
\end{aligned}$$

$$
\begin{aligned}
&= \sqrt{\frac{4\pi}{3}} \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \phi_{l,m} \int \mathrm{d}\hat{\Omega} \Bigg[\sqrt{\frac{1}{2}} \left(-Y^*_{1,1}(\hat{\Omega}) + Y^*_{1,-1}(\hat{\Omega}) \right) \hat{x} \\
&\qquad - i \sqrt{\frac{1}{2}} \left(+Y^*_{1,1}(\hat{\Omega}) + Y^*_{1,-1}(\hat{\Omega}) \right) \hat{y} \\
&\qquad + Y^*_{1,0}(\hat{\Omega}) \hat{z} \Bigg] Y_{l,m}(\hat{\Omega}) \\
&= \sqrt{\frac{4\pi}{3}} \left[\sqrt{\frac{1}{2}} \left(-\phi_{1,1} + \phi_{1,-1} \right) \hat{x} - i \sqrt{\frac{1}{2}} \left(\phi_{1,1} + \phi_{1,-1} \right) \hat{y} + \phi_{1,0} \hat{z} \right] . \qquad \text{(A.20)}
\end{aligned}
$$

Eqs. (A.15)-(A.18) are thus equivalent to

$$
\frac{1}{v} \frac{\partial}{\partial t} \Phi(\mathbf{r}, t) + \mu_a \Phi(\mathbf{r}, t) + \nabla \cdot \mathbf{J}(\mathbf{r}, t) = S_0(\mathbf{r}, t) \; , \qquad \text{(A.21)}
$$

$$
\frac{1}{v} \frac{\partial}{\partial t} \mathbf{J}(\mathbf{r}, t) + \mu_t^{(1)} \mathbf{J}(\mathbf{r}, t) + \frac{1}{3} \nabla \Phi(\mathbf{r}, t) = \mathbf{S_1}(\mathbf{r}, t) \; . \qquad \text{(A.22)}
$$

Here $S_0(\mathbf{r}, t)$ and $\mathbf{S_1}(\mathbf{r}, t)$ are respectively the monopole and dipole moments of the source at position $\mathbf{r}$ and time t as defined in eq. (2.8).

Eq. (A.21) and eq. (A.22) constitute the P_1 approximation to the photon transport equation. The derivation of the diffusion equation from these equations is discussed in section 2.1 starting with eq. (2.9) and eq. (2.10), which correspond to eq. (A.21) and eq. (A.22) respectively.

A.1.2 P_3 Approximation

With the P_1 approximation we had four coupled differential equations to decouple. The P_3 approximation will give us 16 coupled differential equations. In general the P_N approximation will have $(N + 1)^2$ coupled differential equations. To simplify the derivation, we can approximate the one-dimensional transport equation, obtain a differential equation for the fluence, and then extend the one-dimensional result to three dimensions. In one-dimension we need only concern ourselves with the $m = 0$ equations and therefore the P_N approximation will have $N + 1$ coupled differential equations. This simplification works because the photon transport equation does not have a prefered direction, and thus all differential operators that appear in the P_N

equations will be symmetric under rotations (e.g. ∇^2 and ∇^4). We can thus transform the one-dimensional equation to a higher dimension equation by replacing $\frac{\partial^{2n}}{\partial z^{2n}}$ to ∇^{2n} where n is an integer and ∇ is the differential operator for the desired dimensional space. In three dimensions $\nabla = \frac{\partial}{\partial x}\hat{x} + \frac{\partial}{\partial y}\hat{y} + \frac{\partial}{\partial z}\hat{z}$. This simplification does not work if the optical properties are spatially varying. In this case, spatial derivatives of the optical properties appear that are not spherically symmetric.

In one dimension the $\alpha = 0$ equation is

$$\frac{1}{v}\frac{\partial}{\partial t}\phi_{0,0} + \mu_a\phi_{0,0} + \sqrt{\frac{1}{3}}\frac{\partial}{\partial z}\phi_{1,0} = q_{0,0} \ . \tag{A.23}$$

The $\alpha = 1$ equation is

$$\frac{1}{v}\frac{\partial}{\partial t}\phi_{1,0} + \mu_t^{(1)}\phi_{1,0} + \sqrt{\frac{1}{3}}\frac{\partial}{\partial z}\phi_{0,0} + \sqrt{\frac{4}{15}}\frac{\partial}{\partial z}\phi_{2,0} = q_{1,0} \ . \tag{A.24}$$

The $\alpha = 2$ equation is

$$\frac{1}{v}\frac{\partial}{\partial t}\phi_{2,0} + \mu_t^{(2)}\phi_{2,0} + \sqrt{\frac{4}{15}}\frac{\partial}{\partial z}\phi_{1,0} + \sqrt{\frac{9}{35}}\frac{\partial}{\partial z}\phi_{3,0} = q_{2,0} \ . \tag{A.25}$$

The $\alpha = 3$ equation is

$$\frac{1}{v}\frac{\partial}{\partial t}\phi_{3,0} + \mu_t^{(3)}\phi_{3,0} + \sqrt{\frac{9}{35}}\frac{\partial}{\partial z}\phi_{2,0} = q_{3,0} \ . \tag{A.26}$$

We can decouple these equations to find an equation for $\phi_{0,0}$ by back-substitution. First, re-write the equations as

$$\begin{array}{ccccccccc} A\phi_{0,0} & + & B\phi_{1,0} & & & & & = & q_{0,0} \\ C\phi_{0,0} & + & D\phi_{1,0} & + & E\phi_{2,0} & & & = & q_{1,0} \\ & & F\phi_{1,0} & + & G\phi_{2,0} & + & H\phi_{3,0} & = & q_{2,0} \\ & & & & I\phi_{2,0} & + & J\phi_{3,0} & = & q_{3,0} \ . \end{array} \tag{A.27}$$

The coefficients A through J are given by eq. (A.23) through eq. (A.26). First multiply the third line by J, switch the order of J and H, and substitute for $J\phi_{3,0}$ from line

4. Transposing J and H is okay since we are assuming the optical properties are spatially uniform. The third line of eq. (A.27) becomes

$$\begin{aligned} JF\phi_{1,0} + JG\phi_{2,0} + HJ\phi_{3,0} &= Jq_{2,0} \\ JF\phi_{1,0} + JG\phi_{2,0} + Hq_{3,0} - HI\phi_{2,0} &= Jq_{2,0} \\ JF\phi_{1,0} + (JG - HI)\phi_{2,0} &= Jq_{2,0} - Hq_{3,0} \end{aligned} \tag{A.28}$$

Next, multiply the second line of eq. (A.27) by $(JG - HI)$, transpose $(JG - HI)$ and E, and substitute for $(JG - HI)\phi_{2,0}$ from the third line of eq. (A.28). The second line of eq. (A.27) becomes

$$\begin{aligned} (JG - HI)C\phi_{0,0} + (JG - HI)D\phi_{1,0} + E(JG - HI)\phi_{2,0} &= \\ (JG - HI)q_{1,0} & \\ (JG - HI)C\phi_{0,0} + (JG - HI)D\phi_{1,0} + EJq_{2,0} - EHq_{3,0} - EJF\phi_{1,0} &= \\ (JG - HI)q_{1,0} & \\ (JGC - HIC)\phi_{0,0} + (JGD - HID - EJF)\phi_{1,0} &= \\ (JG - HI)q_{1,0} - EJq_{2,0} + EHq_{3,0} & \end{aligned} \tag{A.29}$$

Finally, multiply the first line of eq. (A.27) by $\mathcal{L} = (JGD - HID - EJF)$, transpose $\mathcal{L}$ and B, and substitute for $\mathcal{L}\phi_{1,0}$ from the third line of eq. (A.29). The first line of eq. (A.27) becomes

$$\begin{aligned}
\mathcal{L}A\phi_{0,0} + B\mathcal{L}\phi_{1,0} &= \\
\mathcal{L}q_{0,0} \\
\mathcal{L}A\phi_{0,0} + (BJG - BHI)q_{1,0} - BEJq_{2,0} + BEHq_{3,0} - (BJGC - BHIC)\phi_{0,0} &= \\
\mathcal{L}q_{0,0} \\
(JGDA - HIDA - EJFA - BJGC + BHIC)\phi_{0,0} &= \\
(JGD - HID - EJF)q_{0,0} + (BHI - BJG)q_{1,0} + BEJq_{2,0} - BEHq_{3,0}
\end{aligned} \tag{A.30}$$

Finally, replace the coefficients with their definitions from eq. (A.26), change $\frac{\partial^2}{\partial z^2}$ to ∇^2 and $\frac{\partial^4}{\partial z^4}$ to ∇^4, and we obtain

$$\left[9\nabla^4 + \beta\nabla^2 + \gamma\right]\phi_{0,0}(\mathbf{r},\omega) = Wq_{0,0}(\mathbf{r},\omega) + Xq_{1,0}(\mathbf{r},\omega) + Yq_{2,0}(\mathbf{r},\omega) + Zq_{3,0}(\mathbf{r},\omega) \ , \tag{A.31}$$

where

$$\beta = 90\frac{\omega^2}{v^2} + i\frac{\omega}{v}\left(55\mu_a + 27\mu_t^{(1)} + 35\mu_t^{(2)} + 63\mu_t^{(3)}\right) - \left(27\mu_a\mu_t^{(1)} + 28\mu_a\mu_t^{(3)} + 35\mu_t^{(2)}\mu_t^{(3)}\right) \tag{A.32}$$

$$\gamma = 105(-i\frac{\omega}{v} + \mu_a)(-i\frac{\omega}{v} + \mu_t^{(1)})(-i\frac{\omega}{v} + \mu_t^{(2)})(-i\frac{\omega}{v} + \mu_t^{(3)}) \ . \tag{A.33}$$

The right-hand-side of eq. (A.31) contains the moments of the source distribution where

$$\begin{aligned}
W &= 105\left(-i\frac{\omega}{v} + \mu_t^{(3)}\right)\left(-i\frac{\omega}{v} + \mu_t^{(2)}\right)\left(-i\frac{\omega}{v} + \mu_t^{(1)}\right) - 27\left(-i\frac{\omega}{v} + \mu_t^{(1)}\right)\nabla^2 \\
&\quad -28\left(-i\frac{\omega}{v} + \mu_t^{(3)}\right)\nabla^2
\end{aligned} \tag{A.34}$$

$$X = 27\sqrt{\frac{1}{3}}\ \frac{\partial^3}{\partial z^3} - 105\sqrt{\frac{1}{3}}\left(-i\frac{\omega}{v} + \mu_t^{(3)}\right)\left(-i\frac{\omega}{v} + \mu_t^{(2)}\right)\frac{\partial}{\partial z} \tag{A.35}$$

$$Y = 105\sqrt{\frac{4}{45}}\left(-i\frac{\omega}{v} + \mu_t^{(3)}\right)\nabla^2 \tag{A.36}$$

$$Z = 105\sqrt{\frac{36}{3\cdot 15\cdot 35}}\ \frac{\partial^3}{\partial z^3} \tag{A.37}$$

Solutions to the P_3 equation and comparisons with the diffusion equation are made in section 2.7.

A.2 Correlation Transport Equation

The P_N approximation as described for the photon transport equation can be applied to the correlation transport equation with only a few modifications. The correlation transport equation is

$$\nabla \cdot G_1^T(\mathbf{r}, \hat{\Omega}, \tau)\hat{\Omega} + \mu_t G_1^T(\mathbf{r}, \hat{\Omega}, \tau) = \mu_s \int G_1^T(\mathbf{r}, \hat{\Omega}', \tau) g_1^s(\hat{\Omega}, \hat{\Omega}', \tau) f(\hat{\Omega}, \hat{\Omega}') \mathrm{d}\hat{\Omega}' + S(\mathbf{r}, \hat{\Omega}) \ . \tag{A.38}$$

Here, $G_1^T(\mathbf{r}, \hat{\Omega}, \tau)$ is the unnormalized temporal field correlation function which is a function of position $\mathbf{r}$, direction $\hat{\Omega}$, and correlation time τ. The scattering and absorption coefficients are respectively μ_s and μ_a, and $\mu_t = \mu_s + \mu_a$ is the transport coefficient. Furthermore, $g_1^s(\hat{\Omega}, \hat{\Omega}', \tau)$ is the normalized temporal field correlation function for single scattering, $f(\hat{\Omega}, \hat{\Omega}')$ is the normalized differential cross-section, and $S(\mathbf{r}, \hat{\Omega})$ is the source distribution. The scattering coefficient is the reciprocal of the scattering length, $\mu_s = 1/l$, and the absorption coefficient is the reciprocal of the absorption length, $\mu_a = 1/l_a$. The time dependence (not to be confused with correlation time) has been left out of the equation since I am only considering measurements with CW sources. The time dependence can be included by adding a time-derivative of $G_1^T(\mathbf{r}, \hat{\Omega}, \tau)$ (i.e. $v^{-1}\frac{\partial}{\partial t} G_1^T(\mathbf{r}, \hat{\Omega}, \tau)$) to the left-hand side of eq. (A.38).

In analogy to photon transport, the correlation fluence is

$$G_1(\mathbf{r}, t) = \int \mathrm{d}\hat{\Omega} G_1^T(\mathbf{r}, \hat{\Omega}, \tau) \ , \tag{A.39}$$

while the correlation flux is given by

$$\mathbf{J}_\mathrm{g}(\mathbf{r}, t) = \int \mathrm{d}\hat{\Omega} G_1^T(\mathbf{r}, \hat{\Omega}, \tau)\hat{\Omega} \ . \tag{A.40}$$

The main difference between the correlation transport equation and the photon transport equation is the appearance of $g_1^s(\hat{\Omega}, \hat{\Omega}', \tau)$ in the integral, as discussed in section 4.2.3. The appearance of this angular dependent quantity will result in integrals of three spherical harmonics which are handled in a fashion similar to the handling of $\hat{\Omega} \cdot \nabla \phi_{l,m}(\mathbf{r}, t)$ in the photon transport equation (see section A.1).

Within the P_N approximation $G_1^T(\mathbf{r}, \hat{\Omega}, \tau)$ and the source distribution are expanded as

$$G_1^T(\mathbf{r}, \hat{\Omega}, \tau) = \sum_{l=0}^{N} \sum_{m=-l}^{l} \Gamma_{l,m}(\mathbf{r}, \tau) Y_{l,m}(\hat{\Omega}) \ , \tag{A.41}$$

and

$$S(\mathbf{r}, \hat{\Omega}) = \sum_{l=0}^{N} \sum_{m=-l}^{l} q_{l,m}(\mathbf{r}) Y_{l,m}(\hat{\Omega}) \ . \tag{A.42}$$

For the phase function, we make the reasonable assumption that the amplitude is only dependent on the change in direction of the photon and thus

$$\begin{aligned} f(\hat{\Omega} \cdot \hat{\Omega}') &= \sum_{l=0}^{\infty} \frac{2l+1}{4\pi} g_l P_l(\hat{\Omega} \cdot \hat{\Omega}') \\ &= \sum_{l=0}^{\infty} \sum_{m=-l}^{l} g_l Y_{l,m}^*(\hat{\Omega}') Y_{l,m}(\hat{\Omega}) \ , \end{aligned} \tag{A.43}$$

where P_l is a Legendre Polynomial and the second line is obtained using the angular addition rule [63]. The phase function is normalized and therefore $g_0 = 1$.

The single scattering temporal field correlation function is

$$g_1^s(\hat{\Omega}, \hat{\Omega}', \tau) = \exp\left(-\frac{1}{6} q^2 \left\langle \Delta r^2(\tau) \right\rangle\right) = \exp\left(-\frac{1}{3} k_o^2 \left\langle \Delta r^2(\tau) \right\rangle \left(1 - \hat{\Omega} \cdot \hat{\Omega}'\right)\right) \ , \tag{A.44}$$

where $\langle \Delta r^2(\tau) \rangle$ is the mean square displacement of the scattering particles and $q = 2k_o \sin(\theta/2)$ is the momentum transfer for the scattered photon where θ is the angle between $\hat{\Omega}$ and $\hat{\Omega}'$. For particles undergoing Brownian motion, $\langle \Delta r^2(\tau) \rangle = 6 D_B \tau$ where D_B is the Brownian diffusion coefficient. When $\tau \ll (2 D_B k_o^2)^{-1}$, then eq. (A.44) is Taylor expanded to

$$\begin{aligned} g_1^s(\hat{\Omega}, \hat{\Omega}', \tau) &= 1 - 2 D_B k_o^2 \tau + 2 D_B k_o^2 \tau \left(\hat{\Omega} \cdot \hat{\Omega}'\right) \\ &= 1 - 2 D_B k_o^2 \tau + 2 D_B k_o^2 \tau \frac{4\pi}{3} \sum_{m=-1}^{1} Y_{1,m}^*(\hat{\Omega}') Y_{1,m}(\hat{\Omega}) \ . \end{aligned} \tag{A.45}$$

The second line is obtained using the angular addition rule [63]. Note that $(2D_B k_o^2)^{-1} \approx 10^{-3}$ s when $D_B = 1\text{x}10^{-8}$ cm^2 s^{-1} and the wavelength of light is 514 nm.

Substituting these expansions into the correlation transport equation, eq. (A.38), we obtain

$$\sum_{l=0}^{N} \sum_{m=-l}^{l} \left\{ \left[\hat{\Omega}\cdot\nabla + \mu_t\right] \Gamma_{l,m}(\mathbf{r},\tau) Y_{l,m}(\hat{\Omega}) - q_{l,m} Y_{l,m}(\hat{\Omega}) \right.$$
$$-\mu_s \int \mathrm{d}\hat{\Omega}' \Gamma_{l,m}(\mathbf{r},\tau) Y_{l,m}(\hat{\Omega}') \sum_{l'=0}^{N} \sum_{m'=-l}^{l} g_{l'} Y^*_{l',m'}(\hat{\Omega}') Y_{l',m'}(\hat{\Omega})$$
$$\left. \left[1 - 2D_B k_o^2 \tau + 2D_B k_o^2 \tau \frac{4\pi}{3} \sum_{m''=-1}^{1} Y^*_{1,m''}(\hat{\Omega}') Y_{1,m''}(\hat{\Omega})\right] \right\} = 0 \; . \quad \text{(A.46)}$$

The integral over $\hat{\Omega}'$ can be calculated for the first two terms between the [...]'s on the third line using the spherical harmonic orthogonality relation (eq. (A.8)). Integrating gives

$$\sum_{l=0}^{N} \sum_{m=-l}^{l} \left[\hat{\Omega}\cdot\nabla + \mu_t^{(l)} + g_l k_c\right] \Gamma_{l,m}(\mathbf{r},\tau) Y_{l,m}(\hat{\Omega}) - q_{l,m} Y_{l,m}(\hat{\Omega})$$
$$-k_c \int \mathrm{d}\hat{\Omega}' \Gamma_{l,m}(\mathbf{r},\tau) Y_{l,m}(\hat{\Omega}') \sum_{l'=0}^{N} \sum_{m'=-l}^{l} g_{l'} Y^*_{l',m'}(\hat{\Omega}') Y_{l',m'}(\hat{\Omega})$$
$$\left[\frac{4\pi}{3} \sum_{m''=-1}^{1} Y^*_{1,m''}(\hat{\Omega}') Y_{1,m''}(\hat{\Omega})\right] = 0 \; . \quad \text{(A.47)}$$

New notation is introduced to simplify eq. (A.47): $\mu_t^{(l)} = \mu_s(1-g_l) + \mu_a$ is the reduced transport coefficient (note $\mu_t^{(0)} = \mu_a$) and $k_c = 2\mu_s D_B k_o^2 \tau$ is a dynamic absorption coefficient.

The $Y^*_{1,m''}(\hat{\Omega}') Y^*_{l',m'}(\hat{\Omega}')$ and $Y_{1,m''}(\hat{\Omega}) Y_{l',m'}(\hat{\Omega})$ can be rewritten in terms of single spherical harmonics, given (see Arfken section 12.9 [147])

$$Y_{l,m}(\hat{\Omega}) Y_{1,-1}(\hat{\Omega}) = \sqrt{\frac{3}{8\pi}} B_{l+1}^{m-1} Y_{l+1,m-1}(\hat{\Omega}) - \sqrt{\frac{3}{8\pi}} B_l^{-m} Y_{l-1,m-1}(\hat{\Omega}) \; , \quad \text{(A.48)}$$
$$Y_{l,m}(\hat{\Omega}) Y_{1,0}(\hat{\Omega}) = \sqrt{\frac{3}{4\pi}} A_{l+1}^{m} Y_{l+1,m}(\hat{\Omega}) + \sqrt{\frac{3}{4\pi}} A_l^{m} Y_{l-1,m}(\hat{\Omega}) \; , \quad \text{(A.49)}$$
$$Y_{l,m}(\hat{\Omega}) Y_{1,1}(\hat{\Omega}) = \sqrt{\frac{3}{8\pi}} B_{l+1}^{-m-1} Y_{l+1,m+1}(\hat{\Omega}) - \sqrt{\frac{3}{8\pi}} B_l^{m} Y_{l-1,m+1}(\hat{\Omega}) \; . \quad \text{(A.50)}$$

The coefficients A_l^m and B_l^m are given by

$$A_l^m = \left(\frac{(l-m)(l+m)}{(2l-1)(2l+1)}\right)^{1/2} \tag{A.51}$$

$$B_l^m = \left(\frac{(l-m)(l-m-1)}{(2l-1)(2l+1)}\right)^{1/2} \tag{A.52}$$

The product of spherical harmonics in the integral of eq. (A.47) can be rewritten as

$$\begin{aligned}
&\frac{4\pi}{3}\sum_{l'm'} g_{l'} Y_{l'}^{m'*}(\hat{\Omega}') Y_{l'}^{m'}(\hat{\Omega}) \sum_{m''=-1}^{1} Y_1^{m''*}(\hat{\Omega}') Y_1^{m''}(\hat{\Omega}) \\
&= \frac{4\pi}{3}\sum_{l'm'} g_{l'} \Bigg\{ \\
&+\frac{3}{8\pi}\left[B_{l'+1}^{m'-1} Y_{l'+1}^{m'-1*}(\hat{\Omega}') - B_{l'}^{-m'} Y_{l'-1}^{m'-1*}(\hat{\Omega}')\right]\left[B_{l'+1}^{m'-1} Y_{l'+1}^{m'-1}(\hat{\Omega}) - B_{l'}^{-m'} Y_{l'-1}^{m'-1}(\hat{\Omega})\right] \\
&+\frac{3}{4\pi}\left[A_{l'+1}^{m'} Y_{l'+1}^{m'*}(\hat{\Omega}') + A_{l'}^{m'} Y_{l'-1}^{m'*}(\hat{\Omega}')\right]\left[A_{l'+1}^{m'} Y_{l'+1}^{m'}(\hat{\Omega}) + A_{l'}^{m'} Y_{l'-1}^{m'}(\hat{\Omega})\right] \\
&-\frac{3}{8\pi}\left[B_{l'+1}^{-m'-1} Y_{l'+1}^{m'+1*}(\hat{\Omega}') - B_{l'}^{m'} Y_{l'-1}^{m'+1*}(\hat{\Omega}')\right]\left[B_{l'+1}^{-m'-1} Y_{l'+1}^{m'+1}(\hat{\Omega}) - B_{l'}^{m'} Y_{l'-1}^{m'+1}(\hat{\Omega})\right] \\
&\Bigg\}
\end{aligned} \tag{A.53}$$

Doing the final integral over $\hat{\Omega}'$ we obtain

$$\begin{aligned}
\sum_{l=0}^{N}\sum_{m=-l}^{l} & \left[\hat{\Omega}\cdot\nabla + \mu_t^{(l)} + g_l k_c\right]\Gamma_{l,m}(\mathbf{r},\tau) Y_{l,m}(\hat{\Omega}) - q_{l,m} Y_{l,m}(\hat{\Omega}) \\
-k_c \Gamma_{l,m}\frac{4\pi}{3}\Bigg\{ & + \frac{3}{8\pi} g_{l-1} B_l^m \left[B_l^m Y_l^m(\hat{\Omega}) - B_{l-1}^{-m-1} Y_{l-2}^m(\hat{\Omega})\right] \\
& - \frac{3}{8\pi} g_{l+1} B_{l+1}^{-m-1} \left[B_{l+2}^m Y_{l+2}^m(\hat{\Omega}) - B_{l+1}^{-m-1} Y_l^m(\hat{\Omega})\right] \\
& + \frac{3}{4\pi} g_{l-1} A_l^m \left[A_l^m Y_l^m(\hat{\Omega}) + A_{l-1}^m Y_{l-2}^m(\hat{\Omega})\right] \\
& + \frac{3}{4\pi} g_{l+1} A_{l+1}^m \left[A_{l+2}^m Y_{l+2}^m(\hat{\Omega}) + A_{l+1}^m Y_l^m(\hat{\Omega})\right] \\
& - \frac{3}{8\pi} g_{l-1} B_l^{-m} \left[-B_l^{-m} Y_l^m(\hat{\Omega}) + B_{l-1}^{m-1} Y_{l-2}^m(\hat{\Omega})\right] \\
& + \frac{3}{8\pi} g_{l+1} B_{l+1}^{m-1} \left[-B_{l+2}^{-m} Y_{l+2}^m(\hat{\Omega}) + B_{l+1}^{m-1} Y_l^m(\hat{\Omega})\right] \Bigg\} = 0\ .
\end{aligned} \tag{A.54}$$

Next, we multiply eq. (A.54) by $Y^*_{\alpha,\beta}(\hat{\Omega})$ and integrate over $\hat{\Omega}$. Using the orthogonality relations for the spherical harmonics, eq. (A.8), we arrive at

$$
\begin{aligned}
\mu_t^{(\alpha)}\Gamma_{\alpha,\beta} &+ g_\alpha k_c \Gamma_{\alpha,\beta} \\
-k_c\Big\{ &+ \frac{1}{2}\left[g_{\alpha-1}B^\beta_\alpha B^\beta_\alpha \Gamma_{\alpha,\beta} - g_{\alpha+1}B^\beta_{\alpha+2}B^{-\beta-1}_{\alpha+1}\Gamma_{\alpha+2,\beta}\right] \\
&- \frac{1}{2}\left[g_{\alpha-1}B^{-\beta-1}_{\alpha-1}B^\beta_\alpha \Gamma_{\alpha-2,\beta} - g_{\alpha+1}B^{-\beta-1}_{\alpha+1}B^{-\beta-1}_{\alpha+1}\Gamma_{\alpha,\beta}\right] \\
&+ \left[g_{\alpha-1}A^\beta_\alpha A^\beta_\alpha \Gamma_{\alpha,\beta} + g_{\alpha+1}A^\beta_{\alpha+2}A^\beta_{\alpha+1}\Gamma_{\alpha+2,\beta}\right] \\
&+ \left[g_{\alpha-1}A^\beta_{\alpha-1}A^\beta_\alpha \Gamma_{\alpha-2,\beta} + g_{\alpha+1}A^\beta_{\alpha+1}A^\beta_{\alpha+1}\Gamma_{\alpha,\beta}\right] \\
&- \frac{1}{2}\left[-g_{\alpha-1}B^{-\beta}_\alpha B^{-\beta}_\alpha \Gamma_{\alpha,\beta} + g_{\alpha+1}B^{-\beta}_{\alpha+2}B^{\beta-1}_{\alpha+1}\Gamma_{\alpha+2,\beta}\right] \\
&+ \frac{1}{2}\left[-g_{\alpha-1}B^{\beta-1}_{\alpha-1}B^{-\beta}_\alpha \Gamma_{\alpha-2,\beta} + g_{\alpha+1}B^{\beta-1}_{\alpha+1}B^{\beta-1}_{\alpha+1}\Gamma_{\alpha,\beta}\right] \Big\} \\
&+ \frac{1}{2}B^{\beta-1}_{\alpha+1}\left(\frac{\partial}{\partial x} - i\frac{\partial}{\partial y}\right)\Gamma_{\alpha+1,\beta-1} - \frac{1}{2}B^{-\beta}_\alpha\left(\frac{\partial}{\partial x} - i\frac{\partial}{\partial y}\right)\Gamma_{\alpha-1,\beta-1} \\
&- \frac{1}{2}B^{-\beta-1}_{\alpha+1}\left(\frac{\partial}{\partial x} + i\frac{\partial}{\partial y}\right)\Gamma_{\alpha+1,\beta+1} + \frac{1}{2}B^\beta_\alpha\left(\frac{\partial}{\partial x} + i\frac{\partial}{\partial y}\right)\Gamma_{\alpha-1,\beta+1} \\
&+ A^\beta_{\alpha+1}\frac{\partial}{\partial z}\Gamma_{\alpha+1,\beta} + A^\beta_\alpha \frac{\partial}{\partial z}\Gamma_{\alpha-1,\beta} = q_{\alpha,\beta} \ . \qquad \text{(A.55)}
\end{aligned}
$$

This is a coupled set of linear differential equations for $\Gamma_{\alpha,\beta}$.

To obtain the correlation diffusion equation, we neglect all $\Gamma_{\alpha,\beta}$ and g_α for $\alpha > 1$. The $\alpha = 0$ equation is

$$
\begin{aligned}
&\mu_a\Gamma_{0,0} + k_c(1-g_1)\Gamma_{0,0} + \frac{1}{2}\sqrt{\frac{2}{3}}\left(\frac{\partial}{\partial x} - i\frac{\partial}{\partial y}\right)\Gamma_{1,-1} \\
&-\frac{1}{2}\sqrt{\frac{2}{3}}\left(\frac{\partial}{\partial x} + i\frac{\partial}{\partial y}\right)\Gamma_{1,1} + \sqrt{\frac{1}{3}}\frac{\partial}{\partial z}\Gamma_{1,0} = q_{0,0} \ , \qquad \text{(A.56)}
\end{aligned}
$$

and the $\alpha = 1$ equations are

$$
\mu_t^{(1)}\Gamma_{1,-1} + \left(g_1 - \frac{1}{3}\right)k_c\Gamma_{1,-1} + \frac{1}{2}\sqrt{\frac{2}{3}}\left(\frac{\partial}{\partial x} + i\frac{\partial}{\partial y}\right)\Gamma_{0,0} = q_{1,-1} \ , \qquad \text{(A.57)}
$$

$$
\mu_t^{(1)}\Gamma_{1,0} + \left(g_1 - \frac{1}{3}\right)k_c\Gamma_{1,0} + \sqrt{\frac{1}{3}}\frac{\partial}{\partial z}\Gamma_{0,0} = q_{1,0} \ , \qquad \text{(A.58)}
$$

$$\mu_t^{(1)}\Gamma_{1,1} + \left(g_1 - \frac{1}{3}\right) k_c \Gamma_{1,1} - \frac{1}{2}\sqrt{\frac{2}{3}}\left(\frac{\partial}{\partial x} - i\frac{\partial}{\partial y}\right)\Gamma_{0,0} = q_{1,1} \ . \tag{A.59}$$

Using the definition for the correlation fluence $G_1(\mathbf{r},\tau)$ (eq. (A.39)) and the correlation flux $\mathbf{J}_g(\mathbf{r},\tau)$ (eq. (A.40)), the $\alpha = 0$ and $\alpha = 1$ equations can be rewritten as

$$\mu_a G_1(\mathbf{r},\tau) + \frac{1}{3}\mu_s' k_o^2 \left\langle \Delta r^2(\tau)\right\rangle G_1(\mathbf{r},\tau) + \nabla\cdot\mathbf{J}_g(\mathbf{r},\tau) = S_0(\mathbf{r}) \ , \tag{A.60}$$

$$\mu_t^{(1)}\mathbf{J}_g(\mathbf{r},\tau) + \frac{1}{3}\mu_s\left(g_1 - \frac{1}{3}\right) k_o^2\left\langle \Delta r^2(\tau)\right\rangle \mathbf{J}_g(\mathbf{r},\tau) + \frac{1}{3}\nabla G_1(\mathbf{r},\tau) = \mathbf{S_1}(\mathbf{r}) \ . \tag{A.61}$$

Recall that we have assumed that the correlation $G_1^T(\mathbf{r},\hat{\Omega},\tau)$ is nearly isotropic and that the scattering particles have moved a distance that is much smaller than a wavelength of light. The first assumption is satisfied when $\mu_a \ll \mu_s$ and the scattering is not too anisotropic. The second assumption is satisfied when $k_o^2\left\langle\Delta r^2(\tau)\right\rangle \ll 1$. To keep our equations consistent with these approximations it is necessary to drop terms from eq. (A.61); in particular

$$\mu_s'\mathbf{J}_g(\mathbf{r},\tau) + \frac{1}{3}\nabla G_1(\mathbf{r},\tau) = \mathbf{S_1}(\mathbf{r}) \ . \tag{A.62}$$

Decoupling eq. (A.60) and eq. (A.62) for $G_1(\mathbf{r},\tau)$, we arrive at the correlation diffusion equation

$$\left[-\nabla\cdot\left(\frac{1}{v}D_\gamma\nabla\right) + \mu_a + \frac{1}{3}\mu_s' k_o^2\left\langle\Delta r^2(\tau)\right\rangle\right] G_1(\mathbf{r},\tau) = S_0(\mathbf{r}) - \nabla\cdot\left(\frac{3}{v}D_\gamma \mathbf{S}_1(\mathbf{r})\right) \ , \tag{A.63}$$

where $D_\gamma = v/(3\mu_s')$ is the *photon diffusion coefficient*.

Appendix B

Henyey-Greenstein Phase Function

The normalized Henyey-Greenstein phase function is [141, 139, 140]

$$f(\hat{\Omega} \cdot \hat{\Omega}') = f(\cos\theta) = \frac{1 - g^2}{2\left[1 + g^2 - 2g\cos\theta\right]^{3/2}} \ , \tag{B.1}$$

where θ is the angle between the input direction $\hat{\Omega}'$ and the output direction $\hat{\Omega}$, and g is the scattering anisotropy. The angle θ is in the interval $[0, \pi]$. This phase function is unique because the average cosine of the scattering angle is g,

$$\langle\cos\theta\rangle = \int_0^\pi f(\cos\theta)\cos\theta\sin\theta \mathrm{d}\theta = g \ , \tag{B.2}$$

and higher moments of the scattering angle are g^l,

$$\int_0^\pi f(\cos\theta) P_l(\cos\theta)\sin\theta \mathrm{d}\theta = g^l \ . \tag{B.3}$$

$P_l(\cos\theta)$ is a Legendre polynomial of order l.

Appendix C

Monte Carlo Code

Following is the listing of the Monte Carlo code that I used to simulate the propagation of diffuse photon density waves and temporal correlation through turbid media. The code is written to handle infinite and semi-infinite media which is either homogeneous or contains a spherical inhomogeneity with different optical and dynamical properties. When running simulations with a spherical object the optical properties of the background and object can be anything. The background is assumed static and the object is dynamic.

This code is compiled using

```
gcc -o monte monte.c ran.c ran2.c ran3.c -lm
```

or an equivalent. Parameters for the simulation are entered on the command line using the following format:

```
unix_prompt> monte nphotons musp mua musp2 mua2 radius sz dz DeltaYmax
DeltaYstep output_file
```

`nphotons` is the number of photons to run in the simulation. `musp` and `mua` are the reduced scattering and absorption coefficent of the background medium. `musp2`, `mua2`, and `radius` are the reduced scattering and absorption coefficent and radius of the spherical object (if it exists). `sz` and `dz` are the z coordinates of the source and detector. `DeltaYmax` and `DeltaYstep` determine the range over which the total momentum transfer from moving particles is histogrammed. `output_file` is the file name for the data generated by the simulation.

The code can be compiled in many different modes, each of which runs a simulation for a different geometry. Which mode the code runs in is determined by the #define statements for HOMOGENEOUS, INFINITE, COLLIMATED, SPHERICAL_DETECTOR, and PARTIAL_DYNAMIC in the beginning of the program. If HOMOGENEOUS is defined then the medium is homogeneous, otherwise a spherical object is centered at the origin. If INFINITE is defined then the medium is infinite otherwise it is semi-infinite. The source is collimated in the +z direction if COLLIMATED is defined, otherwise the source is isotropic. If INFINITE and HOMOGENEOUS are defined and COLLIMATED is not defined then the spherical symmetry of the geometry can be exploited by using spherical detectors. This is done by defining SPHERICAL_DETECTOR, otherwise ring detectors which lie in a plane are used. For ring detectors, the detection plane is in the xy plane at the z-coordinate `dz` and the source is at x=y=0 and z=`sz`. For spherical detectors the source is at x=y=z=0. Finally, the medium can be homogeneous with a uniformly distributed static and dynamic component. This is a model of capillary blood flow. This geometry is set by defining PARTIAL_DYNAMIC where VOL_FRAC is defined as the volume fraction (actually P_{blood}, see section 4.4.3) of the dynamic component. If PARTIAL_DYNAMIC is not defined then the system is 100% dynamic.

Two different sets of output are generated. The first set contains the time domain data. A file is generated for each detector position. The file names are `output_file_##.##.tdd` where the `##.##` indicates the detector position and `.tdd` indicates time domain data. The second set contains the total momentum transfer data. Once again a file is generated for each detector position. The file names are `output_file_##.##.DelY` where the `##.##` indicates the detector position and `.DelY` indicates momentum transfer data. The formats are self explanatory.

C.1 monte.c

```
#include<stdio.h>
#include<stdlib.h>
#include<math.h>
```

```
#define HOMOGENEOUS   /* DEFINE IF THE MEDIUM IS HOMOGENEOUS
         OTHERWISE THERE IS A SPHERE AT THE ORIGIN */
#define INFINITE      /* DEFINE IF MEDIUM IS INFINITE OTHERWISE SEMI-INFINITE*/
/*#define COLLIMATED  /* DEFINE IF SOURCE IS COLLIMATED OTHERWISE ISOTROPIC */

#ifdef INFINITE
#ifdef HOMOGENEOUS
#ifndef COLLIMATED
#define SPHERICAL_DETECTOR /* DEFINE IF THE DETECTORS ARE SPHERICAL
      OTHERWISE RING DETECTORS ARE USED */
#endif
#endif
#endif

#ifdef HOMOGENEOUS
/*#define PARTIAL_DYNAMIC   /* DEFINE IF SYSTEM IS UNIFORM BUT PART STATIC
     AND PART DYNAMIC.  ONLY WORKS IF DEF HOMOGENEOUS*/
#define VOL_FRAC 0.1      /* VOLUME FRACTION OD DYNAMIC COMPONENT
     USED ONLY IF PARTIAL_DYNAMIC IS DEFINED */
#endif


#define pi 3.1415926353
#define TRUE 1
#define FALSE 0
#define MAX_TBIN  1040      /* MAXIMUM NUMBER OF TEMPORAL BINS */
#define MAX_DeltaYBIN 2080  /* MAXIMUM NUMBER OF MOMENTUM TRANSFER BINS */
#define MAX_RHOBIN 40       /* MAXIMUM NUMBER OF RADIAL/RHO BINS */

main( argc, argv )
int argc;
char *argv[];
{
  int i,j,q;
  int idum;             /* FOR RANDOM NUMBER GENERATOR */
  int ncall;            /* NUMBER OF CALLS TO RANDOM NUMBER GENERATOR - USED
  BY THE GENERATOR */
  int ABSORBED;         /* FLAG IF PHOTON HAS BEEN ABSORBED */
  int b;                /* TOTAL NUMBER OF PHOTONS TO RUN */
  int p;                /* NUMBER OF PHOTONS RUN SO FAR */
  int OUTSIDE;          /* FLAG IF OUTSIDE SPHERE */
  int rhoindex,tindex,DeltaYindex;  /* INDICES FOR RADIAL/RHO, TIME,
       AND MOMENTUM TRANSFER SCORING */
  int nt,nDeltaY;       /* NUMBER OF TIME AND MOMENTUM BINS NEEDED */
  float rho;            /* rho=sqrt(x*x+y*y) POSITION OF PHOTON */
  float rhostep;        /* WIDTH OF DETECTOR */
  float t,tgate,tbin;   /* CURRENT TIME, GATE TIME, WIDTH OF TEMPORAL BINS */
  float DeltaY;         /* CURRENT MOMENTUM TRANSFER */
  float DeltaYmax, DeltaYstep;
                        /* MAXIMUM MOMENTUM TRANSFER, WIDTH OF MOMENTUM BINS */
  float velocity;       /* PHOTON VELOCITY IN THE MEDIUM */
  float g=0.;           /* ANISOTROPY FACTOR */
  float foo;            /* TEMPORARY VARIABLE */
  float mua,musp,mus;   /* OPTICAL PROPERTIES OF THE BACKGROUND */
  float muainv,musinv;
  float mua2,musp2,mus2; /* OPTICAL PROPERTIES OF THE SPHERE */
  float muainv2,musinv2;
  float radi2,radisq;   /* RADIUS OF THE SPHERE, RADIUS SQUARE */
  float phi,theta,sphi,cphi,stheta,ctheta;
                        /* SCATTERING ANGLES */
  float x,y,z;          /* CURRENT PHOTON POSITION */
  float xold,yold,zold;/* LAST POSITION OF PHOTON */
  float xm,ym,zm,lm;    /* x,y, and z OF PHOTON INTERSECTION WITH A PLANE
  DETECTOR.  lm IS THE LENGTH FROM LAST SCATTERING
  EVENT TO DETECTOR INTERSECTION */
  float r,rold;         /* CURRENT AND LAST RADIAL POSITION OF PHOTON */
  float c1,c2,c3;       /* DIRECTION COSINES */
  float c1o, c2o, c3o; /* OLD DIRECTION COSINES */
  float la;             /* ABSORPTION DISTANCE - RANDOMLY GENERATED FROM MUA */
  float ls;             /* SCATTERING DISTANCE - RANDOMLY GENERATED FROM MUS */
  float sz, dz;         /* SOURCE AND DETECTOR  Z POSITION.  THE SOURCE IS
                           AT X=Y=0 */
  float hgpart1,hgpart2,hgpart3,hgpart4,hgpart5,hgpart6;
                        /* USED IN HENYEY-GREENSTEIN CALCULATION */
  FILE *fp;             /* FILE POINTER FOR SAVING THE DATA */
  double fluxout[MAX_RHOBIN][MAX_TBIN];          /* SCORE THE PHOTON FLUX */
  double fluxin[MAX_RHOBIN][MAX_TBIN];
  double DeltaYout[MAX_RHOBIN][MAX_DeltaYBIN];  /* SCORE THE TOTAL MOMENTUM */
  double DeltaYin[MAX_RHOBIN][MAX_DeltaYBIN];   /* TRANSFER                 */
  float rnm;            /* RANDOM NUMBER */
  float ran( int *idum, int *ncall );           /* FUNCTION DECLARATION */
  float B,C,L,T,DELL,T1,T2,LSP,LAP,LSP2,LAP2,B2;
```

```
            /* USED FOR SPHERE INTERSECTION ROUTINE */
            /* B,C to be used in B^2-4AC calculation! */
            /* L, T are also for cross passing, entering sphere etc checks */
            /* B2=B^2-4AC*/
       /* T1,T2,T are for parameterizations */
       /* DELL=delta L*/
       /* LSP: ls temp */
       /* LAP : la temp */
char filenm[32];     /* FILE NAME FOR DATA FILE */


/* GET THE COMMAND LINE ARGUMENTS */
if( argc!=12 ) {
 printf( "usage:  monte   nphotons musp mua musp2 mua2  radius  sz dz  DeltaYmax DeltaYstep output_file\n" );
  exit(1);
}

/* GET THE NUMBER OF PHOTONS TO MIGRATE */
sscanf( argv[1], "%f", &foo );  b = (int)foo;

/* GET THE OPTICAL PROPERTIES */
/* mua & musp are for background medium */
/* mua2 & musp2  are for the spherical tumor, all variables with
   ´2´ as the last  character are for the tumor */
sscanf( argv[2], "%f", &musp );    mus = musp/(1.-g);  musinv = 1./mus;
sscanf( argv[3], "%f", &mua );  muainv = 1. / mua;
sscanf( argv[4], "%f", &musp2 );  mus2= musp2/(1.-g);  musinv2= 1./mus2;
sscanf( argv[5], "%f", &mua2 );  muainv2 = 1. / mua2;

/* GET THE SPHERE RADIUS */
/* radi2 is the radius of the spherical tumor */
/* radisq is for cross pass calculation */
sscanf( argv[6], "%f", &radi2 );radisq=radi2*radi2;

/* SOURCE AND DETECTOR Z POSITION */
sscanf( argv[7], "%f", &sz );
sscanf( argv[8], "%f", &dz );

/* RANGE OF MOMENTUM TRANSFERS AND BIN STEP */
sscanf( argv[9], "%f", &DeltaYmax );
sscanf( argv[10], "%f", &DeltaYstep );

/* INITIALIZE OTHER PARAMETERS */
velocity = 2.9979e10 / 1.333;    /* PHOTON VELOCITY IN WATER */
g = 0.;                          /* SCATTERING ANISOTROPY */
tbin=20e-12 ; tgate=10.24e-9;    /* TEMPORAL BIN WIDTH AND GATE */
rhostep=0.1;                     /* DETECTOR WIDTH */

/* CALCULATE THE NUMBER OF TEMPORAL AND MOMENTUM BINS THAT ARE NEEDED */
nt = tgate/tbin;
nDeltaY = DeltaYmax/DeltaYstep+1;

/* MAKE SURE THAT ENOUGH MEMORY HAS BEEN ALLOCATED FOR THE NEEDED BINS */
if( nt>MAX_TBIN ) {
  printf( "Maximum number of time bins exceeded." );
  exit(1);
}
 if( nDeltaY>MAX_DeltaYBIN ) {
  printf( "Maximum number of DeltaY bins exceeded." );
  exit(1);
}

/* INITIALIZE THE FLUX TO BE ZERO */
for( i=0; i<MAX_RHOBIN; i++ )
  for( j=0; j<nt; j++ ) {
    fluxin[i][j] = 0.;
    fluxout[i][j] = 0.;
  }
/* INITIALIZE DeltaY TO ZERO */
for( i=0; i<MAX_RHOBIN; i++ )
  for( j=0; j<nDeltaY; j++ ) {
    DeltaYin[i][j] = 0.;
    DeltaYout[i][j] = 0.;
  }

/* NUMBER PHOTONS EXECUTED SO FAR */
p=0;

/* SEED THE RANDOM NUMBER GENERATOR - A LARGE NEGATIVE NUMBER IS REQUIRED */
idum = -149249;
ncall = 0;         /* NUMBER OF CALLS MADE TO THE GENERATOR */
```

```
  /* START MIGRATING THE PHOTONS */
  /* GENERATING PHOTONS UNTIL NUMBER OF PHOTONS EXECUTED (p) IS EQUAL TO THE
     NUMBER TO BE GENERATED (b) */

  while (p<b){
    OUTSIDE=FALSE;     /* START OUTSIDE THE OBJECT */
    ABSORBED=FALSE;    /* PHOTON NOT ABSORBED YET */

    t=0.;              /* START PHOTON AT TIME = 0 */
    DeltaY = 0.;       /* NO SCATTERING FROM A MOVING PARTICLE YET.
  ZERO MOMENTUM TRANSFER */
    ++p;               /* INCREMENT THE PHOTONS EXECUTED COUNTER */

    /* INITIAL SOURCE POSITION */
    x=0.; y=0.; z=sz;        /* CURRENT POSITION */
    xold=x; yold=y; zold=z;  /* PREVIOUS POSITION */

    /* RADIAL POSITION OF PHOTON
       USED FOR CHECKING FOR INTERSECTIONS WITH SPHERICAL DETECTORS
       AND THE SPHERICAL OBJECT */
    r = sqrt(x*x+y*y+z*z);         /* RADIAL POSITION OF PHOTON */
    rold = r;                      /* OLD RADIAL POSITION */

    /* INITIAL DIRECTION OF PHOTON */
#ifdef COLLIMATED
    /* COLLIMATED ALONG Z-AXIS */
    c1=0.; c1o=c1;
    c2=0.; c2o=c2;
    c3=1.; c3o=c3;
#endif
#ifndef COLLIMATED
    /* ISOTROPIC */
    rnm = ran(&idum,&ncall);
    phi=2*pi*rnm;
    cphi=cos(phi);
    sphi=sin(phi);
    rnm = ran(&idum,&ncall);
    theta=acos(1.-2.*rnm);
    ctheta=cos(theta);
    stheta=sin(theta);
    c1 = stheta*cphi;
    c2 = stheta*sphi;
    c3 = ctheta;
    c1o = c1;
    c2o = c2;
    c3o = c3;
#endif

    /* LOOP UNTIL TIME EXCEEDS GATE, PHOTON IS ABSORBED, OR PHOTON ESCAPES */
#ifndef INFINITE   /* SEMI-INFINITE MEDIUM */
    while ( t<tgate && ABSORBED==FALSE && z>=sz ) {
#endif
#ifdef INFINITE    /* INFINITE MEDIUM */
    while ( t<tgate && ABSORBED==FALSE ) {
#endif

      /* CALCULATE SCATTERING AND ABSORPTION LENGTHS */

#ifdef HOMOGENEOUS /* HOMOGENEOUS MEDIUM */
      rnm = ran(&idum,&ncall);
      ls = -musinv * log(rnm);
      rnm = ran(&idum,&ncall);
      la = -muainv * log(rnm);
      OUTSIDE=TRUE;
      if(ls<la) {
L=ls;
      }
      else {
L=la;
ABSORBED=TRUE;
      }

      /* ACCUMULATE THE MOMENTUM TRANSFER FROM A MOVING PARTICLE */
#ifndef PARTIAL_DYNAMIC
      DeltaY += 1.-c1*c1o-c2*c2o-c3*c3o;
#endif
#ifdef PARTIAL_DYNAMIC
      rnm = ran(&idum,&ncall);
      if( rnm<VOL_FRAC )  DeltaY += 1.-c1*c1o-c2*c2o-c3*c3o;
#endif
#endif
```

```
#ifndef HOMOGENEOUS /* HETEROGENEOUS MEDIUM, I.E. A SPHERE IS PRESENT */
      /* CHECK IF WE ARE OUTSIDE THE SPHERE, OR INSIDE THE SPHERE */
      if(radi2<r){
rnm = ran(&idum,&ncall);
ls=-musinv *log(rnm);
rnm = ran(&idum,&ncall);
la=-muainv *log(rnm);
OUTSIDE=TRUE;
      }
      else {

/*INCREMENT TOTAL WAVEVECTOR TRANSFER IF INSIDE SPHERE*/
DeltaY += 1.-c1*c1o-c2*c2o-c3*c3o;

rnm = ran(&idum,&ncall);
ls=-musinv2*log(rnm);
rnm = ran(&idum,&ncall);
la=-muainv2*log(rnm);
OUTSIDE=FALSE;
      }

      /* CHECK FOR INTERSECTIONS WITH THE SURFACE OF THE SPHERE */

      /* CALCULATE A,B,C */
      rold = r;
      B=(xold*c1+yold*c2+zold*c3);
      C=rold*rold-radisq;
      B2=B*B-C;

      /* CALCULATE MINIMUM DISTANCE */
      if(ls<la) {
L=ls;
      }
      else {
L=la;
ABSORBED=TRUE;
      }

      /* FINE TUNE */
      if (OUTSIDE){
if (B2>0){
  T1=(-B+sqrt(B2));
  T2=(-B-sqrt(B2));

  /* FIND IF WE INTERSECTED THE TUMOR */
  /* I.E ENTERED IT */
  if((T1>0 && T1<L) || (T2>0 && T2<L)) {

    /* FIND MINIMUM OF T1, T2*/
    if (T1<T2){
      DELL=T1;
      T=T2;
    }
    else{
      DELL=T2;
      T=T1;
    }
    L=DELL;
    LSP=(ls-DELL)*musinv/muainv2;
    LAP=(la-DELL)*muainv/muainv2;

    /* CHECK IF WE CROSSED OUT THE TUMOR */
    if(LSP>(T-DELL) && LAP>(T-DELL))  {
      L=T;
      LSP2=(LSP-T+DELL)*musinv2/musinv;
      LAP2=(LAP-T+DELL)*muainv2/muainv;
      if(LSP2<LAP2){
L+=LSP2;
ABSORBED=FALSE;
      }
      else {
L+=LAP2;
ABSORBED=TRUE;
      }
    }

    /*STILL INSIDE THE TUMOR */
    else  {
      if(LSP<LAP){
L+=LSP;
ABSORBED=FALSE;
```

```
      }
      else{
L+=LAP;
ABSORBED=TRUE;
      }
    }
  }
}

/* END OF INTERSECTION WITH TUMOR */
      }

      /* INSIDE TUMOR */
      else  {
T1=(-B+sqrt(B2));
T2=(-B-sqrt(B2));

/* FIND IF WE INTERSECTED THE TUMOR */
/* I.E EXITED IT */
if((T1>0 && T1<L) || (T2>0 && T2<L))  {

  /* FIND MAXIMUM OF T1, T2*/
  if (T1>T2){
    DELL=T1;
  }
  else{
    DELL=T2;
  }
  L=DELL;
  LSP=(ls-DELL)*musinv/musinv2;
  LAP=(la-DELL)*muainv/muainv2;

  if(LSP<LAP){
    L+=LSP;
    ABSORBED=FALSE;
  }
  else {
    L+=LAP;
    ABSORBED=TRUE;
  }
}
      }
      /*END OF INSIDE TUMOR */
#endif

      /* CALCULATE THE NEW POSITION */
      xold = x;
      yold = y;
      zold = z;
      rold = r;

      x=xold+L*c1;
      y=yold+L*c2;
      z=zold+L*c3;
      r=sqrt(x*x+y*y+z*z);

      /* SCORE THE PHOTON */

      /* INCREMENT THE TIME */
      t+=L/velocity;

      /* SCORE THE PHOTON WITH A RING DETECTOR */
#ifndef SPHERICAL_DETECTOR
      if( z<dz && zold>dz )  {
lm=(zold-dz)/(zold-z)*L;
xm=xold+lm*c1;
ym=yold+lm*c2;
rho=sqrt(xm*xm+ym*ym);
rhoindex=(int)floor(rho/rhostep);
/* tindex = (t+lm/velocity)/tbin;*/
tindex = t/tbin;
DeltaYindex=(int)ceil(DeltaY/DeltaYstep);
if( rhoindex<MAX_RHOBIN && tindex<MAX_TBIN ) {
  fluxout[rhoindex][tindex]+=-1./c3;  /* THE EFFECTIVE WIDTH OF THE
 DETECTOR VARIES WITH THE
 ANGLE OF INCIDENCE.  NORMALIZE
 OUT THIS DEPENDENCE ON ANGLE*/
/*   fluxout[rhoindex][tindex]++;*/
  if( DeltaYindex<MAX_DeltaYBIN )
    DeltaYout[rhoindex][DeltaYindex]++;
}
      }
```

```
#ifdef INFINITE
      if( z>dz && zold<dz )  {
lm=(zold-dz)/(zold-z)*L;
xm=xold+lm*c1;
ym=yold+lm*c2;
rho=sqrt(xm*xm+ym*ym);
rhoindex=(int)floor(rho/rhostep);
/* tindex = (t+lm/velocity)/tbin;*/
tindex = t/tbin;
DeltaYindex=(int)ceil(DeltaY/DeltaYstep);
if( rhoindex<MAX_RHOBIN && tindex<MAX_TBIN ) {
  fluxin[rhoindex][tindex]+=1./c3;  /* THE EFFECTIVE WIDTH OF THE
 DETECTOR VARIES WITH THE
 ANGLE OF INCIDENCE.  NORMALIZE
 OUT THIS DEPENDENCE ON ANGLE*/
/*   fluxin[rhoindex][tindex]++;*/
  if( DeltaYindex<MAX_DeltaYBIN )
    DeltaYin[rhoindex][DeltaYindex]++;
}
      }
#endif
#endif

      /* SCORE THE PHOTON WITH SPHERICAL DETECTORS */
#ifdef SPHERICAL_DETECTOR
      tindex = t/tbin;
      DeltaYindex=(int)ceil(DeltaY/DeltaYstep);
      if( r<rold ) {
rhoindex = (int)ceil(r/rhostep);
while( (float)rhoindex*rhostep<rold ) {
  if( rhoindex<MAX_RHOBIN ) {
    fluxin[rhoindex][tindex]++;
    if( DeltaYindex<MAX_DeltaYBIN )
      DeltaYin[rhoindex][DeltaYindex]++;
  }
  rhoindex++;
}
      }
      if( r>rold ) {
rhoindex = (int)ceil(rold/rhostep);
while( (float)rhoindex*rhostep<r ) {
  if( rhoindex<MAX_RHOBIN ) {
    fluxout[rhoindex][tindex]++;
    if( DeltaYindex<MAX_DeltaYBIN )
      DeltaYout[rhoindex][DeltaYindex]++;
  }
  rhoindex++;
}
      }
#endif


      /* CALCULATE THE NEW SCATTERING ANGLE ASSUMING ISOTROPIC SCATTERING */
      rnm = ran(&idum,&ncall);
      phi=2*pi*rnm;
      cphi=cos(phi);
      sphi=sin(phi);
      rnm = ran(&idum,&ncall);
      theta=acos(1.-2*rnm);
      ctheta=cos(theta);
      stheta=sin(theta);

      /* CALCULATE THE NEW SCATTERING ANGLE USING HENYEY-GREENSTEIN */
/*      phi=2*pi*rnm;
      cphi=cos(phi);
      sphi=sin(phi);
      rnm = ran(&idum,&ncall);
      hgpart1=(1.+(g*g));
      hgpart2=(1.-(g*g));
      hgpart3=(1.-g+(2.*g*rnm));
      hgpart4=hgpart3*hgpart3;
      hgpart5=1/(2.*g);
      hgpart6=(hgpart2)*(hgpart2);
      foo = (hgpart1-(hgpart6/hgpart4))*(hgpart5);
      theta=acos(foo);
      stheta=sin(theta);
      ctheta=cos(theta);*/

      c1o = c1;
      c2o = c2;
      c3o = c3;
```

```
      c1 = stheta*cphi;
      c2 = stheta*sphi;
      c3 = ctheta;

    } /* LOOP UNTIL END OF SINGLE PHOTON */
  } /* LOOP UNTIL ALL PHOTONS EXHAUSTED */



  /* SAVE TIME DOMAIN DATA USING A FORMAT UNDERSTOOD BY PMI */
  for( q=1; q<MAX_RHOBIN; q++ ) {
    rho = rhostep * ((float)q);
    sprintf( filenm, "%s_%05.2f.tdd", argv[11], rho );
    fp=fopen( filenm, "w");
    fprintf( fp, "%d %e 2000\n", nt, tgate );
    fprintf( fp, "0 0 %f %d 0\n",sz, b );
#ifndef SPHERICAL_DETECTOR
    fprintf( fp, "%f 0 %f\n", rho+rhostep/2, dz);
#endif
#ifdef SPHERICAL_DETECTOR
    fprintf( fp, "%f 0 0\n", rho);
#endif
    for( tindex=0; tindex<nt; tindex++ )
#ifndef SPHERICAL_DETECTOR
      fprintf(fp,"%lf\n",2.*(float)(fluxin[q][tindex]+fluxout[q][tindex])/(pi*rhostep*rhostep+2*pi*rhostep*rho));
#endif
#ifdef SPHERICAL_DETECTOR
      fprintf(fp,"%lf\n",2.*(float)(fluxin[q][tindex]+fluxout[q][tindex])/(4.*pi*rho*rho));
#endif
    fclose(fp);
  }

  /* SAVE MOMENTUM TRANSFER DATA */
  for( q=1; q<MAX_RHOBIN; q++ ) {
    rho = rhostep * ((float)q);
    sprintf( filenm, "%s_%05.2f.DelY", argv[11], rho );
    fp=fopen( filenm, "w");
    fprintf( fp, "%d %e %e\n", nDeltaY, DeltaYmax, DeltaYstep );
    fprintf( fp, "0 0 %f %d 0\n",sz, b );
#ifndef SPHERICAL_DETECTOR
    fprintf( fp, "%f 0 %f\n", rho+rhostep/2, dz);
#endif
#ifdef SPHERICAL_DETECTOR
    fprintf( fp, "%f 0 0\n", rho);
#endif
    for( DeltaYindex=0; DeltaYindex<nDeltaY; DeltaYindex++ )
#ifndef SPHERICAL_DETECTOR
      fprintf(fp,"%lf\n",2.*(float)(DeltaYin[q][DeltaYindex]+DeltaYout[q][DeltaYindex])
                         /(pi*rhostep*rhostep+2*pi*rhostep*rho));
#endif
#ifdef SPHERICAL_DETECTOR
      fprintf(fp,"%lf\n",2.*(float)(DeltaYin[q][DeltaYindex]+DeltaYout[q][DeltaYindex])/(4.*pi*rho*rho));
#endif
    fclose(fp);
  }

}
```

C.2 ran.c

I use a combination of two random number generators from Numerical Recipes in C [149]. This particular routine was strongly suggested by Dr. Murray Penney at GE-CRD in Schenectady, NY. Dr. Penney has thoroughly tested the randomness of this routine.

```
#include <stdio.h>
#include <math.h>
```

```
static long idum2;

float ran( int *idum, int *ncall )
{
  float rn;
  float ran3( int *idum );
  float ran2( long *idum2 );

  *ncall = *ncall + 1;
  if( *ncall==1 ) idum2 = *idum*0.79;
  if( fmod(*ncall,1e6)==0 )  *idum=-1111-99999*ran2(&idum2);
  rn = ran3(idum);

  if( rn<1e-4 )  rn=1.e-4*ran3(idum);
  if( rn==0 )  rn=1e-12;

  return rn;
}
```

C.3 ran2.c

This routine is from Numerical Recipes in C [149].

```
#include <math.h>

#define M 714025
#define IA 1366
#define IC 150889

float ran2(idum)
long *idum;
{
static long iy,ir[98];
static int iff=0;
int j;
void nrerror();

if (*idum < 0 || iff == 0) {
iff=1;
if ((*idum=(IC-(*idum)) % M) < 0) *idum = -(*idum);
for (j=1;j<=97;j++) {
*idum=(IA*(*idum)+IC) % M;
ir[j]=(*idum);
}
*idum=(IA*(*idum)+IC) % M;
iy=(*idum);
}
j=1 + 97.0*iy/M;
if (j > 97 || j < 1) nrerror("RAN2: This cannot happen.");
iy=ir[j];
*idum=(IA*(*idum)+IC) % M;
ir[j]=(*idum);
return (float) iy/M;
}

#undef M
#undef IA
#undef IC
```

C.4 ran3.c

This routine is from Numerical Recipes in C [149].

```
#define MBIG 1000000000
#define MSEED 161803398
#define MZ 0
#define FAC (1.0/MBIG)
```

```
float ran3(idum)
int *idum;
{
static int inext,inextp;
static long ma[56];
static int iff=0;
long mj,mk;
int i,ii,k;

if (*idum < 0 || iff == 0) {
iff=1;
mj=MSEED-(*idum < 0 ? -*idum : *idum);
mj %= MBIG;
ma[55]=mj;
mk=1;
for (i=1;i<=54;i++) {
ii=(21*i) % 55;
ma[ii]=mk;
mk=mj-mk;
if (mk < MZ) mk += MBIG;
mj=ma[ii];
}
for (k=1;k<=4;k++)
for (i=1;i<=55;i++) {
ma[i] -= ma[1+(i+30) % 55];
if (ma[i] < MZ) ma[i] += MBIG;
}
inext=0;
inextp=31;
*idum=1;
}
if (++inext == 56) inext=1;
if (++inextp == 56) inextp=1;
mj=ma[inext]-ma[inextp];
if (mj < MZ) mj += MBIG;
ma[inext]=mj;
return mj*FAC;
}

#undef MBIG
#undef MSEED
#undef MZ
#undef FAC
```

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