Biomedical Optics VI

Diffusion equation

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Approximations

- The transport equation is difficult to solve analytically. In order to find an analytical solution we need to simplify the problem:
- Discretisation methods $N(\mathrm{r},\mathrm{s},t) = \sum_i N(\mathrm{r},\mathrm{s}_i,t)$
  - discrete ordinates method
  - 2-flux method or Kubelka-Munk theory
  - Adding-double method
- Expansion methods
  - Diffusion theory
- Probabilistic methods
  - Monte Carlo simulations

The P_N - approximation

- A formal method of solving a differential equation is to find a solution to its homogenous part and expand the general solution in terms of the homogenous solution obtained.
- Another approach would be to expand the radiance or photon distribution function in well-known appropriate function series. This is performed in the diffusion approximation.

$$N(\mathrm{r},\mathrm{s},t) = N(\mathrm{r},t)\sum a_i(\mathrm{r},t)\Psi_i(\mathrm{s})$$

Diffusion approximation

- One of the most useful approaches for tissue light interaction is the diffusion approximation, as it can be solved analytically for simple geometries. The diffusion approximation has been used extensively in photon propagation modeling in tissue in the time domain, as well as in the frequency domain and in the steady state.

Diffusion approximation

- The basic idea behind the diffusion approximation is to expand the functions in the transport equation into spherical harmonics, and to use only the lowest order in the expansion. Thus the position and directional variables can be separated into new functions. Expanding the distribution function N(r,s,t) yields:

$$N(\mathrm{r},\mathrm{s},t) = \sum_{l=0}^{\infty}\sum_{m=-l}^{+l}\sqrt{\frac{2l+1}{4\pi}}N_{lm}(\mathrm{r},t)Y_{lm}$$

Spherical harmonics

- The spherical harmonics are the angular portion of the solution to Laplace's equation in spherical coordinates where azimuthal symmetry is not present.
- Spherical harmonics constitute a complete set of expansions of wave functions. Frequently used in quantum mechanics since they are eigenfunctions to the angular momentum operators in central force problems.

Spherical harmonics

- The spherical harmonics form an orthogornal set , since

$$\int_0^{2\pi}\int_0^{\pi}(Y_l^m(\theta,\varphi))^* Y_{l'}^{m'}(\theta,\varphi)\sin\theta d\theta d\varphi = \delta_{l,l'}\delta_{m,m'}$$

Spherical harmonics

- Definition

$$Y_l^m(\theta,\varphi) = \sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}}(-1)^m e^{im\varphi}P_l^m(\cos\theta)$$

where

$$P_l^m(\zeta) = \frac{(1-\zeta)^{m/2}}{2^l\cdot l!}\frac{d^{l+m}}{d\zeta^{l+m}}(\zeta^2-1)^l; m \le l$$

are the associated Legendre polynomials

Spherical harmonics

- The first few spherical harmonics are:

$$Y_0^0 = \frac{1}{\sqrt{4\pi}}$$

$$Y_1^0 = \sqrt{\frac{3}{4\pi}}\cos\theta$$

$$Y_1^{\pm 1} = \pm\sqrt{\frac{3}{8\pi}}e^{\pm i\varphi}\sin\theta$$

The P_1-approximation

- Truncating the expansion after the terms would yield

$$N(\mathrm{r},\mathrm{s},t) = \sqrt{\frac{1}{4\pi}}L_{00}(\mathrm{r},t)Y_{00}(\mathrm{s}) + \sqrt{\frac{3}{4\pi}}\sum_{m=-1}^{1}L_{lm}(\mathrm{r},t)Y_{lm}(\mathrm{s})$$

- This expression could now be inserted into the transport equation, which after integration over s would give four equations and four unknowns.

The vector approach

- Another approach is to observe that Y_{00} is a scalar and that Y_{1m} (m=0, ±1) represent the three components of a vector. The expression for the photon distribution function N thus can be substituted by

$$N(\mathbf{r},\mathbf{s},t) = A(\mathbf{r},t) + \mathbf{B}(\mathbf{r},t)\cdot\mathbf{s}$$

- where A is the isotropic distribution and **B** the linear gradient of the photon distribution function, respectively, and **s** the vector of the gradient.

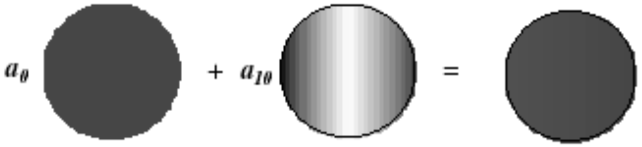
Arbitrary point in space

- An arbitrary point in space can be expressed as coordinate values for a defined set of base vectors. $\mathbf{r} = x\hat{\mathbf{x}} + y\hat{\mathbf{y}} + z\hat{\mathbf{z}}$
- To have a unique set of coordinates for each point the base vectors need to be orthogonal, i.e. etc. $\hat{\mathbf{x}}\cdot\hat{\mathbf{y}} = 0$
- For a multidimensional function the base vectors need to be function, but the principle of expansion is otherwise identical

Diffusion: schematically

$$N = a_0 Y_0^0 + \sum_{m=-1}^{1} a_{1m} Y_1^m = A + \mathbf{B} \cdot \mathbf{s}$$

Assume for the illustration that $A = 1$, $B_x = 0.1$, $B_y = B_z = 0$



Y_0^0 $\quad$ Y_1^0

Photon density function ρ(r,t)

- To determine A, this expression is integrated over ω:

$$\rho(\mathbf{r},t) = \int N(\mathbf{r},\mathbf{s},t)\,d\Omega = \int (A + \mathbf{s}\cdot\mathbf{B})\,d\Omega$$

where ρ(r,t) is the photon density. The last term on the right-hand-side is equal to zero. This yields the expression for A:

$$A = \frac{1}{4\pi}\rho(\mathbf{r},t)$$

Photon current density

- To determine B, the expression is first multiplied by s and then integrated over ω:

$$\int \mathbf{s}N(\mathbf{r},\mathbf{s},t)\,d\Omega = \int \mathbf{s}(A + \mathbf{s}\cdot\mathbf{B})\,d\Omega$$

- The left-hand-side is the definition of the photon current density divided by the velocity of light. The first term on the right-hand-side is equal to zero. This yields the expression for B:

$$\mathbf{B} = \frac{3}{4\pi c}\mathbf{J}(\mathbf{r},t)$$

Diffusion approximation

- Putting the expressions for A and B together yields the angular expansion of N.

$$N(\mathbf{r},\mathbf{s},t) = \frac{1}{4\pi}\left[\rho(\mathbf{r},t) + \frac{3}{c}\mathbf{J}(\mathbf{r},t)\cdot\mathbf{s}\right]$$

- In a similar way the source function can be expanded and written as.

$$\mathbf{q}(\mathbf{r},\mathbf{s},t) = \frac{1}{4\pi}\left[\mathbf{q}_0(\mathbf{r},t) + 3\mathbf{q}_1(\mathbf{r},t)\cdot\mathbf{s}\right]$$

Insertion in transport equation

$$\frac{\partial}{\partial t}\left[\rho + \frac{3}{c}\mathbf{J}\cdot\mathbf{s}\right] = -c\,\mathbf{s}\nabla\left[\rho + \frac{3}{c}\mathbf{J}\cdot\mathbf{s}\right] - c\mu_t(\mathbf{r})\left[\rho + \frac{3}{c}\mathbf{J}\cdot\mathbf{s}\right] +$$

$$c\mu_t(\mathbf{r})\int_{4\pi} p(\mathbf{s}\cdot\mathbf{s}')\left[\rho + \frac{3}{c}\mathbf{J}\cdot\mathbf{s}'\right]d\Omega' + \mathbf{q}_0 + 3\mathbf{q}_1\cdot\mathbf{s}$$

$$\int_{4\pi} p(\mathbf{s}\cdot\mathbf{s}')d\Omega' = 1 \text{ and } g = \frac{\int_{4\pi} p(\mathbf{s}\cdot\mathbf{s}')(\mathbf{s}\cdot\mathbf{s}')d\Omega'}{\int_{4\pi} p(\mathbf{s}\cdot\mathbf{s}')d\Omega'}$$

Rearrangements yields

$$\frac{\partial\rho}{\partial t} + \frac{3}{c}\frac{\partial\mathbf{J}\cdot\mathbf{s}}{\partial t} = -c(-\mathbf{s}\nabla - \mu_t + \mu_s)\rho + 3(-\mathbf{s}\cdot\nabla - \mu_t + g\mu_s)\mathbf{J}\cdot\mathbf{s} + \mathbf{q}_0 + 3\mathbf{q}_1\cdot\mathbf{s}$$

$$\mu_{tr} = (1-g)\mu_s + \mu_a = \mu_s' + \mu_a$$

$$\frac{1}{c}\left[\frac{\partial\rho}{\partial t} + \frac{3}{c}\frac{\partial\mathbf{J}\cdot\mathbf{s}}{\partial t}\right] = (-\mathbf{s}\nabla - \mu_a)\rho + \frac{3}{c}(-\mathbf{s}\cdot\nabla - \mu_{tr})\mathbf{J}\cdot\mathbf{s} + \frac{1}{c}\mathbf{q}_0 + \frac{3}{c}\mathbf{q}_1\cdot\mathbf{s}$$

Mathematical simplification I

- Now, if this expression is integrated over Ω and use

  $$\int(\mathbf{s}\cdot\mathbf{A})d\Omega = 0 \qquad \int(\mathbf{s}\cdot\mathbf{A})(\mathbf{s}\cdot\mathbf{B})d\Omega = \frac{4\pi}{3}\mathbf{A}\cdot\mathbf{B}$$

  $$\frac{1}{c}\frac{\partial\rho}{\partial t} = -\mu_a\rho - \frac{1}{c}\nabla\mathbf{J} + \frac{1}{c}\mathbf{q}_0$$

- If the equation instead first is multiplied by **s** and then integrated over Ω using

Mathematical simplification II

- Here we make some approximations. Assuming that we have an isotropic source, i.e. $q_1=0$, at steady-state, we obtain Fick's law from this equation:

$$\int\mathbf{s}(\mathbf{s}\cdot\mathbf{A})d\Omega = \frac{4\pi}{3}\mathbf{A}$$

$$\frac{1}{c^2}\frac{\partial\mathbf{J}}{\partial t} = -\frac{1}{3}\nabla\rho - \frac{\mu_{tr}}{c}\mathbf{J} + \frac{1}{c}\mathbf{q}_1$$

$$\mathbf{J} = -cD\nabla\rho$$

The diffusion coefficient

- Here we introduce an important definition, the diffusion coefficient:

$$D = \frac{1}{3\mu_{tr}} = \frac{1}{3(\mu_a + (1-g)\mu_s)}$$

- Putting Fick's law into Eq. (1) we arrive at the final expression, the diffusion equation:

$$\frac{1}{c}\frac{\partial p}{\partial t} - \nabla D \nabla \rho + \mu_a \rho = \frac{1}{c}\mathbf{q}_0$$

The Diffusion Equation!

- By assuming a homogenous medium, that means that the diffusion coefficient D is constant and using the relation that the fluence rate is related to the photon density by:

$$\Phi(\mathbf{r},t) = ch\nu\rho(\mathbf{r},t)$$

- one arrives in the diffusion equation as it is usually presented in the field of biomedical optics:

$$\frac{1}{c}\frac{\partial}{\partial t}\Phi(\mathbf{r},t) - D\nabla^2\Phi(\mathbf{r},t) + \mu_a\Phi(\mathbf{r},t) = S(\mathbf{r},t)$$

Diffusion approximation validity

- The diffusion equation is valid only if the propagating light is diffuse and this implies that the reduced scattering coefficient is much larger than the absorption, i.e. $(1-g)\mu_s >> \mu_a$. The source and detector must also be separated in space and time to allow that the light is diffuse when it reaches the detector.

Point source solution

- The solution to the diffusion equation for an infinite homogenous slab with a short pulse isotropic point source is $S(\mathbf{r},t) = \delta(0,0)$

$$\Phi(\mathbf{r},t) = c(4\pi Dct)^{-3/2}\exp(-\frac{\mathrm{r}^2}{4Dct} - \mu_a ct)$$