

## Direction Cosines and Polarization Vectors for Monte Carlo Photon Scattering

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**Abstract**—*New ways to calculate the direction cosines and polarization vectors for Monte Carlo photon scattering are developed and presented. The new approach for direction cosines is more physical, easier to understand, straightforward to implement, and—for simulations involving polarized photons—slightly faster than the traditional approach. The polarization vector after scatter is also presented.*

### I. TRADITIONAL METHOD FOR DIRECTION COSINES

Carter and Cashwell<sup>1</sup> presented a scheme, which is used in many Monte Carlo codes, for finding the direction cosines of a photon after a scatter. For a photon with unit direction vector  $\mathbf{\Omega} = \langle u, v, w \rangle$  that is then scattered with polar angle  $\theta$  and azimuthal angle  $\phi$ , the scattered direction vector is

$$\mathbf{\Omega}' = \begin{bmatrix} u' \\ v' \\ w' \end{bmatrix} = \begin{cases} \begin{bmatrix} \sqrt{1 - \mu^2} \cos \phi \\ \sqrt{1 - \mu^2} \sin \phi \\ \frac{\mu w}{|w|} \end{bmatrix} & \text{if } |w| \sim 1 \\ \begin{bmatrix} u\mu + (uw \cos \phi - v \sin \phi) \frac{\sqrt{1 - \mu^2}}{\sqrt{1 - w^2}} \\ v\mu + (vw \cos \phi + u \sin \phi) \frac{\sqrt{1 - \mu^2}}{\sqrt{1 - w^2}} \\ w\mu - \cos \phi \sqrt{1 - \mu^2} \sqrt{1 - w^2} \end{bmatrix} & \text{otherwise,} \end{cases} \quad (1)$$

using  $\mu = \cos \theta$  and  $\sqrt{1 - \mu^2} = \sin \theta$ . These relationships come from a transformation of coordinates so that the original photon direction is on the  $z$  axis, scattering with angles  $\theta$  and  $\phi$ , and then the coordinates are transformed back to the laboratory frame. These expressions were originally derived from rotations through angles expressed as complex numbers by Cashwell and Everett.<sup>2</sup>

The same result can be found without a coordinate transformation. The direction  $\phi = 0$  is defined to be a unit vector lying on the plane perpendicular to  $\mathbf{\Omega}$  and also lying in a plane that contains the projection of  $\mathbf{\Omega}$  on the  $x$ - $y$  plane, pointing downward. This vector in the  $\phi = 0$  direction,  $\mathbf{q}_1$ , is then  $1/\sqrt{1 - w^2} \langle uw, vw, w^2 - 1 \rangle$ . To define the direction of increasing  $\phi$ , the direction of  $\phi = \pi/2$ ,  $\mathbf{q}_2$ , can be chosen such that  $\mathbf{q}_2 = \mathbf{\Omega} \times \mathbf{q}_1$ . This gives

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$\mathbf{q}_2 = 1/\sqrt{1-w^2} \langle -v, u, 0 \rangle$  and completely defines  $\phi$  for the original photon  $\mathbf{\Omega}$ . This is shown in Fig. 1. For the special case of  $|w| \sim 1$ ,  $\mathbf{q}_1$  can be defined as  $\langle 1, 0, 0 \rangle$  and  $\mathbf{q}_2$  as  $\langle 0, 1, 0 \rangle$ .

From the foregoing definitions, the new direction  $\mathbf{\Omega}'$  can be expressed as a linear combination of the three orthogonal vectors  $\mathbf{\Omega}$ ,  $\mathbf{q}_1$ , and  $\mathbf{q}_2$ :

$$\mathbf{\Omega}' = \mathbf{\Omega} \cos \theta + \mathbf{q}_1 \cos \phi \sin \theta + \mathbf{q}_2 \sin \phi \sin \theta . \tag{2}$$

By inserting the components of  $\mathbf{q}_1$ ,  $\mathbf{q}_2$ , and  $\mathbf{\Omega}$ , the scattered vector is found to be

$$\mathbf{\Omega}' = \begin{bmatrix} u' \\ v' \\ w' \end{bmatrix} = \begin{bmatrix} u \cos \theta + \cos \phi \sin \theta \frac{uw}{\sqrt{1-w^2}} + \sin \phi \sin \theta \frac{-v}{\sqrt{1-w^2}} \\ v \cos \theta + \cos \phi \sin \theta \frac{vw}{\sqrt{1-w^2}} + \sin \phi \sin \theta \frac{u}{\sqrt{1-w^2}} \\ w \cos \theta + \cos \phi \sin \theta \frac{w^2-1}{\sqrt{1-w^2}} + \sin \phi \sin \theta \frac{0}{\sqrt{1-w^2}} \end{bmatrix} \tag{3}$$

$$= \begin{bmatrix} u\mu + (uw \cos \phi - v \sin \phi) \frac{\sqrt{1-\mu^2}}{\sqrt{1-w^2}} \\ v\mu + (vw \cos \phi + u \sin \phi) \frac{\sqrt{1-\mu^2}}{\sqrt{1-w^2}} \\ w\mu - \cos \phi \sqrt{1-\mu^2} \sqrt{1-w^2} \end{bmatrix} , \tag{4}$$

which is a result identical to that of Carter and Cashwell. Using the components of the special case for  $\mathbf{q}_1$  and  $\mathbf{q}_2$  and taking  $\mathbf{\Omega} \sim \langle 0, 0, \pm 1 \rangle$  will then give the special case of Carter and Cashwell.

For some routines (for example, biasing routines), the initial and scattered photon directions are known, and the two scatter angles  $\theta$  and  $\phi$  need to be found. This can be done with

$$\mu = \mathbf{\Omega} \cdot \mathbf{\Omega}' = uu' + vv' + ww' , \tag{5}$$

$$\cos \phi = \frac{\mathbf{q}_1 \cdot \mathbf{\Omega}'}{\sqrt{1-\mu^2}} = \frac{1}{\sqrt{1-\mu^2} \sqrt{1-w^2}} \times (uwu' + vvv' + w'(w^2-1)) , \tag{6}$$

and

$$\sin \phi = \frac{\mathbf{q}_2 \cdot \mathbf{\Omega}'}{\sqrt{1-\mu^2}} = \frac{1}{\sqrt{1-\mu^2} \sqrt{1-w^2}} \times (uv' - vu') , \tag{7}$$

being careful of the special cases of  $\mu = \pm 1$  and  $w = \pm 1$ . Two equations are needed for  $\phi$  so that it may be specified over the entire range of  $[-\pi, \pi]$ . In ForTran, the dual argument arctangent function  $\phi = \text{atan } 2[uv' - vu', uwu' + vvv' + w'(w^2-1)]$  will report  $\phi$  over the whole range.

### II. A SIMPLIFIED APPROACH

The Carter and Cashwell approach to finding the new direction cosines works but is unnecessarily difficult to

comprehend physically and is somewhat arbitrary in its definition of the azimuthal angle. Coordinate transformations or arbitrarily defining the  $\phi = 0$  direction based on the laboratory coordinate system are not easy to understand, and they break down for some initial directions ( $w = \pm 1$ ), which forces the programmer to set up special cases.

When the Carter and Cashwell technique is applied to polarized radiation, extra complications arise in

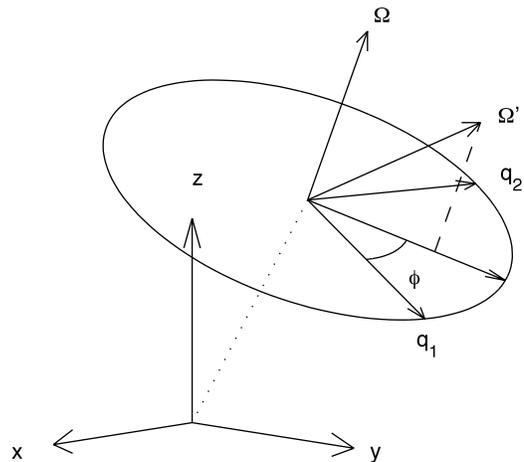


Fig. 1. Geometry of a scatter from direction  $\mathbf{\Omega}$  to  $\mathbf{\Omega}'$  similar to the Carter and Cashwell approach. The azimuthal angle is in the plane perpendicular to the  $\mathbf{\Omega}$  direction, which is shown here by the circle.

calculating the scattered azimuthal angle. Another rotation is required to find where the polarization vector is located in relation to the  $\phi = 0$  direction. The scatter angle is then added to that angle.

An alternate approach is to recognize that a photon traveling in direction  $\Omega$  with an electric field vector  $\mathbf{p}$  (normal to  $\Omega$ ) is really carrying around its own coordinate system. With the definition of the third vector  $\mathbf{t} = \Omega \times \mathbf{p}$ , an orthogonal system of base vectors is complete. The scattered vector  $\Omega'$  can then be written in terms of these base vectors, the polar scatter angle  $\theta$ , and the azimuthal angle  $\phi$ , measured in the plane perpendicular to  $\Omega$ . This gives

$$\Omega' = \Omega \cos \theta + \mathbf{p} \cos \phi \sin \theta + \mathbf{t} \sin \phi \sin \theta . \quad (8)$$

Note that the  $\phi = 0$  direction is aligned with  $\mathbf{p}$  and  $\phi$  increases toward  $\mathbf{t}$ . This is quite convenient since differential scattering cross sections are given in terms of  $\phi$  measured from the direction of the polarization vector. This is illustrated in Fig. 2.

Using the notation  $\Omega = \langle u, v, w \rangle$  and  $\mathbf{p} = \langle p_u, p_v, p_w \rangle$ ,  $\mathbf{t}$  is easily found to be  $\langle vp_w - wp_v, wp_u - up_w, up_v - vp_u \rangle$ , and the scattered direction cosines can be written as

$$\Omega' = \begin{bmatrix} u' \\ v' \\ w' \end{bmatrix} = \begin{bmatrix} u \cos \theta + p_u \cos \phi \sin \theta + (vp_w - wp_v) \sin \phi \sin \theta \\ v \cos \theta + p_v \cos \phi \sin \theta + (wp_u - up_w) \sin \phi \sin \theta \\ w \cos \theta + p_w \cos \phi \sin \theta + (up_v - vp_u) \sin \phi \sin \theta \end{bmatrix} \quad (9)$$

$$= \begin{bmatrix} u\mu + (p_u \cos \phi + (vp_w - wp_v) \sin \phi) \sqrt{1 - \mu^2} \\ v\mu + (p_v \cos \phi + (wp_u - up_w) \sin \phi) \sqrt{1 - \mu^2} \\ w\mu + (p_w \cos \phi + (up_v - vp_u) \sin \phi) \sqrt{1 - \mu^2} \end{bmatrix} . \quad (10)$$

Comparing Eqs. (1) and (10), one sees that this photon-coordinate approach has a few more operations but does not contain the "if" logic for the special case. The new approach also has one less square root. When each method was coded in ForTran 77 on a Sun Ultra 2 computer for a polarized photon-slab penetration problem, the new approach was faster than the Carter and Cashwell method by 6%. Of course, in a large code, this small difference probably will not be noticed. Speed is not the attraction of this new approach; its simplicity is.

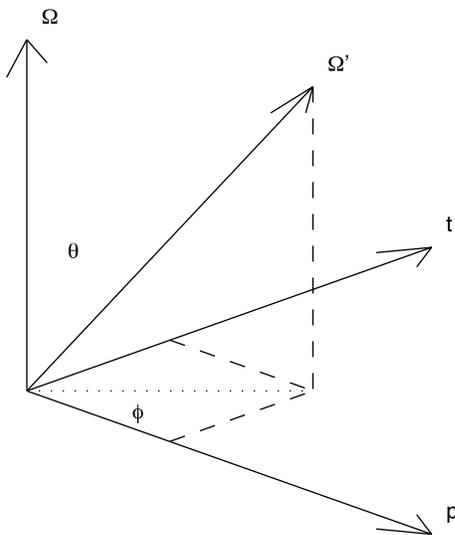


Fig. 2. Geometry of a scatter from direction  $\Omega$  to  $\Omega'$  using the photon-coordinate approach. The azimuthal angle is in the plane perpendicular to the  $\Omega$  direction.

Given the original photon vector  $\Omega$  and the scattered photon vector  $\Omega'$ , the angles of scatter can be found by the dot product of each component ( $\Omega, \mathbf{p}, \mathbf{t}$ ) with the scattered photon vector giving

$$\cos \theta = \Omega \cdot \Omega' , \quad (11)$$

$$\cos \phi = \frac{\mathbf{p} \cdot \Omega'}{\sqrt{1 - \mu^2}} , \quad (12)$$

and

$$\sin \phi = \frac{\mathbf{t} \cdot \Omega'}{\sqrt{1 - \mu^2}} . \quad (13)$$

The only special case here is when  $\mu = \pm 1$ , where  $\phi$  can be set to 0. In ForTran, again using the dual argument arctangent function,  $\phi$  can be found over the entire range of  $[-\pi, \pi]$  with  $\phi = \text{atan} 2[\mathbf{t} \cdot \Omega', \mathbf{p} \cdot \Omega']$ .

### III. POLARIZATION

If the polarization of the photon is being considered, the new electric field vector  $\mathbf{p}'$  of the scattered photon must be found. Namito, Ban, and Hirayama<sup>3</sup> and Vincze et al.<sup>4</sup> state that  $\mathbf{p}'$  lies in the plane defined by the electric field vector of the original photon  $\mathbf{p}$  and the scattered photon direction  $\Omega'$ . Of course, the new polarization vector  $\mathbf{p}'$  must also be perpendicular to  $\Omega'$ . Since these three vectors are all in one plane, the third can be expressed as a combination of the first two:

$$\mathbf{p} = \mathbf{p}'(\mathbf{p} \cdot \mathbf{p}') + \Omega'(\mathbf{p} \cdot \Omega') . \quad (14)$$

Since everything is in a plane, these are all unit vectors, and  $\mathbf{p}' \perp \boldsymbol{\Omega}'$ , then  $(\mathbf{p} \cdot \mathbf{p}')^2 + (\mathbf{p} \cdot \boldsymbol{\Omega}')^2 = 1$ . Inserting this and solving for  $\mathbf{p}'$  gives

$$\mathbf{p} = \mathbf{p}' \sqrt{1 - (\mathbf{p} \cdot \boldsymbol{\Omega}')^2} + \boldsymbol{\Omega}' (\mathbf{p} \cdot \boldsymbol{\Omega}') \quad (15)$$

$$\mathbf{p}' = \frac{\mathbf{p} - \boldsymbol{\Omega}' (\mathbf{p} \cdot \boldsymbol{\Omega}')}{\sqrt{1 - (\mathbf{p} \cdot \boldsymbol{\Omega}')^2}} \quad (16)$$

Both Namito, Ban, and Hirayama<sup>3</sup> and Vincze et al.<sup>4</sup> describe in words where the polarization vector is located after scatter but neither state the direction mathematically, as is done here.

A coherent scatter maintains the polarization of the photon. An incoherent scatter does not, with a depolarization probability of<sup>3</sup>

$$(1 - P) = \frac{E'/E + E/E' - 2}{E'/E + E/E' - 2 \sin^2 \theta \cos^2 \phi} \quad (17)$$

where  $E$  is the original photon energy and  $E/E' = 1 + (E/mc^2)(1 - \cos \theta)$ . Namito, Ban, and Hirayama<sup>3</sup> state that when a photon is depolarized, the direction of the polarization vector should be sampled from either  $\mathbf{p}'$  or  $\boldsymbol{\Omega}' \times \mathbf{p}'$  (which is equal to  $\boldsymbol{\Omega}' \times \mathbf{p}' / \sqrt{1 - (\mathbf{p} \cdot \boldsymbol{\Omega}')^2}$ ).

Note that the new electric field direction becomes undefined when  $\mathbf{p} \parallel \boldsymbol{\Omega}'$ . This is not a problem since the coherent scatter cross section is zero for scatter in those directions ( $\theta = \pi/2$  and  $\phi = 0$  or  $\pi$ ). The incoherent cross section for scatter in these directions is not zero, but the depolarization probability is one. The new electric field vector direction can be picked as any direction perpendicular to  $\boldsymbol{\Omega}'$ .

So, for coherent scatter, the new electric field direction is

$$\mathbf{p}' = \frac{\mathbf{p} - \boldsymbol{\Omega}' (\mathbf{p} \cdot \boldsymbol{\Omega}')}{\sqrt{1 - (\mathbf{p} \cdot \boldsymbol{\Omega}')^2}} \quad (18)$$

For incoherent scatter, a determination by a random variable for depolarization is made first. If the photon will be depolarized, another random number  $\xi$  is picked. Then,

$$\mathbf{p}' = \begin{cases} \text{any unit vector } \perp \boldsymbol{\Omega}' & \text{if } \mathbf{p} \parallel \boldsymbol{\Omega}' \\ \frac{\mathbf{p} - \boldsymbol{\Omega}' (\mathbf{p} \cdot \boldsymbol{\Omega}')}{\sqrt{1 - (\mathbf{p} \cdot \boldsymbol{\Omega}')^2}} & \text{not depolarized or } \xi > 0.5 \\ \frac{\boldsymbol{\Omega}' \times \mathbf{p}}{\sqrt{1 - (\mathbf{p} \cdot \boldsymbol{\Omega}')^2}} & \text{depolarized and } \xi \leq 0.5 \end{cases} \quad (19)$$

#### IV. UNPOLARIZED PHOTONS

This new approach can also be used in problems involving unpolarized photons. Since there is no electric field vector  $\mathbf{p}$ , one has to be picked before the scatter. Any vector perpendicular to  $\boldsymbol{\Omega}$  will suffice;  $\mathbf{p} =$

$1/\sqrt{1-w^2} \langle -v, u, 0 \rangle$  is a simple choice. Of course, one has to check for  $|w| \sim 1$  and put in some "if" logic to avoid a division by zero. If this is the case,  $\mathbf{p}$  can be defined as  $\langle 1, 0, 0 \rangle$ .

Now the new method has the problem of the special case, just like the original Carter and Cashwell approach. With a few more operations of Eq. (10) over Eq. (1), combined with the time of finding a new polarization vector, the photon-coordinate approach takes  $\sim 8\%$  more time than the Carter and Cashwell approach. However, in a large code, this slight time difference is likely to be insignificant.

This new approach is still easy to understand and has a physical basis: If the radiation is unpolarized, then the electric field vector should be a random direction perpendicular to  $\boldsymbol{\Omega}$  at any given time. Since unpolarized photon scattering cross sections are uniform in  $\phi$ , the direction of  $\phi = 0$  is not really important, as shown by the Carter and Cashwell approach. As long as  $\phi$  can be sampled over the entire  $2\pi$  range for any given direction  $\boldsymbol{\Omega}$ , the approach is consistent, and the results will be correct.

The best way to incorporate this new approach for unpolarized radiation may be to pick a random polarization direction ( $\perp \boldsymbol{\Omega}$ ) after picking the source photon. This  $\mathbf{p}$  vector would be updated after each scatter, never bothering to pick whether or not to depolarize. Any code developed with this system for unpolarized radiation would be very easy to upgrade to handle polarized radiation.

#### V. SUMMARY

This note has done three things. First, a simplified derivation of the Carter and Cashwell formulas for direction cosines showed how arbitrary the approach is. Second, a new approach for direction cosines, which uses the polarization vector and the original direction vector as the base of a coordinate system, was developed and presented. Finally, concise mathematical formulas were presented for calculating the polarization vector after a scatter.

Compared to the transformation of coordinate systems that is used by most Monte Carlo programmers, this new approach for direction cosines is easy to understand, easy to implement, and works very naturally with the angular differential cross sections for polarized photon scattering. For codes that simulate polarized radiation, this new approach offers a small speedup.

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#### REFERENCES

1. L. L. CARTER and E. D. CASHWELL, "Particle-Transport Simulation with the Monte Carlo Method," Technical Information Center, Office of Public Affairs, U.S. Energy Research and Development Administration (1975).
2. E. D. CASHWELL and C. J. EVERETT, *A Practical Manual on the Monte Carlo Method for Random Walk Problems*, p. 103, Pergamon Press, New York (1959).
3. Y. NAMITO, S. BAN, and H. HIRAYAMA, "Implementation of Linearly-Polarized Photon Scattering Into the EGS4 Code," *Nucl. Instrum. Methods A*, **332**, 277 (1993).
4. L. VINCZE, K. JANSSENS, F. ADAMS, M. L. RIVERS, and K. W. JONES, "A General Monte Carlo Simulation of ED-XRF Spectrometers—II. Polarized Monochromatic Radiation, Homogeneous Samples," *Spectrochi. Acta, Part B*, **50**, 127 (1995).