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Comparison of Quadrature Schemes in DOM for Anisotropic Scattering Radiative Transfer Analysis

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Running Head: DOM Quadrature for Anisotropic Scattering

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Abstract

The commonly implemented level-symmetric $S_N$ quadrature set for the discrete-ordinates method suffers from a limitation in discrete direction number to avoid physically unrealistic weighting factors. This limitation can have an adverse impact for determining radiative transfer, as directional discretization results in angular false scattering errors due to distortion of scattering phase-function in addition to ray effect. To combat this limitation, several higher-order quadrature schemes with no directional limitation were developed. Here four higher-order quadrature sets (Legendre-Equal Weight, Legendre-Chebyshev, Triangle Tessellation, and Spherical Ring Approximation) are implemented for determination of radiative transfer in a 3-D cubic enclosure containing participating media. Heat fluxes obtained at low direction number are compared to the $S_N$ quadrature and Monte Carlo predictions to gauge and compare quadrature accuracy. Investigation into the reduction/elimination of angular false scattering with increase in direction number, including heat flux accuracy with respect to Monte Carlo and computational efficiency, is presented. It is found that while the higher-order quadrature sets are able to effectively minimize angular false scattering, the amount of directions required is extremely large, and thus it is more computationally efficient to implement proper phase-function normalization to obtain accurate results.
Nomenclature

$$A^{ll}$$ Normalization coefficients
$$g$$ Asymmetry factor
$$I$$ Radiative intensity ($$W/m^2sr$$)
$$M$$ Total number of discrete directions
$$r$$ Position vector
$$s$$ Unit direction vector
$$w$$ Discrete direction weight

Greek Symbols

$$\sigma_a$$ Absorption coefficient ($$m^{-1}$$)
$$\sigma_s$$ Scattering coefficient ($$m^{-1}$$)
$$\mu, \eta, \xi$$ Direction cosines
$$\Phi$$ Scattering phase-function
$$\Phi$$ Normalized scattering phase-function
$$\phi$$ Radiation direction azimuthal angle ($$^\circ$$)
$$\Theta$$ Scattering angle ($$^\circ$$)
$$\theta$$ Radiation direction polar angle ($$^\circ$$)
$$\omega$$ Scattering albedo, = $$\sigma_s/(\sigma_a + \sigma_s)$$

Subscripts

$$b$$ Blackbody
$$HG$$ Heneyy-Greenstein
$$N$$ DOM Quadrature index

Superscripts

$$'$$ Radiation incident direction
$$l, l'$$ Radiation directions
$$l'l'$$ From direction $$l'$$ into direction $$l$$

Introduction

The Discrete-Ordinates Method (DOM) [1-3] is a commonly implemented approximate method for determining radiative transfer, achieved by numerically solving the Equation of Radiative Transfer (ERT). For processes where radiation is the dominant mode of heat transfer, such as high-temperature
combustion and material processing [4-7] or biomedical therapeutic applications involving ultrafast interaction of laser light with biological tissue [8-12], complete and precise solutions of the ERT are required for accurate radiative transfer modeling. Analytic solution of the ERT is extremely difficult for practical applications where light scattering exists, and thus accurate yet efficient numerical solutions of the ERT are desired.

The DOM was first proposed by Chandrasekhar [1] for atmospheric and astrophysical radiation, then applied to solving the neutron-transport equation, and later extended for use in radiative heat transfer. Works by Fiveland [13,14] and Truelove [15] used the DOM to determine steady-state radiative transfer in 2-D and 3-D enclosures containing participating media. Later, Guo and Kumar expanded the DOM for use in solving the transient ERT [16,17] in order to accurately determine ultrafast radiative transfer in participating media. Further works by Guo and co-authors used the transient DOM (TDOM) to accurately model short-pulsed irradiation of turbid media [11,12], laser-tissue welding and soldering [10], and pulse train irradiation using Duhamel’s superposition theorem [5,18].

In the DOM, the continuous angular variation is approximated using a finite set of discrete radiation directions with corresponding directional weighting factors. The choice of discrete direction quadrature set for the DOM is generally arbitrary, although the chosen directions must satisfy certain moment conditions [19]. The most commonly used quadrature set is the $S_N$ quadrature, also referred to as Level-Symmetric quadrature [19,20], where the total number of directions is $M = N(N + 2)$. However, this quadrature scheme has an inherent directional limitation, as for $S_{20}$ and greater, the moment matching criteria produce unrealistic negative weighting factors [20]. It is well known that the DOM suffer from ray effect [21] due to imprecise approximation of the continuous angular variation, and thus the directional limitation restricts the adaptivity of the $S_N$ quadrature. In practical participating media where scattering can be highly anisotropic, such as biological tissue, poor angular discretization also results in a lack of scattered energy conservation in the system [22]. Correction of this problem via traditional phase-function normalization technique can result in substantial distortion/alternation in scattering phase-function [23-26], an error recently classified as a second type of false scattering due to angular discretization [27,28], or “angular false scattering” in contrast to the terminology “spatial false scattering” due to space discretization [21]. A phase-function normalization technique recently developed by the current authors [24-28], which implements a second constraint to simultaneously conserve scattered energy and scattering asymmetry factor, has been shown to accurately predict
radiative transfer in both 2-D axisymmetric cylindrical [24-26] and 3-D cubic enclosures [27,28] and eliminate/minimize the angular false scattering.

Since errors due to angular false scattering manifest solely due to angular discretization, sufficient increases in the number of discrete directions used to solve the ERT may minimize this error. In order to effectively analyze this hypothesis, higher-order quadrature sets with no directional limitation are required. Recently, several higher-order quadrature sets have been developed. Longoni and Haghighat [29] developed the Legendre-Equal Weight \((P_N-EW)\) and Legendre-Chebyshev \((P_N-T_N)\) quadrature sets using the Gauss-Legendre quadrature technique [30]. Two purely geometric quadrature sets, the \(T_N\) triangle-tessellation quadrature [31] and the Spherical Ring Approximation \((SRAP_N)\) quadrature [32], were specifically developed to counter directional-limitations of the traditional level-symmetric quadrature sets. Analysis of the impact of directional increase on angular false scattering errors using these quadrature sets is important, as the necessity of using an artificial phase-function normalization correction to produce accurate radiative transfer predictions may not be needed.

In this study, the impact of higher-order quadrature sets for 3-D radiative transfer in highly anisotropic scattering media is investigated. Radiative heat fluxes determined using higher-order quadratures are compared to \(S_N\) results and Monte Carlo solutions [23] to gauge their accuracy. Distortions in heat flux profiles due to angular false scattering after scattered energy normalization are examined for all quadratures with increasing direction number. Additionally, application of Hunter and Guo’s normalization technique on higher-order quadrature is investigated. Finally, computational efficiency for DOM with higher-order quadratures is examined, and a determination of whether it is more practical to increase direction number or simply implement phase-function normalization is made.

**Discretization of ERT**

The steady-state ERT of radiation intensity \(l\) in a gray, absorbing-emitting, and anisotropically scattering medium can be written in the following form, using general vector notation [3]:

\[
\mathbf{s} \cdot \nabla l(r, \mathbf{s}, t) = - \left( \sigma_a + \sigma_s \right) l(r, \mathbf{s}, t) + \sigma_a l_b(r, t) + \frac{\sigma_s}{4\pi} \int l(r, \mathbf{s'}, t)\Phi(\mathbf{s'}, \mathbf{s}) d\Omega'
\]  

The term on the left-hand side of the ERT represents the spatial gradients of radiative intensity. The first term on the right-hand side represents the attenuation of intensity due to both absorption and out-scattering; the second term represents the contribution of blackbody emission to radiative intensity, and
the final term accounts for intensity augmentation due to radiative energy in-scattering from a given direction $\mathbf{s}'$ into a second direction $\mathbf{s}$.

For a general 3-D enclosure defined using the Cartesian coordinate system, Eq. (1) can be expanded into a set of simultaneous partial differential equations in discrete directions $\mathbf{s}^l$ using the DOM, as follows:

$$
\mu^l \frac{\partial I^l}{\partial x} + \eta^l \frac{\partial I^l}{\partial y} + \xi^l \frac{\partial I^l}{\partial z} = -\left(\sigma_a + \sigma_{sm}\right)I^l + S^l, \quad l = 1,2,\ldots,M
$$

(2a)

$$
S^l = \sigma_a I_b + \frac{\sigma_s}{4\pi} \sum_{l' \neq l} w^{l'l'} I^{l'}
$$

(2b)

$$
\sigma_{sm} = \sigma_s \left(1 - \frac{1}{4\pi} w^l \Phi^l\right)
$$

(2c)

where $M$ is the total number of discrete radiation directions; $\mu = \sin \theta \cos \phi$, $\eta = \sin \theta \sin \phi$, and $\xi = \cos \theta$ are direction cosines corresponding to the x-, y-, and z-directions, respectively, and $\theta$ and $\phi$ are the polar and azimuthal angles corresponding to radiation direction $\mathbf{s}^l$. In the source term of Eq. (2b), the in-scattering integral from Eq. (1) has been replaced by a discrete quadrature summation, which represents the in-scattering of diffuse radiative intensity. In this summation, $w^{l'l'}$ is the DOM directional weighting factor corresponding to radiation direction $\mathbf{s}^{l'}$, and $\Phi^{l'l'}$ is the diffuse scattering phase-function between arbitrary radiation directions $\mathbf{s}^{l'}$ and $\mathbf{s}^l$. Eq. (2c) defines a modified scattering coefficient $\sigma_{sm}$, following the treatment of Chai et al. [33], in which the forward-scattering term is extracted from the diffuse intensity in-scattering summation and treated as transmission as a means of improving DOM computational efficiency for radiative transfer in strongly-scattering media.

The Mie scattering phase-function $\Phi$ is generally highly oscillatory in nature, and can be expressed as an infinite series of Legendre polynomials, as follows:

$$
\Phi(\theta) = 1 + \sum_{i=1}^{\infty} C_i P_i(\cos \theta)
$$

(3)

where $\theta$ is the scattering angle between radiation directions $\mathbf{s}'$ and $\mathbf{s}$, and the coefficients $C_i$ are determined via Mie theory. While it is possible to exactly implement the Mie phase function in
numerical simulation, the highly oscillatory nature makes such implementation difficult. To avoid this issue, phase-function approximations, such as the Henyey-Greenstein (HG) phase-function approximation, are commonly used. The HG phase function is desirable for highly anisotropic scattering media, as it is able to accurately capture strong-forward scattering peaks. The analytic form of the HG phase function is as follows:

$$\Phi_{HG}(\theta) = \frac{1 - g^2}{[1 + g^2 - 2g \cos(\theta)]^{1.5}}$$  (4)

where the overall phase-function asymmetry factor $g$ is a measure of the average cosine of the scattering angle $\theta$.

In order to solve Eqs. 2(a-c), the domain of interest is subdivided into small control volumes, while the spatial derivative is approximated using traditional control-volume methods. In order to obtain sufficient solution accuracy, the spatial grid sizes should be taken as small as possible [33] with the consideration that increases in grid refinement can substantially increase both computational memory and solution time. In addition to spatial grid, the DOM quadrature scheme must be specified at the outset to fully define the angular distribution of $M$ discrete radiation directions, with each direction represented by direction cosines and a weighting factor.

After defining the computational grid, quadrature scheme and medium properties, Eqs. 2(a-c) can be solved using a control-volume marching scheme [17]. For brevity, further details on DOM solution procedure are not repeated here, but are readily available in standard text [3] and in the authors’ previous publications [16,17].

**DOM Quadrature Schemes**

In general, the choice of quadrature scheme for the DOM is arbitrary. However, DOM quadrature sets are normally developed around directional moment condition satisfaction [3]. After directional discretization, the $m^{th}$-order moment conditions can be expressed as follows for the three direction cosines:
\[
\frac{1}{4\pi} \sum_{i=1}^{M} (\mu^i)^m w^i = \frac{1}{4\pi} \sum_{i=1}^{M} (\eta^i)^m w^i = \frac{1}{4\pi} \sum_{i=1}^{M} (\xi^i)^m w^i = \begin{cases} 0 \quad m = 1,3,5,7,... \\ \frac{1}{m+1} \quad m = 0,2,4,6,... \end{cases}
\]

(5)

The conditions in Eq. (5) are commonly referred to as odd- or even-moment conditions, depending on the value of \( m \). The simplest moment condition arises when \( m = 0 \), providing the following constraint on the directional weighting factors:

\[
\frac{1}{4\pi} \sum_{i=1}^{M} w^i = 1
\]

(6)

The most commonly implemented quadrature set is the \( S_N \) quadrature, also known as level-symmetric quadrature [19]. The total number of directions for the \( S_N \) level-symmetric quadrature set is \( M = N(N + 2) \), where \( N \) is an even integer. The \( S_N \) quadrature fully satisfies both reflectional and rotational symmetries about all coordinate axes. In the principal octant, \( S_N \) discrete directions are arranged on \( \frac{N}{2} \) directional levels of constant polar angle (and thus, constant \( \xi \)), with \( \frac{N}{2} - i + 1 \) directions on the \( i^{th} \) level, \( i = 1,2,\ldots,\frac{N}{2} \) [31]. The rotational and reflectional symmetries of the quadrature set can be used to map discrete directions in the principal octant onto the remainder of the unit sphere. In addition, the directions and weighting factors satisfy both the zeroth and first order moment conditions \( (m = 0, 1 \text{ in Eq. (5)})) \), as well as all subsequent even conditions \( (m \geq 2) \). Further details on the development and derivation of the \( S_N \) quadrature set are not presented here, for brevity, but are readily available elsewhere [3, 19].

While use of the \( S_N \) level-symmetric quadrature set is common for DOM simulations, it comes with a significant limitation. For \( N \geq 20 \ (M \geq 440 \text{ directions}) \), satisfaction of the directional moment conditions leads to unrealistically negative weighting factors [20], meaning that there is an upper limit on the total number of discrete directions that can be used in a simulation.

**Legendre Equal-Weight and Legendre-Chebyshev Quadratures**

Longoni and Haghighat [29] proposed both the Legendre-Equal Weight \( (P_N-\text{EW}) \) and Legendre-Chebyshev \( (P_N-\text{T}_N) \) quadrature sets, which are determined using the Gauss-Legendre quadrature technique [30]. These quadrature sets have the same level arrangement and total number of directions as previously described for the \( S_N \) quadrature, although the directions and weighting factors differ.
For both quadratures, the values of $\xi_i$ in the principal octant corresponding to the $i^{th}$ level of constant polar angle are taken to be the $\frac{N}{2}$ positive roots of the $N^{th}$-order Legendre polynomial $P_N(x)$, with $\xi_1 < \xi_2 < \cdots < \xi_{\frac{N}{2}}$. The weighting factor $w_i$ corresponding to a given direction on the $i^{th}$ polar level is calculated as follows:

$$w_i = \frac{\pi}{\left(\frac{N}{2} - i + 1\right)} \left(1 - \xi_i^2\right) \left(\frac{dP_N}{dx}\right)_{x=\xi_i}, \quad i = 1, ..., \frac{N}{2}$$

where $\frac{N}{2} - i + 1$ is the total number of equally-weighted directions on each level.

The difference between the $P_N$-EW and $P_N$-$T_N$ quadrature sets appears in the determination of the azimuthal angle for a given direction. For the $P_N$-EW quadrature, the azimuthal angle is determined using equal partitioning of the octant for a given polar level, whereas for the $P_N$-$T_N$ quadrature the azimuthal angles on each level are taken as the roots of the Chebyshev polynomials of the first kind. Thus, the azimuthal angle corresponding to the $j^{th}$ direction on the $i^{th}$ polar level becomes:

$$\phi_{i,j} = \begin{cases} \frac{j\pi}{2\left[\frac{N}{2} - i + 2\right]}, & P_N - EW \\ \frac{\pi[N + 3 - 2i - 2j]}{2[N + 2 - 2i]}, & P_N - T_N \end{cases}$$

where $i = 1, ..., \frac{N}{2}$ and $j = 1, ..., \frac{N}{2} - i + 1$. Once the azimuthal angle is known, the remaining direction cosines $\mu$ and $\eta$ are easily determined. Both the $P_N$-EW and $P_N$-$T_N$ quadrature sets accurately satisfy the zeroth and first order moment conditions. The $P_N$-$T_N$ quadrature also completely satisfies even-moment condition for all direction cosines. The $P_N$-EW quadrature similarly satisfies even moment conditions for $\xi$, but the equipartitioning of azimuthal angle produces noticeable errors in the even-moment summations for $\mu$ and $\eta$ [29].

**Triangle Tessellation ($T_N$) and Spherical Ring Approximation (SRAP$_N$)**

The Triangle Tessellation ($T_N$) quadrature set was developed by Thurgood et al. [31] as an alternative to directionally restrictive quadrature sets. This quadrature set is purely geometric in construction. In this quadrature, the surface of the unit sphere is divided into $M = 8N^2$ continuous
regions \((N^2 \text{ regions per octant})\), where the index \(N\) is an integer \(\geq 1\). Construction of the quadrature set can be achieved in three steps. Firstly, the principal octant is mapped onto an equilateral basal triangle, with vertices at points \((1,0,0)\), \((0,1,0)\), and \((0,0,1)\). Next, the basal triangle is tessellated into \(N^2\) smaller equilateral triangles, whose side lengths are \(1/N\) times the basal triangle side length (i.e., each side of the basal triangle is divided into \(N\) segments). Finally, the basal triangle and tessellations are mapped onto the surface of the unit sphere. The direction cosines for each region can be calculated using simple mapping, as follows:

\[
\begin{align*}
\mu &= \frac{x_c}{\sqrt{x_c^2 + y_c^2 + z_c^2}}, & \eta &= \frac{y_c}{\sqrt{x_c^2 + y_c^2 + z_c^2}}, & \xi &= \frac{z_c}{\sqrt{x_c^2 + y_c^2 + z_c^2}} \\
\end{align*}
\]

where \((x_c, y_c, z_c)\) is the coordinate locating the centroid of the tessellated triangular region in the basal plane. Mapping of triangular regions onto the unit sphere produces spherical triangles, and the weighting factor corresponding to a given discrete direction is calculated as the area of the spherical triangle through which the direction passes. Directions and weights for the remaining octants can be determined through rotational and reflectional symmetry.

A second purely geometric DOM quadrature set is the Spherical Ring Approximation \((SRAP_N)\), introduced by Li et al. [32], where the index \(N\) is an integer \(\geq 2\). Once again, we focus on development of the quadrature in the principal octant, and use symmetries to determine directions in the remaining octants. To determine the quadrature, the surface of the unit sphere in the principal octant is divided into \(N\) total spherical “rings”, with the topmost “ring” reducing to a crown [32]. Working from the top crown element downward, each spherical ring is divided into additional spherical elements. The number of elemental divisions in successive spherical rings constitutes an arithmetic progression, with the topmost crown containing two spherical elements, and every successive ring containing one additional element. With divisions in this manner, each spherical element will have an equal solid angle, and thus an equal elemental surface area.

The discrete directions are determined, for a given element, by locating the centroid \((x_c, y_c, z_c)\) of the elemental solid angle. These coordinates are then transformed using Eq. (9) above into direction cosine form. As with the \(T_N\) quadrature, the weighting factors correspond to the elemental surface area. Since all elements in the \(SRAP_N\) quadrature have identical areas, every direction is equally weighted. The total number of directions in the \(SRAP_N\) quadrature across all octants is
\[ M = 8 \cdot (2 + 3 + 4 + \cdots + (N + 1)) = 8 \sum_{i=2}^{N+1} i = 4N(N + 3) \]

(10)

Thus, the weighting factor for each direction becomes \( w = \frac{4\pi}{M} \).

Thurgood et al. [31] and Li et al. [32] showed that the \( T_N \) and \( SRAP_N \) quadratures, respectively, were accurate in their prediction of first order moments. Thurgood et al. [31] stresses that the \( T_N \) quadrature set is generally less accurate than the \( S_N \) quadratures of similar direction number, but the \( T_N \) quadrature has no directional limit. Li et al. [32] compared the \( T_N \) and \( SRAP_N \) quadratures, noticing good agreement in calculation of half moments. However, they clarified that the \( T_N \) quadrature may suffer from numerical errors, due to the fact that the discrete directions are calculated using the centroids of the tessellated triangles before mapping onto the unit sphere. This mapping does not guarantee that \( T_N \) directions directly pass through the elemental solid angle centroids, as the \( SRAP_N \) directions are designed.

Figures 1(a-d) depict the principal octant directional distributions and weighting factors for the \( P_{16} - T_{16} \), \( P_{16} \)-EW, \( T_6 \), and \( SRAP_7 \) quadrature sets, respectively. All quadrature sets have \( M = 288 \) discrete directions, except for \( SRAP_7 \) (\( M = 280 \)). The weighting factors are indicated by the spectrum shading of each point in the plots. As described, the weighting factors on each level for the \( P_{16} \)-EW and \( P_{16} - T_{16} \) quadrature sets are identical, and the difference in the azimuthal angles on each level can be clearly seen. The directional distribution of the \( T_6 \) quadrature set reflects the use of triangular elements, and is the only set that does not exhibit specific levels of constant polar angle. The weighting factors for \( SRAP_7 \) are identical for every discrete direction. It is interesting to note that the magnitude of the maximum weighting factor is very similar for all the four high-order quadrature sets (\( w_{\text{max}} \sim 0.045 - 0.06 \)).

**Phase-Function Normalization**

It is well recognized that overall scattered energy conservation should be preserved after directional discretization of the continuous angular variation. For isotropic scattering, this is not such a concern because conversation is exactly satisfied for any given DOM quadrature set. For anisotropic scattering, however, satisfaction of the moment conditions of Eq. (5) is not sufficient to ensure scattered energy conservation, and thus an additional constraint is required. Scattered energy conservation can
be achieved through phase-function normalization, after which the following condition must be satisfied:

\[
\frac{1}{4\pi} \sum_{l=1}^{M} \Phi^{l'} w^l = 1, \quad l' = 1, 2, \ldots, M
\]  

(11)

where \( \Phi^{l'} \) is the discrete value of normalized phase function.

One simple technique that ensures scattered energy conservation after directional discretization was described by Kim and Lee [22], and is as follows:

\[
\Phi^{l'} = \Phi^{l'} \ast \left( \frac{1}{4\pi} \sum_{l=1}^{M} \Phi^{l'} w^l \right)^{-1}
\]  

(12)

While scattered energy normalization using the above form corrects the issue of scattered energy conservation, recent works [23-28] have shown that this approach significantly skews the overall shape and asymmetry factor of the anisotropic scattering phase-function, which lead to large errors in radiative transfer predictions. In order to maintain phase-function asymmetry factor, and thus the scattering properties of the original phase function, the following constraint must be satisfied after directional discretization and phase-function normalization [24]:

\[
\frac{1}{4\pi} \sum_{l=1}^{M} \Phi^{l'} \cos \Theta^{l'} w^l = g, \quad l' = 1, 2, \ldots, M
\]  

(13)

It is essential that both Eqs. (11) and (13) are conserved after directional discretization, in order to obtain accurate radiative transfer solutions. Numerical errors brought on when Eq. (13) is not satisfied can be characterized as a second type of false scattering due to the angular discretization, or “angular false scattering” [27,28]. Angular false scattering should not be confused with traditional false scattering (numerical diffusion errors due to spatial discretization), as it is independent of the spatial discretization.

Hunter and Guo [24-28] recently developed a phase-function normalization technique which guarantees accurate satisfaction of Eqs. (11) and (13), simultaneously. The phase function is normalized in the following manner:
\[
\Phi^{il'} = (1 + A^{il'}) \Phi^{il}
\]

Taking directional symmetry into account (\(\Phi^{il'} = \Phi^{il}\)), the linear system of equations comprised of Eq. (14) and Eqs. (11) and (13) is underdetermined, as there are \(2M\) equations and \(M(M + 1)/2\) unknown normalization parameters. The desired normalization parameters \(A^{il'}\) which satisfy scattered energy and asymmetry factor conservation accurately can be determined via the minimum-norm solution of this system, which is easily obtained using least-squares approximation or pseudo-inversion.

When applying Hunter and Guo’s technique, care must be taken to avoid issues with computational memory overflow. The coefficient matrix in this linear system has \(M^3 + M^2\) total elements (\(2M\) rows corresponding to the number of equations, and \(M(M + 1)/2\) columns corresponding to the number of unknowns). However, out of these elements, only \(2M^2\) have a non-zero value, meaning that the fraction of non-zero elements is on the order of \(M^{-1}\). Therefore, in order to maximize computational efficiency, the coefficient matrix can be defined as sparse so that memory is only used for the non-zero terms. This will reduce the total memory for Hunter and Guo’s normalization technique from \(O(M^3)\) to \(O(M^2)\). Table 1 lists the computational memory storage required for the coefficient matrix for both full and sparse matrix storage, as well as the percentage of non-zero elements, for various discrete direction numbers. For 24 total directions, only 8% of the coefficient matrix elements are non-zero. Sparse storage of the coefficient matrix reduces memory storage by 63.0%. For lower direction numbers, computational memory overflow is not a concern. However, as the number of directions increases, this becomes a major issue. For example, in order to store the coefficient matrix for \(M = 2024\) discrete directions (where only 0.10% of elements are non-zero), the computer would require over 61 GB of RAM, which is roughly 8-12 times more RAM than the average CPU contains nowadays. Sparse storage reduces this memory requirement to 0.282 GB of RAM, reducing the requirement by 99.5% to a value which can be easily stored on average CPU’s. The data in Table 1 clearly indicates the use of proper sparse matrix storage and computation for efficient application of Hunter and Guo’s normalization technique.

As previously mentioned, application of the scattered energy normalization of Eq. (12) is guaranteed to explicitly conserve scattered energy in the system, but may result in angular false scattering. Therefore, investigation of the magnitude of angular false scattering due to alteration of the discretized asymmetry factor after application of Eq. (12) is crucial. According to the isotropic scaling
law [34,35], the change in scattering effect brought about by distortion of $g$ is manifested in the
difference of $(1-g)$. Thus, by analyzing the difference in $(1-g)$ after application of scattered energy
normalization, additional information about the necessity of conserving asymmetry factor can be
obtained.

Figure 2 plots percentage difference in $(1-g)$ after scattered energy normalization for the five
quadrature sets versus number of discrete directions. In this case, a value of $g = 0.9300$ is specified
before directional discretization. All five quadrature sets exhibit similar behavior, with dramatic
decreases in scattering effect change occurring with direction number increase. Deviations of >90% are
witnessed for the lowest-order quadrature for all quadrature schemes. Application of Eq. (12) results in
altered $g$ values of 0.9609, 0.9624, 0.9617, 0.9614, and 0.9627 for the $S_{16}, P_{16}$-EW, $P_{16}$-$T_N$, $T_6$ ($M = 288$ for all), and $SRAP_T$ ($M = 280$) quadratures, respectively, which correspond to changes in scattering
effect of 44.1%, 46.3%, 45.3%, 44.9%, and 46.7%, respectively. Changes in scattering effect of less than
10% are first realized around $M = 1000$ for all four higher-order quadratures. At greater direction
numbers ($M = 2024$ for $P_{44}$-EW and $P_{44}$-$T_{44}$, $M = 2048$ for $T_{16}$, and $M = 2016$ for $SRAP_{21}$), the changes in
scattering effect become 3.29%, 1.57%, 2.57%, and 1.14%, respectively, indicating that some error due
to angular false scattering may still exist in radiative transfer predictions. In general, scattering effect
changes for $P_N$-$T_N$ and $SRAP_N$ are slightly smaller than those for $T_N$ and $P_N$-EW, which could be a result
of better moment-condition satisfaction. Substantial increases in direction number result in the percent
change in scattering effect converging towards 0%, indicating an advantage of non-limited quadrature
sets. However, extremely fine angular grids must be applied in order to effectively minimize scattering
effect changes after scattered energy normalization is applied. When Hunter and Guo’s technique is
applied, $g$ is accurately conserved, and no change in scattering effect exists.

Results and Discussion

While Figure 2 gives a preliminary indication of the impact of improper phase-function
normalization on DOM solutions with various quadrature sets, it is necessary to examine the impact of
phase-function normalization on actual radiative transfer predictions, determined using the various
quadrature sets, to draw a more concrete conclusion.

For this study, a benchmark test problem involving steady-state radiative transfer in a cubic
enclosure of edge length $L$ is investigated. The cubic enclosure houses an optically thick ($\tau = (\sigma_a +$
\( \sigma_s L = 10.0 \), purely scattering \((\omega = 1.0)\) medium, which anisotropically scatters radiant energy with asymmetry factor \(g = 0.93\). In order to ensure invariance with further spatial grid refinement, the spatial grid for all simulations is taken as \( (N_x \times N_y \times N_z) = 27 \times 27 \times 27 \), and the positive differencing scheme is implemented [3]. The spatial coordinates are non-dimensionalized as follows: \( x^* = x/L, y^* = y/L, \) and \( z^* = z/L \). To further simplify the problem, the cube edge length \( L \) is taken to be unity.

The medium and enclosure walls are taken to be cold and black, except for the wall at \( z^* = 0 \), which is taken as a diffuse, blackbody emitter with unity emissive power. The workstation used for simulation is a Dell Optiplex 780, with an Intel Core 2 processor and 4.0 GB of RAM. Radiative transfer solutions using the DOM with the five quadrature schemes are generated using the FORTRAN computing language. For simulations where Hunter and Guo’s normalization procedure is applied, the diffuse normalization parameter coefficients \( A_{i''} \) are pre-determined using MATLAB’s built-in least-squares solver, and imported into FORTRAN.

As a means of analyzing the impact of both phase-function normalization and choice of DOM quadrature set, Figure 3(a-b) compares radiative heat flux determined using the DOM to a reference Monte Carlo (MC) solution [23]. The radiative heat flux \( Q \) is calculated at the centerline of the wall directly opposite from the diffuse source, i.e. \( Q(x^*, y^* = 0.5, z^* = 1.0) \), and is plotted versus location \( x^* \). The reference MC solution for this test problem, presented by Boulet et al. [23], implements over 4 million quanta per reference control volume. DOM solutions are presented, for all five discussed quadrature sets, using both scattered energy normalization and Hunter and Guo’s normalization.

In Figure 3(a), radiative heat fluxes are presented for DOM quadrature with discrete direction number on the order of the \( S_4 \) quadrature \((M = 24)\). The \( T_2 \) \((M = 32)\) and \( SRAP_2 \) \((M = 40)\) quadrature sets are applied for this analysis, as their direction numbers are the closest possible to that of the \( S_4 \) quadrature. When only the scattered energy normalization of Eq. (12) is applied, heat flux profiles differ greatly from the reference MC solution for all quadratures. The maximum percentage differences with respect to MC for \( S_4, P_4 – EW, P_4 – T_4, T_2, \) and \( SRAP_2 \) are 222%, 111%, 110%, 131%, and 68.8%, respectively. All quadratures overpredict the MC heat flux at all medium locations except for \( SRAP_2 \). In fact, the \( SRAP_2 \) profile does not make physical sense, as the heat flux should be highest at \( x^* = 0.50 \) in this situation. When Hunter and Guo’s technique is applied, and asymmetry factor is conserved in addition to the scattered energy conservation, differences from the MC solution decrease. The maximum percentage differences for the five quadratures decrease to 92.9%, 18.9%, 16.7%, 41.1%, and 23.8%, respectively. While the solutions are vastly improved, errors in comparison to MC still have high
magnitude due to ray effect, since only a small number of directions are being used to approximate the continuous angular variation. It is noteworthy to mention that the four higher-order quadrature sets predict more closely to MC than the $S_N$ quadrature, regardless of normalization, indicating their potential as a more accurate alternative to the $S_N$ quadrature for lower direction numbers.

Figure 3(b) compares radiative heat fluxes determined using quadratures on the order of the $S_B$ quadrature ($M = 80$). The $T_3$ and $SRAP_3$ quadratures ($M = 72$) are chosen for comparison, as their discrete direction number is closest to that of $S_B$. The heat fluxes generated using scattered energy normalization overpredict the MC solution at all locations significantly for all quadrature sets, although the increase in direction number over the results seen in Figure 3(a) has dramatically reduced the discrepancy. Maximum percentage differences from MC reach for $48.8\%$, $58.5\%$, $54.3\%$, $74.0\%$, and $62.0\%$ for $S_B$, $P_B$-EW, $P_B$-$T_B$, $T_3$, and $SRAP_3$, respectively. Application of Hunter and Guo’s technique results in vast improvement, as all five quadratures produce heat fluxes within $10\%$ of the MC value at all locations, indicating that the increase in direction number has more effectively mitigated ray effect error.

For Figures 4(a-b), instead of plotting radiative heat flux directly, the percentage difference in heat flux from the reference MC solution vs. $x^*$ is directly presented for the various DOM quadratures. Percentage differences shown in these figures are calculated as $\frac{Q_{DOM} - Q_{MC}}{Q_{MC}} \times 100\%$, so that the sign of the percentage difference indicates heat flux over- or underpredictions. For Figure 4(a), quadratures on the order of the $S_{12}$ quadrature ($M = 168$) are examined, with $T_5$ ($M = 200$) and $SRAP_5$ ($M = 160$) selected as the closest quadratures to that particular direction number. For Figure 4(b), quadratures on the order of the $S_{16}$ quadrature ($M = 288$) are examined, with only $SRAP_7$ ($M = 280$) having a different direction number.

When only scattered energy normalization is applied to the $S_{12}$-order quadratures in Figure 4(a), all five quadratures continue to drastically overpredict the MC solution at all locations, with maximum differences of $42.0\%$, $40.6\%$, $41.8\%$, $30.0\%$, and $39.8\%$ occurring for $S_{12}$, $P_{12}$-EW, $P_{12}$-$T_{12}$, $T_5$, and $SRAP_5$, respectively. The $T_5$ quadrature predicts more accurately at all locations than the other four quadratures, due to the fact that it contains more than 30 extra directions. In general, differences between DOM and MC heat flux decrease with increasing $x^*$. The $S_{12}$ quadrature produces similar heat flux values to the $P_{12}$-$T_{12}$ and $SRAP_5$ quadratures near $x^* = 0$ and $x^* = 0.5$, but differs greatly near $x^* = 0.25$. Similarly, the two Legendre quadratures exhibit nearly identical behavior near $x^* = 0$, but vastly
different trends as the location is moved towards the wall center. When Hunter and Guo’s technique is applied, all five quadratures produce heat flux profiles that differ by less than 7% in absolute value. Except for a small portion of $x^*$ for the $T_5$ quadrature, DOM heat fluxes underpredict the MC value at all locations. The $S_{12}$ quadrature is the least accurate on average, with an average underprediction of 5.06%, while the $T_5$ quadrature is the most accurate due to the higher direction number, with an average underprediction of just 0.12%.

As the direction numbers are further increased to the $S_{16}$ order in Figure 4(b), errors due to angular false scattering when only scattered energy normalization is applied continue to decrease at all locations, according to the trend in Figure 2. However, the differences in heat flux when compared to MC are still significant, with maximum differences of 35.9%, 28.3%, 27.7%, 26.4%, and 22.4% for $S_{16}$, $P_{16}$-EW, $P_{16}$-$T_{16}$, $SRAP_7$, and $T_6$, respectively. At all locations, the $S_{16}$ quadrature set deviates more greatly from MC than the four higher-order quadratures, while the $T_6$ quadrature exhibits the smallest differences. Additionally, the differences in heat flux in Figure 4(b) exhibit similar trends with respect to $x^*$ as those in Figure 4(a). Percentage differences strictly decrease with increasing $x^*$ for the $P_N$-$T_N$, $T_N$, and $SRAP_N$ quadratures, while the $S_N$ and $P_N$-EW quadrature sets exhibit both increases and decreases in percentage difference with increasing $x^*$. Application of Hunter and Guo’s technique reduces the discrepancies with respect to MC to less than 6% in absolute value for all quadratures. In addition, it is seen that the DOM heat fluxes underpredict the MC values for all quadratures and locations. The average percentage differences are -2.27%, -2.82%, -3.00%, -0.56%, and -1.69% for the five quadrature sets. Generally, errors of these magnitudes are considered acceptable, due to both statistical errors inherent in the MC method, and discretization errors inherent in the DOM.

The results from Figures 3(a-b) and 4(a-b) mirror the expectations from analysis of the change in scattering effect in Figure 2. Increases in direction number produce DOM heat flux profiles that are more accurate in comparison with MC when only scattered energy normalization is applied, due to a reduction of angular false scattering. However, the errors between DOM and MC still have significant magnitude for all $S_{16}$ equivalent quadrature sets, corresponding to the ~40% changes in scattering effect seen in Figure 2 for these quadratures. In general, the four higher-order quadratures tend to conform to MC solutions with equal or higher accuracy than the $S_N$ quadrature, but angular false scattering errors are still prevalent. To effectively minimize angular false scattering and improve DOM solution accuracy for $M \leq 288$ discrete directions, Hunter and Guo’s normalization technique can be implemented, with errors > 10% occurring only for the lowest-order quadrature due to ray effect.
As discussed before, increase in the number of discrete directions can effectively reduce errors due to ray effect and angular false scattering. Figures 5(a-d) examine the percent difference in diffuse heat flux between the reference MC and DOM solutions vs. discrete direction number at four different values of $x^*$: $x^*$ = 0.02, 0.10, 0.30, and 0.50, respectively. The profiles are generated for the four higher-order quadrature sets using either only scattered energy normalization or Hunter and Guo’s technique. In Figure 5(a), corresponding to $x^*$ = 0.02, increase in direction number when scattered energy normalization is applied causes the differences between MC and DOM heat flux to decrease for all quadrature sets, corresponding to the decrease in scattering effect change in Figure 2. However, it is important to note that the percent differences do not converge to zero. Instead, they slowly converge to a slightly negative percentage, due to statistical/numerical errors inherent in both MC and DOM methods. For example, for the $P_{44}^4$ - $T_{44}$, $P_{44}$-EW, $T_{16}$, and $SRAP_{21}$ quadratures (which have $M$ = 2024, 2024, 2048, and 2016 discrete directions, respectively), the percent differences between MC and DOM heat fluxes are -1.26%, -0.19%, -1.41%, and -1.60%, respectively. In order to obtain heat fluxes that differ by less than 5% when scattered energy normalization is applied, between $M$ = 750 and 1000 directions must be used, depending on the quadrature set. Conversely, if Hunter and Guo’s technique is applied, absolute difference of less than 5% is attained for all quadratures except $P_N$-EW when $M$ = 288. In fact, an increase in discrete directions does not appear to have a substantial effect on the heat fluxes generated using Hunter and Guo’s technique. Percent differences for the $P_N$-TN, $P_N$-EW, $T_N$, and $SRAP_N$ quadratures only improve by 0.94%, 1.08%, 0.07%, and 0.66%, respectively, over the range of discrete directions shown when Hunter and Guo’s technique is applied, indicating that higher-order directionality may not be necessary if asymmetry factor is accurately conserved after discretization.

Similar results are seen for the three remaining values of $x^*$ in Figures 5(b-d). For the two locations that are closest to the wall center ($x^*$ = 0.30 and 0.50), more prominent discrepancies between the four quadrature sets exist for scattered energy normalization. The $P_N$-EW quadrature more greatly overpredicts the MC solution than the other quadrature sets over the range of discrete directions. In fact, for these two locations, while the other quadratures have started to underpredict the MC solution, heat fluxes generated by $P_N$-EW have converged more slowly, and continue to overpredict the MC solution at high direction number. In order to obtain a percentage difference of less than 5% at $x^*$ = 0.50, the $P_N$-EW requires 1368 discrete directions ($P_{36}$-EW), while the other quadratures only require 840 ($P_{28}$-T$_{28}$), 524 ($T_8$), and 832 ($SRAP_{13}$) discrete directions. For all locations, it appears that the heat fluxes determined with both scattered energy normalization and Hunter and
Guo’s techniques converge towards similar steady-state values, but Hunter and Guo’s technique converges much more quickly.

The necessity of Hunter and Guo’s normalization for highly anisotropic scattering stems from deviations in scattered energy and asymmetry factor conservation caused by a limited representation of the angular discretization. The advent of higher-order quadrature sets with no directional limit provides the possibility that, with sufficiently large discrete direction number, both scattered energy and asymmetry factor may be accurately conserved without the use of phase-function normalization. This concept is examined in Figure 6, in which DOM heat flux profiles generated with the $P_{N}-T_{N}$ quadrature with extremely high direction number and no phase-function normalization are compared to the reference MC solution. Profiles are presented for the $P_{44}-T_{44}$, $P_{52}-T_{52}$, and $P_{64}-T_{64}$ quadratures, which have $M = 2024, 2808$, and $4224$ discrete directions, respectively.

The three non-normalized profiles show a converging trend as direction number increases. For the $P_{44}-T_{44}$ quadrature, differences of between 27-30% exist for all locations when compared to the MC solution. At this quadrature, the discretized $g$ is distorted to $g = 0.9453$, corresponding to a 21.9% change in scattering effect. While scattered energy is conserved well enough to actually obtain a heat flux profile (i.e., the solution of the ERT does converge), the angular grid is still too coarse to obtain accurate solutions. As the number of directions is increased to $M = 2808$ for the $P_{52}-T_{52}$ quadrature, the discretized $g$ decreases to $g = 0.9356$, and discrepancies between DOM and MC reduce to less than 10% for all locations. For the extreme $P_{64}-T_{64}$ quadrature, the differences between MC and DOM are less than 1.4% for all locations. This solution corresponds to a discretized $g$ of 0.9313, which still results in a 1.9% change in scattering effect. For comparison, applying the scattered energy normalization of Eq. (12) to this quadrature reduces the discretized $g$ to 0.9301, which corresponds to a 0.14% scattering effect change. This profile underpredicts the MC solution by less than 2.5% at all locations, conforming to the results of Figures 5(a-d).

While the preceding results have shown that higher-order DOM quadrature sets have the advantage of minimizing errors, a major disadvantage of higher-order quadrature sets lies in computational efficiency, as increases in discrete direction number directly result in both higher computational convergence times and greater computational committed memory. Figure 7 examines the computational convergence time, in minutes, versus number of discrete directions for various quadrature sets. For low direction number, all five quadrature sets converge in similar amounts of time, with convergence times of ~ 13 minutes seen for $S_{16}$ equivalent quadratures. As the number of
directions increases, convergence time dramatically increases in a non-linear fashion. For example, looking at the $P_N$-$T_N$ quadrature, increases in direction number to $M = 624$, 840, 1088, 1368, and 2024 result in convergence times of 98, 195, 325, 557, and 1330 minutes, respectively. Although it is not presented in this figure, obtaining the more accurate non-normalized $P_{64}$-$T_{64}$ solution in Figure 6 required 7107 minutes (4.94 days) to converge. These extremely high convergence times illustrate the impracticality of using higher-order quadratures to obtain accurate radiative transfer solutions. In general, to obtain accurate solutions, it is more practical and efficient to use Hunter and Guo’s normalization technique, as it is able to obtain accurate solutions with far fewer number of directions. For example, as seen in Figures 5(a-d), achieving percent differences of 6% or less at all $x^*$ locations required at least 840 directions for the $P_N$-$T_N$ quadrature with scattered energy normalization. Using Hunter and Guo’s technique, heat fluxes determined for 168 discrete directions already attain such an accuracy, which reduces the computational time requirement by 98%, from ~ 195 minutes to 4 minutes.

Figure 8 examines the DOM total computational committed memory (determined through the operating system) for both scattered energy normalization and Hunter and Guo’s technique versus number of discrete directions. It is important to note that the amount of computational memory solely depends on the spatial and angular grid sizes, and is independent of quadrature scheme. At low direction number, computational memory for each normalization technique is comparable. As direction number increases, the computational memory for Hunter and Guo’s technique begins to increase over that of scattered energy normalization, due to the necessity of storing the $O(M^2)$ coefficient matrix. However, this increase in memory for Hunter and Guo’s technique is not an issue, because Figures 5(a-d) showed that increases in direction number did not drastically improve solution accuracy. Taking the same example as previously discussed for Figure 7, 840 directions are required to obtain solution accuracy of <6% for the $P_N$-$T_N$ quadrature set when compared to MC, while only 168 directions are required when Hunter and Guo’s technique is applied. This reduction in discrete directions results in a reduction in computational memory of 78.9% (0.27 GB to 0.06 GB).

**Conclusions**

In this study, the use of higher-order DOM quadrature schemes to calculate radiative transfer accurately in highly anisotropic scattering media is examined, and the impact of phase-function normalization technique on radiative transfer predictions is analyzed. The following conclusions can be made:
(1) For low direction numbers ($M \leq 288$), the four higher-order schemes conform with equal or better accuracy to MC solutions as the directionally-limited $S_N$ quadrature.

(2) Angular false scattering due to a lack of phase-function asymmetry factor conservation occurs for all quadratures after application of only scattered energy normalization.

(3) Substantial increase in direction number will effectively minimize angular false scattering and ray effect for all quadrature schemes, increasing the accuracy of DOM heat fluxes when compared with MC. However, a consequence of this is a dramatic increase in computational time and memory requirements, making this strategy less practical.

(4) Hunter and Guo’s normalization technique, which minimizes angular false scattering for all direction numbers, produces heat flux profiles that accurately conform to MC for all quadratures and direction numbers except the very lowest order ($M = 24$) due to ray effect. Increases in direction number produce minimal improvement to DOM heat fluxes when this technique is applied.

(5) Application of Hunter and Guo’s normalization is a practical and efficient method to accurately determine radiative transfer in highly anisotropic scattering media, due to substantial reductions in computational time and memory over traditional scattered energy normalization.

References


Table 1: Computational memory analysis of normalization parameter coefficient matrix in Hunter and Guo’s normalization technique

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