SOME RECENT DEVELOPMENTS IN RADIATIVE TRANSFER COMPUTATION

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ABSTRACT

This keynote focuses on recent development of my own research group on the discovery and re-examination of numerical errors and their physical meanings in the discretization and solution of the integro-differential equation of radiation transfer. Among discretization-based numerical methods, such as the discreteordinates and the finite-volume methods, two shortcomings were well known, i.e., false scattering and ray effect. We will see that the so-called “false scattering” actually affects the attenuation term, i.e., both absorption and out-scattering. Both “false scattering” and ray effect errors exhibit dependence on both spatial and angular discretization. In radiation transfer in anisotropic scattering media, errors due to alteration of the asymmetry factor and phase function exist due to angular discretization; and they cause false in-scattering. The error in discretized asymmetry factor can be corrected via Hunter and Guo’s methods of phase function normalization.

KEYWORDS: Radiative heat transfer, Computational methods, Numerical errors, Light scattering.

1. INTRODUCTION

In scientific exploration and engineering problems, such as combustion and fire, high-temperature manufacturing, atmospheric radiation, renewable solar energy, space exploration, and laser material processing, thermal radiation is the dominant mode of energy transfer [1, 2]. Numerical methods have garnered increasing attention in the field of radiation heat transfer, as they provide effective alternatives to costly experimentation and their efficiency and accuracy has been improved with the advance of computational technology [3-9]. A beam of light experiences absorption and scattering when it passes through a participating medium, and reflection and refraction at boundary/interface. With the presence of light in-scattering term, the Equation of Radiation Transfer (ERT) has an integro-differential nature, which makes it a formidable task to obtain analytical solution, and thus numerical methods, such as the finite volume method (FVM) and discrete-ordinates method (DOM), are preferred. Solution of the ERT involves numerical discretization in both the spatial and angular domains, which result in two well-known numerical errors - false scattering and ray effect in the DOM [6]. Such types of errors exist in all ERT-discretization based methods including the FVM that seemed to gain more attention than the DOM. As noticed by Hunter and Guo [10], however, many new angular discretization schemes have been developed in recent years and they have overcome the directional limit in traditional S_N schemes. Though FVM has better flexibility, DOM has shown better efficiency in both CPU time and memory usages [11, 12].

The terminology of “false scattering” error was initially named by S.V. Patankar – a heat transfer legend - according to communication with Patanker’s former student and co-author John Chai during CHT-15 held at Rutgers in May 2015. “False scattering” was defined as a direct result of spatial discretization practice, and is significant in multi-dimensional problems where spatial grid lines and radiation directions are misaligned, although it still persists in 1-D problems [7, 13]. It is sometimes referred to as “numerical smearing” by some

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other researchers [13]. The magnitude of this error was found to depend on both spatial grid resolution and chosen spatial differencing scheme. Ray effect stems from the approximation of the double integral in total solid angle 4π using a finite number of discrete directions [6]. Lack of appropriate angular resolution can lead to physically unrealistic bumps and oscillations in the intensity field. Ray effect exists in any method where angular discretization exists, although the degree of error magnitude may differ for different solution methods and different directional quadrature schemes [10]. The prevailing notion in the field is that ray effect and “false scattering” errors are “separate” from each other, although they have been shown to exhibit compensatory effects in some situations, such that reduction of one error may increase another error [13]. Kamdem Tagne [14] claimed ray effect elimination in DOM and FVM for isotropically scattering media using refined azimuthal discretization. As long as the number of angular discretization is finite, ray effect cannot be eliminated completely, but could be reduced to a negligible level in my opinion.

For four decades the conservation of scattered energy in radiation transfer computation has been well observed. Nevertheless, the importance of preserving the scattering angle was just fully discovered by Hunter and Guo [15] in 2011. Angular discretization would alter the phase function, and most importantly the value of asymmetry factor, which is an average cosine of scattering angle. Alteration of phase function really means false scattering, as phase function is defined as the angular distribution of radiation intensity scattered by a particle at a given wavelength. Discrepancy between given and discretized asymmetry factor values indicates breakdown of conservation of scattering angle. To correct this issue, one approach is phase-function normalization, which was commonly adopted for conserving scattered energy in DOM. Normalization of phase function must now satisfy two constrains – preservation of scattered asymmetry factor and conservation of scattered energy. This has also shown effectiveness in FVM [16]. A comparison study of various normalization conditions was presented in ref [17].

Though there are many excellent studies by others that have contributed to the advance and development of radiative transfer computation in recent years, this keynote focuses on reviewing our own studies due to author’s limited capability. I have realized the disparity between physical asymmetry factor and its discretized value for a few years. I knew that it could be a major cause why big differences in results exist among different approaches in radiation transfer computation. It was until early 2011 when I guided my former graduate student Brian Hunter into this problem. Hunter was extremely skillful in mathematics and program coding. I gave him the task to satisfy conservation constrains in both scattered energy and angle through normalization of phase function, and he tackled the problem via introducing a normalization matrix with minimum norm and this first method worked fantastically and was published in 2012 [15]. H. T. Kamdem Tagne read our paper and came out a normalization scheme to conserve only asymmetry factor via modifying the forward-scattering peak of phase function, and found that conserving asymmetry factor is more critical than conserving scattered energy. Kamdem Tagne’s such a paper may not be available in a journal, though I recommended it. Kamdem Tagne pinpointed me to an early study of Mishchenko et al. [18], in which this same idea was initiated to conserve scattered energy. Rather than mathematically altering every value of the discretized phase function, Mishchenko’s method altered phase function at only the forward point. However, this one-equation method cannot be applied to satisfy both scattered energy and asymmetry factor, because two constrains require two equations. Quickly I had a solution – modifying both the forward-scattering peak and backward-scattering valley. I deduced the formulae and asked Hunter to coding it. We completed the whole work in a month, resulting in our second normalization method [19] published in 2014. This new method has the advantage of retaining the phase-function value for the majority of directional combination, as well as being computationally savvy and easy to implement. This simple method was later found to produce unrealistic negative phase-function value at several directions in some situations. However, negative-intensity correction can be employed to resolve this issue [17].

In the same period when young student Hunter was enjoying the many productive results in discovering conservation of asymmetry factor, I have been persuading him to re-examine the relations between ray effect and “false scattering” errors (this was an extra request beyond his dissertation). Three months after his Ph.D. defence, we completed a new paper [20], in which the dependence of “false scattering” and ray effect on both spatial and angular discretization was revealed, and proportionality expressions for various orders of numerical truncation error were derived. Thereafter, I have been looking into the real physical meaning of the “false scattering” error.
I had intensive discussion in private and in public talks with one of the term inventors, J. Chai, during CHT-15. I insisted that the so-called “false scattering” error physically affects absorption as well as scattering; it introduces error from the same radiation direction, either increasing or decreasing the magnitude of attenuation, depending on the numerical scheme adopted. It is not an in-scattering contribution from other radiation directions. Mathematically, the “false scattering” error is a product of the radiation intensity and a power function of the ratio between spatial grid to directional cosine.

2. MATHEMATICAL MODELS

In general vector notation, the steady-state ERT of radiation intensity I can be expressed as follows, for a gray, absorbing-emitting, and scattering medium:

\[ \vec{S} \cdot \nabla I(\vec{r}, \vec{s}) = -(\sigma_a + \sigma_s)I(\vec{r}, \vec{s}) + \sigma_a I_b(\vec{r}) + \frac{\sigma_s}{4\pi} \iint I(\vec{r}, \vec{s}') \Phi(\vec{s}', \vec{s}) d\Omega' \]  

(1)

Using the DOM, Eq. (1) can be expanded into a simultaneous set of partial differential equations in finite discrete directions for a 3-D enclosure, based on Cartesian coordinates, in the following dimensionless form:

\[ \mu^l \frac{\partial I^l}{\partial \tau_x} + \eta^l \frac{\partial I^l}{\partial \tau_y} + \zeta^l \frac{\partial I^l}{\partial \tau_z} = -I^l + (1 - \omega)I_b + \frac{\omega}{4\pi} \sum_{l=1}^M w^l \Phi I^l I_{l'}, \quad l = 1, 2, ..., M \]  

(2)

where \( \tau_j = (\sigma_a + \sigma_s)j \) for \( j = x, y, z \), and the scattering albedo \( \omega = \sigma_s/(\sigma_a + \sigma_s) \). The continuous angular integral of radiation scattering is replaced by a sum over \( M \) total discrete directions, defined by both polar angle \( \theta^l \) and azimuthal angle \( \phi^l \). To solve Eq. (2) using an iterative control-volume (CV) marching procedure, the spatial domain of interest is discretized into numerous CVs, and the spatial derivatives are approximated using CV conservation methods. Additional details on the DOM and solution procedure can be found in textbooks.

2.1 Numerical Truncation Error

Numerical diffusion error arises due to domain spatial discretization. Consider three representative discretization schemes (the step scheme, diamond scheme, and QUICK scheme) for the derivative \( \mu^l \frac{\partial I^l}{\partial \tau_x} \) in a 1-D CV [20]:

\[ \mu^l \left( \frac{\partial I^l}{\partial \tau_x} \right)_i \equiv \mu^l \left( \frac{I^l_i - I^l_{i-1}}{\Delta \tau_x} \right)_{ste p} \equiv \mu^l \left( \frac{I^l_{i+1} - I^l_{i-1}}{2\Delta \tau_x} \right)_{dia m} \equiv \mu^l \left( \frac{3I^l_{i+1} + 3I^l_{i-1} - 7I^l_{i+1} + I^l_{i-2}}{8\Delta \tau_x} \right)_{Q U I C K} \]  

(3)

where \( \Delta \tau_x = (\sigma_a + \sigma_s)\Delta x \). Derivative approximation introduces numerical truncation error, which can be readily determined using Taylor Series analysis. The highly-stable step scheme attains first order \( O(\Delta \tau_x^2) \) accuracy with respect to grid size \( \Delta \tau_x \), while the diamond and QUICK schemes are second-order accurate \( O(\Delta \tau_x^4) \).

In general, Taylor Series analysis shows that the numerical error inherent in an \( O(\Delta \tau_x^n) \) spatial differencing scheme \( |E_{x,i}^{ln}| \propto \left| \mu^l (\Delta \tau_x^2)\frac{\partial^{n+1}(I^l)}{\partial \tau_x^{n+1}} \right| \). From the ERT, \( \mu^l \frac{\partial I^l}{\partial \tau_x} \sim -I^l \), and thus \( \frac{\partial^{n+1}(I^l)}{\partial \tau_x^{n+1}} \sim \left( -\frac{1}{\mu^l} \right)^n I^l \). The following proportionality relationship for numerical truncation error is derived:

\[ |E_{x,i}^{ln}| \propto \left( \frac{\Delta \tau_x}{\mu^l} \right)^n |I^l| \]  

(4)

From Eq. (4), it is apparent that numerical truncation error comes from the same radiation direction. It increases or decreases the attenuation (the first term on the right-hand side in Eq. (2)) due to absorption and out-scattering, depending on whether it is positive or negative. This error can be reduced by either refining spatial grid density, reducing medium optical thickness, or by using higher-order spatial schemes. To confine numerical truncation error, \( \left( \frac{\Delta \tau_x}{\mu^l} \right) \) should be < 1. If it equals to unity, the error will be the same order of the real attenuation term; if > 1, the error induced would be even greater than the real attenuation term.
Numerical truncation itself was widely believed to be “independent” of angular discretization. However, Eq. (4) illustrates that numerical truncation error depends directly on the ratio of spatial grid size to discrete direction cosine magnitude. Therefore, refinement of angular grid will actually increase numerical smearing error for constant grid size, due to reduction in $\mu_l$. Moreover, the total numerical smearing error can be expressed using the root-sum-squares method as follows, for 3-D problems:

$$E_{NS} = \sqrt{\sum_{l=1}^{M} \left[ (E_{x,l,n})^2 + (E_{y,l,n})^2 + (E_{z,l,n})^2 \right]}$$

(5)

Eq. (5) reinforces the dependence of overall numerical truncation error on angular discretization, showing that increasing $M$ (i.e., refining angular direction/reducing ray effect) will increase $E_{NS}$.

2.2 Ray Effect

Ray effect error results from the approximation of the continuous angular variation of radiation scattering via a finite number of discrete directions and is comprised of two components: (1) local error and (2) propagation error. The local component arises from the difference between the exact scattering integral and the approximate summation for each discrete direction. Additionally, local ray effect error also exists in the determination of radiative quantities of interest, such as heat flux and incident radiation. The propagation component of ray effect error arises from the propagation of rays. Consider the 2-D computational domain in Figure 1a, where a diffuse emitter is located at the bottom wall and the medium is purely absorbing. For simplicity, the diffuse radiation is approximated using two radiation directions (A & A’), represented by the dashed lines. Tracing rays in these two directions from the source wall illustrates the expansion of the radiation sphere with increasing propagation distance, resulting in no direct ray interception at CVs 1-4. Physically, all CVs should receive radiation from the diffuse emitter. This prevailing notion was broadly adopted to explain ray effect. As seen in Figure 1b, however, the propagating rays are actually incorporated into adjacent CV boundaries, and the radiation sphere effectively resets with new CVs of interest. Therefore, the arrows in Figure 1b represent a more appropriate view of ray propagation during DOM calculation. For example, ray 1 in CV-1 is affected by ray A, and ray 1’ is affected by ray A’. Ray 3 in CV-3 is additionally impacted by ray A via ray 1, and so on. As a matter of fact, all CVs in the calculation domain do receive radiation from the emitter in practical DOM calculations. Due to the finite number of rays during propagation, errors arise. Increasing ray number $M$ is the most effective way to reduce ray effect. Ray effect error was widely thought to be independent of spatial discretization. This statement may not be true. Through refinement of the spatial grid (see Figure 1c), one can see that ray propagation error can be effectively reduced without increasing ray number. Additionally, according to the Beer-Lambert Law, in a given CV, intensity decays exponentially with $\Delta \tau$. Thus, by refining the spatial grid, the magnitude of ray attenuation in a given CV is significantly decreased, which could enhance local errors of ray effect. Therefore, the possibility exists that changes in spatial grid can have a significant impact on ray effect, although no practical method to separate these errors from grid-dependent numerical smearing errors is apparent.

![Figure 1](image-url)
Considering the relationship in Eq. (4), reduction of propagation ray effect via spatial grid refinement (reduction of $\Delta \tau_x$) can additionally reduce numerical smearing error. However, it should be emphasized again, increasing discrete direction number $M$ under constant $\Delta \tau_x$ will reduce the minimum values of $\mu^l$, dramatically increasing the corresponding $E^l_x$ errors. Thus, reduction in $\mu^l$ requires a corresponding reduction in $\Delta \tau_x$ so that both ray effect and numerical truncation errors are minimized.

2.3 Angular False Scattering
Angular false scattering, mainly the non-preservation of asymmetry factor after angular discretization in highly anisotropic scattering media has been well documented in a series publications of Hunter and Guo [15, 17, 19]; and thus, it is not detailed here. Interested readers could refer to those publications and some other works by the same authors not cited here. It should be noted that the error in asymmetry factor could be eliminated.

3. RESULTS AND DISCUSSION
An analysis of the impact of numerical errors on radiative transfer predictions in a cubic enclosure using the DOM is presented. Unless otherwise stated, the positive spatial differencing scheme, which guarantees positive intensities and can attain up to 2nd-order accuracy and the SRAP$_N$ geometric, equal-weight quadrature scheme [21] are implemented in calculations.

An illustration of numerical truncation errors is presented in Figure 2, in which dimensionless heat fluxes generated at the centerline of the wall opposite the source wall in the benchmark problem described in ref. [22] are plotted for various spatial grid resolutions and numerical schemes. In order to solely gauge errors due to numerical smearing, $M = 160$ discrete directions are used, as a direction-independency test revealed that such direction number limits ray effect error. DOM heat fluxes are compared to benchmark Monte Carlo (MC) predictions. Figure 2 shows that errors due to numerical truncation are highly prevalent for lower spatial resolutions in the thicker medium ($\tau = 10.0$). Improvement in spatial grid resolution improves conformity to MC predictions. For $\tau = 1.0$, numerical truncation errors are minimal for all spatial grid resolutions, as $\Delta \tau_x \ll 1$ for most grids used. With use of high order numerical scheme, the results match MC data better.

![Figure 2: Illustration of numerical truncation error due to spatial discretization (MC results from [22]).](image)

An illustration of ray effect error due to finite angular discretization is presented in Figure 3. To ensure grid independency and limit numerical truncation error, the spatial grid is taken to be $\Delta x^* = 0.04$. Angular resolution has a profound impact when the medium is thin ($\tau = 1.0$), as ray effect manifests as unrealistic bumps in the heat flux profiles. Increase in angular resolution mitigates ray effect error. For the thick medium ($\tau = 10.0$), ray effect is minimal, due to the large increase in scattering events in a CV, reducing ray propagation errors. This is consistent with the findings of Chai et al. [6] and Raithby [7]. The percentage error in heat flux shows that refining angular grid resolution reduces ray effect error. Ray effect error decreases with increasing
optical thickness for all examined spatial grids, due to an increase in total scattering events and ray attenuation. Error due to ray effect is less than 2% for $\Delta\Omega^l \leq 0.0785$ ($M \geq 160$) for all optical properties, indicating that further refinement of angular resolution is unnecessary to generate accurate results. Comparing the results in Figures 2 and 3, it appears that while ray effect is dominant for thinner media, numerical truncation is dominant for thicker media. It is also noticed that reduction of $\Delta\tau$ can reduce both error types without corresponding or necessary change in $M$ or $\mu$. However, an increase in $M$ mandates a necessary decrease in $\Delta\tau$, in order to ensure minimization of both error sources.

![Figure 3: Impact of discrete direction number and optical thickness on ray effect error.](image)

![Figure 4: Comparison of individual and combined numerical errors vs. asymmetry factor.](image)

Figure 4 examines the individual and combined effects of numerical errors. For the low scattering medium, the combined ray effect and truncation error is generally less than each of their individual errors. The combined ray effect and angular false scattering error is the largest in general. For the purely scattering medium, the total error combining the three errors is the largest.

4. CONCLUSIONS

The impacts of numerical errors, namely numerical truncation, ray effect, and angular false scattering, on radiation transfer prediction are investigated and examined in detail. Proportionality expressions are derived for numerical truncation error, and ray effect is further classified into local and propagation components. The analysis revealed the relationship between numerical truncation and the ratio $\Delta\tau_x/\mu^l$, indicating dependence on
both angular and spatial discretization. It becomes critical to ensure that ratio is less than unity, to ensure minimal numerical truncation error. It also clarified that the spatial numerical truncation error affects both absorption and scattering, and should not be called false scattering. Ray propagation errors can be reduced via spatial grid refinement, while local error can be reduced via increasing Δτ. Most importantly, reduction of Δτ is able to reduce both numerical truncation and propagation ray effect without a necessary change in direction number, although an increase in direction number mandates a necessary decrease in Δτ in order to minimize both error sources. Numerical truncation error affects both absorption and scattering and should not be categorized as false scattering. Angular false scattering can be eliminated using Hunter and Guo’s phase-function normalization methods.

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