Truncation of the scattering phase matrix for vector radiative transfer simulation

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Abstract

This short communication interprets the delta-fit technique in a context of similarity transformation and the correction to the source function, and derives the analogous form of the method to be applied for the scattering phase matrix. To adapt the delta-fit method to radiative transfer, the mathematically exact form of the similarity principle is used in the theoretical development. Some examples of relevant radiative transfer simulations are also presented for atmospheric ice particles. The performance of the adopted delta-fit method is comparable to the delta-M method with single scattering correction except for worse delta-fit performance for polarized radiance calculations in forward directions.

Keywords: Truncation, phase matrix, vector radiative transfer

1. Introduction

In the application of vector radiative transfer solvers to simulate, for example, ice cloud reflectivity and transmissivity, the presence of large particles triggers a trade-off between the accuracy and speed of the simulation. The scattering properties of such large particles cannot be appropriately represented for the radiance simulation with an affordable directional resolution (number of streams). Anisotropic scattering in the planetary atmosphere has been a major challenge, and Sobolev [1] discusses multiple methods of approximation for highly anisotropic scattering problems. Current common practice is to adapt a truncation technique to minimize error due to the reduced directional resolution used in the numerical radiative transfer simulations.

The δ -fit method developed by Hu et al. [2] fits the scattering phase function with a limited number of Legendre polynomials to accurately simulate the radiance. The method contrasts with the δ -M method developed by Wiscombe [3], which focuses on accurate flux simulation. Each method starts with the following plane-parallel radiative transfer equation:

$$-\mu \frac{\partial I}{\partial \tau} = -I(\tau, \mu, \phi) + \frac{\varpi(\tau)}{4\pi} \int_{-1}^1 d\mu' \int_0^{2\pi} \mathcal{P}(\tau, \cos \Theta) I(\tau, \mu', \phi') d\phi' + (1 - \varpi)B(T), \quad (1)$$

where τ is optical thickness, μ is the cosine of the zenith angle, ϕ is the azimuth angle, $I(\tau, \mu, \phi)$ is the radiance propagating along the direction (μ, ϕ) , ϖ is the single scattering albedo, $\mathcal{P}(\cos \Theta)$ is the phase function value at scattering angle Θ , and $B(T)$ is the blackbody emission at temperature T .

Each method uses the following similarity transformation, which defines scaled variables with an arbitrary factor f in the form:

$$\tau^* = (1 - f\varpi)\tau, \quad (2)$$

$$\varpi^* = \frac{1 - f}{1 - f\varpi} \varpi, \quad (3)$$

$$\mathcal{P}^*(\cos(\Theta)) = \frac{1}{1 - f} [\mathcal{P}(\cos \Theta) - 4\pi f \delta(1 - \cos \Theta)], \quad (4)$$

where $\delta(1 - \cos \Theta)$ is the Dirac delta function peaked in the forward scattering direction. Substituting Eqs. (2)-(4) into Eq. (1) yields the same form for the radiative transfer equation but now for the scaled quantities indicated by the asterisk symbol; namely,

$$-\mu \frac{\partial I}{\partial \tau^*} = -I(\tau^*, \mu, \phi) + \frac{\varpi^*(\tau^*)}{4\pi} \int_{-1}^1 d\mu' \int_0^{2\pi} \mathcal{P}^*(\tau^*, \cos \Theta) I(\tau^*, \mu', \phi') d\phi' + (1 - \varpi^*)B(T). \quad (5)$$

In the classic approach (e.g. [4]), the original phase function $\mathcal{P}(\cos \Theta)$ is approximated by the sum of a delta function and a phase function without a forward peak $\mathcal{P}_{trunc}^*(\cos \Theta)$.

$$\mathcal{P}(\cos \Theta) \approx (1 - f)\mathcal{P}_{trunc}^*(\cos(\Theta)) + 4\pi f \delta(1 - \cos \Theta), \quad (6)$$

and the similarity transformation is derived as a consequence of the approximation. Eqs. (2)-(4) define an approximate radiative transfer problem in the classic approach.

However, the similarity transformation itself is mathematically exact [5, 6], and it is beneficial for our discussion to accept the exact similarity transformation to unambiguously derive the vectorized form of the δ -fit method. Specifically, we

interpret Eqs. (2)-(4) as definitions of scaled quantities τ^* , ϖ^* , and $\mathcal{P}^*(\cos(\theta))$ without approximations. When Eqs. (2)-(4) are strictly satisfied, the solution of Eq. (5) gives an exact solution of the original radiative transfer equation Eq. (1).

By accepting the exact similarity transformation, truncation techniques are seen as optimization techniques. Truncation techniques simultaneously adjust parameter f and $\mathcal{P}_N^*(\cos(\theta))$, which is a reconstructed phase function from N coefficients (c.f. Eq. (14)), to reduce the error in the flux or radiance. A similar interpretation is attempted by Mitrescu [6], who showed that the parameter f depends on the truncation method and the number of streams, in addition to the original phase function. Some systematic evaluations of these truncation techniques have been reported in the literature [7, 8].

This short communication applies the framework discussed above, and interprets the δ -fit method as a correction to the source function, following the approach taken by Rozanov and Lyapustin [7]. The outcome of the theoretical development is an adaptation of the δ -fit method to vector radiative transfer. Some adjustments of the present method are provided for numerical implementation as a user-friendly computer program.

2. The δ -fit method

This section briefly summarizes the δ -fit method based on the original paper by Hu et al. [2]. The traditional δ -fit method starts with the expansion of the phase function in terms of Legendre polynomials $P_s(x)$,

$$\mathcal{P}(x) = \sum_{s=0}^{\infty} \alpha_1^{(s)} P_s(x), \quad (7)$$

where $x = \cos \Theta$ and $\alpha_1^{(s)}$ is the expansion coefficient of order s . The δ -fit method approximates this phase function with a limited number of coefficients N that are the result of fitting in the form:

$$\hat{\mathcal{P}}_N(x) = \sum_{s=0}^N \hat{\alpha}_1^{(s)} P_s(x), \quad (8)$$

where a hat indicates that the quantity is a result of fitting.

The standard least squares method is employed to minimize the sum of squared differences between 1 and the ratio of the reconstructed phase function $\hat{\mathcal{P}}_N(x)$ to the original phase function $\mathcal{P}(x)$:

$$\varepsilon = \sum_{i=1}^m \left(\frac{\hat{\mathcal{P}}_N(x_i)}{\mathcal{P}(x_i)} - 1 \right)^2 w_i, \quad (9)$$

where w_i is the step-function weight defined by the truncation angle Θ_{trc} .

$$w_i = \begin{cases} 1, & x < \cos \Theta_{trc} \\ 0, & x \geq \cos \Theta_{trc}. \end{cases} \quad (10)$$

Linear least square fitting based on Eq. (9) by singular vector decomposition yields a set of coefficients $\hat{\alpha}_1^{(s)}$. Once a set of coefficients is obtained, the similarity transformation of the radiative transfer equation is utilized to satisfy the normalization condition of the phase function. Specifically, the following scaling adjustments are applied:

$$1 - f = \hat{\alpha}_1^{(0)}, \quad (11)$$

$$\hat{\alpha}_1^{(s)*} = \frac{\hat{\alpha}_1^{(s)}}{1-f}. \quad (12)$$

The scaling factor (truncation factor) f and fitted, scaled expansion coefficients $\hat{\alpha}_1^{(s)*}$ are used in an arbitrary solver of the scaled radiative transfer equation.

The fitting process in Eq. (9) can be rewritten as a linear least square fitting with weight inversely proportional to the variance in the tabulated phase function in the form:

$$\varepsilon/\varepsilon_1^2 = \sum_{i=1}^m (\hat{\mathcal{P}}_N(x_i) - \mathcal{P}(x_i))^2 \frac{w_i}{(\varepsilon_1 \mathcal{P}(x_i))^2}, \quad (13)$$

where ε_1 is the precision of the phase function. Note that $(\varepsilon_1 \mathcal{P}(x_i))^2$ is the variance of the phase function at the i th data point. The variance is due to the numerical implementation of light scattering calculations and the numerical representation of a phase function. The precision, ε_1 , is chosen as the largest value among machine precision, table precision, and the relative error in the numerical algorithm.

3. Source function correction by the δ -fit method

The effect of truncation is that the reconstructed phase function:

$$\mathcal{P}_N^*(x) = \sum_{s=0}^N \alpha_1^{(s)*} P_s(x) \quad (14)$$

may not fully describe the scaled phase function $\mathcal{P}^*(x)$ defined in Eq. (4). Note that the scaled radiative transfer equation (Eq. (5)) gives an exact solution only when $\mathcal{P}^*(x) = \mathcal{P}_N^*(x)$. This condition is usually not achieved because the delta function in $\mathcal{P}^*(x)$ requires an infinite number of coefficients to be fully expanded.

The error of the reconstructed phase function affects the radiative transfer equation through modifying the source function. Since the formal solution of the radiative transfer equation is an integral of the source function, the solution is affected by the error in the source function. For simplicity, we limit our discussion to cases with no emission. The untruncated source function is written as:

$$J(\tau^*, \mu, \phi) = \frac{\varpi^*}{4\pi} \int_{-1}^1 d\mu' \int_0^{2\pi} \mathcal{P}^*(\cos \Theta) I(\tau^*, \mu', \phi') d\phi', \quad (15)$$

and the truncated source function is written as:

$$J_N(\tau^*, \mu, \phi) = \frac{\varpi^*}{4\pi} \int_{-1}^1 d\mu' \int_0^{2\pi} \mathcal{P}_N^*(\cos \Theta) I(\tau^*, \mu', \phi') d\phi', \quad (16)$$

so the error in the source function is $J_N(\tau^*, \mu, \phi) - J(\tau^*, \mu, \phi)$. As the total radiance is a sum of direct solar radiation and diffuse radiation, the source function error can be written as the sum of two terms:

$$\begin{aligned} & J_N(\tau^*, \mu, \phi) - J(\tau^*, \mu, \phi) \\ &= \frac{\varpi^*}{4\pi} \int_{-1}^1 d\mu' \int_0^{2\pi} [\mathcal{P}_N^*(\cos \Theta) - \mathcal{P}^*(\cos \Theta)] I_{dir}(\tau^*, \mu', \phi') d\phi' \\ &+ \frac{\varpi^*}{4\pi} \int_{-1}^1 d\mu' \int_0^{2\pi} [\mathcal{P}_N^*(\cos \Theta) I_{diff,N}(\tau^*, \mu', \phi') \\ &- \mathcal{P}^*(\cos \Theta) I_{diff}(\tau^*, \mu', \phi')] d\phi'. \end{aligned} \quad (17)$$

where $I_{dir}(\tau^*, \mu', \phi')$ is the direct solar radiation, $I_{diff,N}(\tau^*, \mu', \phi')$ is the diffuse radiation with the truncated phase function, and $I_{diff}(\tau^*, \mu', \phi')$ is the diffuse radiation with the untruncated phase function.

It is well known that the radiance computed with the δ -M truncation shows a significant oscillation about the true value (e.g., Fig. 2). This is primarily because the

oscillation in the reconstructed phase function (see, Fig. 1 in [9]) propagates through the first term of Eq. (17) to cause the radiance error [7]. The oscillation mainly originates from the first term of Eq. (17) because the direct solar radiation $I_{dir}(\tau^*, \mu', \phi')$ is far more anisotropic than diffuse radiation $I_{diff}(\tau^*, \mu', \phi')$, which is a result of multiple scattering.

In the δ -fit method, a set of fitted coefficients $\hat{\alpha}_1^{(s)}$ that minimize the difference between the reconstructed phase function $\hat{\mathcal{P}}_N(x)$ and the original phase function $\mathcal{P}(x)$ is used after scaling. The resulting reconstructed scaled phase function $\hat{\mathcal{P}}_N^*(x)$ is close to $\mathcal{P}^*(x)$ because $\mathcal{P}(x)$ and $(1-f)\mathcal{P}^*(x)$ are identical except in the exact forward scattering direction. Specifically, we have

$$\hat{\mathcal{P}}_N^*(x) = \mathcal{P}^*(x) + \varepsilon_{fit}(x), \quad (18)$$

where the error of fitting $\varepsilon_{fit}(x)$ is small except between the forward scattering direction and a direction a few degrees from the specified truncation angle.

The δ -fit method minimizes the source function error by using $\hat{\mathcal{P}}_N^*(x)$, which is close to $\mathcal{P}^*(x)$. The source function error for the δ -fit method is as follows:

$$\begin{aligned} J_{fit,N}(\tau^*, \mu, \phi) - J(\tau^*, \mu, \phi) &= \frac{\overline{\omega}^*}{4\pi} \int_{-1}^1 d\mu' \int_0^{2\pi} \varepsilon_{fit}(\cos \Theta) I_{dir}(\tau^*, \mu', \phi') d\phi' \\ &+ \frac{\overline{\omega}^*}{4\pi} \int_{-1}^1 d\mu' \int_0^{2\pi} [\hat{\mathcal{P}}_N^*(\cos \Theta) I_{diff,N}(\tau^*, \mu', \phi') \\ &- \mathcal{P}^*(\cos \Theta) I_{diff}(\tau^*, \mu', \phi')] d\phi'. \end{aligned} \quad (19)$$

Equation (19) shows that the δ -fit method reduces the first term of the source function error in Eq. (18), and improves the accuracy of radiance computation.

Another approach to the source function correction is the TMS method [9]. Essentially, it applies $(1 - f)^{-1}\mathcal{P}(x) = \mathcal{P}^*(x) + 4\pi f(1 - f)^{-1}\delta(1 - \cos \Theta)$ for the single scattering source function and $\hat{\mathcal{P}}_N^*(x)$ for the multiple scattering source function. As multiple scattering is less anisotropic, this approach also significantly improves the accuracy of the radiance. Rozanov and Lyapustin [7] theoretically showed how the TMS method reduces the error. The disadvantage of the method is that a spurious delta function appears in the first-order source function, resulting in an inaccurate transmissivity. This shortcoming is corrected by the IMS method [9] to significantly reduce the error in the transmissivity calculation.

Correction of the source term by these two approaches might not conserve the low-order moments, so these methods are not suitable for flux calculations. The δ -M method [3] is designed to keep the lower order expansion coefficients for accurate flux computations. The contrast of the δ -fit method and the δ -M method originates from conserving different characteristics of the original phase function through truncations. The δ -fit method conserves the shape of the original phase function while the δ -M method conserves the expansion coefficients. As these two characteristics cannot be conserved simultaneously, a proper truncation technique should be selected based on the purpose.

4. Extending the δ -fit method in scattering matrix expansion

The vector radiative transfer equation for plane-parallel media is formulated with Stokes vector $\mathbf{I}(\tau, \mu, \phi)$ and phase matrix $\mathbf{Z}(\tau, \mu, \mu', \phi, \phi')$ as follows [10,11].

$$\begin{aligned}
-\mu \frac{\partial \mathbf{I}}{\partial \tau} = & -\mathbf{I}(\tau, \mu, \phi) + \frac{\varpi(\tau)}{4\pi} \int_{-1}^1 d\mu' \int_0^{2\pi} \mathbf{Z}(\tau, \mu, \mu', \phi, \phi') I(\tau, \mu', \phi') d\phi' \\
& + (1 - \varpi) \mathbf{B}(T),
\end{aligned} \tag{20}$$

where particles and their scattering plane mirror images are randomly oriented.

The similarity transformation also holds for the vector radiative transfer equation.

The reader is referred to [12] for the derivation.

Equation (20) is transformed by defining scaled variables as follows.

$$\tau^* = (1 - f\varpi)\tau, \tag{21}$$

$$\varpi^* = \frac{1 - f}{1 - f\varpi} \varpi, \tag{22}$$

$$\mathbf{Z}^*(\mu, \mu', \phi, \phi') = \frac{1}{1 - f} [\mathbf{Z}(\mu, \mu', \phi, \phi') - 4\pi f \mathbf{E} \delta(1 - \cos \Theta)]. \tag{23}$$

The phase matrix $\mathbf{Z}(\mu, \mu', \phi, \phi')$ is related to the scattering matrix $\mathbf{F}(\cos \Theta)$ by

$$\mathbf{Z}(\mu, \mu', \phi, \phi') = \mathbf{L}(-\sigma_2) \mathbf{F}(\cos \Theta) \mathbf{L}(\sigma_1), \tag{24}$$

where $\mathbf{L}(-\sigma_2)$ and $\mathbf{L}(\sigma_1)$ are rotation matrices of the second and third elements of the Stokes vector. The matrix $\mathbf{E}$ is the 4×4 identity matrix. Since the second term of Eq. (23) appears only in the exact forward scattering direction, the rotation matrices do not modify the identity matrix. This implies that Eq. (23) can be written in the following form:

$$\mathbf{F}^*(\mu, \mu', \phi, \phi') = \frac{1}{1 - f} [\mathbf{F}(\mu, \mu', \phi, \phi') - 4\pi f \mathbf{E} \delta(1 - \cos \Theta)]. \tag{25}$$

Denoting the elements of the scattering matrix as follows:

$$\mathbf{F}(\cos \Theta) = \begin{pmatrix} a_1(\cos \Theta) & b_1(\cos \Theta) & 0 & 0 \\ b_1(\cos \Theta) & a_2(\cos \Theta) & 0 & 0 \\ 0 & 0 & a_3(\cos \Theta) & b_2(\cos \Theta) \\ 0 & 0 & -b_2(\cos \Theta) & a_4(\cos \Theta) \end{pmatrix}, \quad (26)$$

the unique elements are expanded in terms of generalized spherical functions

$P_{q,r}^{(s)}(x)$:

$$a_1(x) = \sum_{s=0}^{\infty} \alpha_1^{(s)} P_{0,0}^{(s)}(x) = \sum_{s=0}^{\infty} \alpha_1^{(s)} P_s(x), \quad (27)$$

$$a_2(x) + a_3(x) = \sum_{s=0}^{\infty} [\alpha_2^{(s)} + \alpha_3^{(s)}] P_{2,2}^{(s)}(x), \quad (28)$$

$$a_2(x) - a_3(x) = \sum_{s=0}^{\infty} [\alpha_2^{(s)} - \alpha_3^{(s)}] P_{2,-2}^{(s)}(x), \quad (29)$$

$$a_4(x) = \sum_{s=0}^{\infty} \alpha_4^{(s)} P_{0,0}^{(s)}(x), \quad (30)$$

$$b_1(x) = \sum_{s=0}^{\infty} \beta_1^{(s)} P_{0,2}^{(s)}(x), \quad (31)$$

$$b_2(x) = \sum_{s=0}^{\infty} \beta_2^{(s)} P_{0,2}^{(s)}(x). \quad (32)$$

By defining $a_{\pm}(x) = a_2(x) \pm a_3(x)$ and $\alpha_{\pm}^{(s)} = \alpha_2^{(s)}(x) \pm \alpha_3^{(s)}(x)$, Eqs. (28) and (29)

are written as the following:

$$a_+(x) = \sum_{s=0}^{\infty} \alpha_+^{(s)} P_{2,2}^{(s)}(x), \quad (33)$$

$$a_-(x) = \sum_{s=0}^{\infty} \alpha_-^{(s)} P_{2,-2}^{(s)}(x). \quad (34)$$

The application of the δ -fit method is based on the same principle as in the scalar version. In an analogy to Eq. (18), we have

$$\widehat{\mathbf{F}}_N^*(x) = \mathbf{F}^*(x) + \varepsilon_{fit}(x) \quad (35)$$

Similar to the scalar case, elements in the scaled scattering matrix $\mathbf{F}^*(x)$ are identical to the elements of the original scattering matrix $\mathbf{F}(x)$ times the factor $(1 - f)^{-1}$ except in the exact forward direction (c.f. Eq. (25)). Therefore, the fitting process should minimize the differences between the original scattering matrix and the reconstructed scattering matrix, given by

$$\varepsilon_{a_p} = \sum_{i=0}^m \left(\frac{\hat{a}_{p,N}(x_i)}{a_p(x_i)} - 1 \right)^2 w_i , \quad (36)$$

$$\varepsilon_{b_q} = \sum_{i=0}^m \left(\frac{\hat{\beta}_{q,N}(x_i)}{b_q(x_i)} - 1 \right)^2 w_i . \quad (37)$$

Equation (36) is applied to diagonal elements ($p = 1, +, -, 4$), whereas Eq. (37) is applied to off-diagonal elements ($q = 1, 2$). All fittings are conducted independently, and the free parameter f is determined by the normalization constraints for $\mathbf{F}^*(x)$ and $\widehat{\mathbf{F}}_N^*(x)$.

$$1 - f = \hat{a}_1^{(0)} \quad (38)$$

Note that parameter f is solely determined by the fitting of $a_1(x)$. This guarantees the consistency between scalar and vector versions of the δ -fit method. The final coefficient set for $\widehat{\mathbf{F}}_N^*(x)$ is obtained by scaling all coefficients from the fitting Eqs. (36) and (37):

$$\hat{\alpha}_p^{(s)*} = \frac{\hat{\alpha}_p^{(s)}}{1-f}, \quad (39)$$

$$\hat{\beta}_q^{(s)*} = \frac{\hat{\beta}_q^{(s)}}{1-f}. \quad (40)$$

5. Theoretical comparison with other approaches

There are some other approaches to adapt the δ -fit method to fit a scattering matrix. Zhai et al. [13] used the standard δ -fit method to fit $a_1(x)$, and applied a scaling to obtain other matrix elements to fit. Their scaling is as follows:

$$a_{p,Z}^*(x) = \frac{a_p(x)}{a_1(x)} \hat{a}_{1N}^*(x), \quad (41)$$

$$b_{q,Z}^*(x) = \frac{b_q(x)}{a_1(x)} \hat{a}_{1N}^*(x), \quad (42)$$

where Z indicates that the phase matrix elements in the left hand side is to be fitted by their method.

The rationale for this treatment is the consistency of ratios a_p/a_1 and b_p/a_1 in all scattering directions. Ignoring the exact forward scattering direction and using Eqs. (25) and (35), we can rewrite Eqs. (41) and (42) as follows:

$$a_{p,Z}^*(x) = \frac{(1-f)a_p^*}{(1-f)a_1^*} [a_1^* + \varepsilon_{fit}(x)] = \left[1 + \frac{\varepsilon_{fit}(x)}{a_1^*} \right] a_p^*(x), \quad (43)$$

$$b_{q,Z}^*(x) = \frac{(1-f)b_q^*}{(1-f)a_1^*} [a_1^* + \varepsilon_{fit}(x)] = \left[1 + \frac{\varepsilon_{fit}(x)}{a_1^*} \right] b_q^*(x). \quad (44)$$

Note that these relations are strictly applicable except for the exact forward scattering direction. As discussed in the previous section, $\varepsilon_{fit}(x)$ is small except at small scattering angles. Therefore, the present approach and the approach

suggested by Zhai et al. [13] fit nearly the same function to obtain the expansion coefficients in side- to back-scattering directions.

Another adaptation proposed by Sanghavi and Stephens [12] also uses the standard δ -fit method to obtain coefficients $\hat{a}_p^{(s)*}$. The other reconstructed diagonal elements in the scattering matrix are as follows (see, Eq. 38 in [12]) :

$$\hat{a}_{2,N,S}^*(x) = \hat{a}_{2,N}^*(x) - f \sum_{s=0}^N \frac{2s+1}{1-f} \left[P_{2,2}^{(s)}(x) + P_{2,-2}^{(s)}(x) \right], \quad (45)$$

$$\hat{a}_{3,N,S}^*(x) = \hat{a}_{3,N}^*(x) - f \sum_{s=0}^N \frac{2s+1}{1-f} \left[P_{2,2}^{(s)}(x) - P_{2,-2}^{(s)}(x) \right], \quad (46)$$

$$\hat{a}_{4,N,S}^*(x) = \hat{a}_{4,N}^*(x) - f \sum_{s=0}^N \frac{2s+1}{1-f} P_{0,0}^{(s)}(x). \quad (47)$$

where S indicates that the phase matrix element is computed by Sanghavi's method. The second terms in Eqs, (45)-(47) are small when the number of expansion coefficients N is large.

6. Adjustments for numerical implementation

Unlike phase functions, scattering phase matrix elements often have zeros (neutral points) at some scattering angles. As obvious from Eq. (13), the original δ -fit method uses the weight $(\varepsilon_1 \mathcal{P}(x_i))^{-2}$, which is undefined at the aforementioned points. It is also counterintuitive that the accuracy of light scattering computation increases near neutral points. For this reason, we introduce an additional error term ε_2 to the weighting. The weighted fittings of the scattering phase matrix elements are performed by minimizing the following quantities:

$$\varepsilon'_{a_1} = \sum_{i=1}^m (\hat{a}_{1N}(x_i) - a_1(x_i))^2 \frac{w_i}{[\varepsilon_1 a_1(x_i)]^2 + [\varepsilon_2]^2}, \quad (46)$$

$$\varepsilon'_{a_+} = \sum_{i=1}^m (\hat{a}_{+N}(x_i) - a_+(x_i))^2 \frac{w_i}{[\varepsilon_1 a_2(x_i)]^2 + [\varepsilon_1 a_3(x_i)]^2 + [\varepsilon_2]^2}, \quad (47)$$

$$\varepsilon'_{a_-} = \sum_{i=1}^m (\hat{a}_{-N}(x_i) - a_-(x_i))^2 \frac{w_i}{[\varepsilon_1 a_2(x_i)]^2 + [\varepsilon_1 a_3(x_i)]^2 + [\varepsilon_2]^2}, \quad (48)$$

$$\varepsilon'_{a_4} = \sum_{i=1}^m (\hat{a}_{4N}(x_i) - a_4(x_i))^2 \frac{w_i}{[\varepsilon_1 a_4(x_i)]^2 + [\varepsilon_2]^2}, \quad (49)$$

$$\varepsilon'_{b_1} = \sum_{i=1}^m (\hat{b}_{1N}(x_i) - b_1(x_i))^2 \frac{w_i}{[\varepsilon_1 b_1(x_i)]^2 + [\varepsilon_2]^2}, \quad (50)$$

$$\varepsilon'_{b_4} = \sum_{i=1}^m (\hat{b}_{2N}(x_i) - b_2(x_i))^2 \frac{w_i}{[\varepsilon_1 b_2(x_i)]^2 + [\varepsilon_2]^2}. \quad (51)$$

Note that $a_1(x_i), \dots, b_2(x_i)$ are original scattering phase matrix elements, and $\hat{a}_{1N}(x_i), \dots, \hat{b}_{2N}(x_i)$ are reconstructed scattering phase matrix elements from N coefficients. Our experiments show that $\varepsilon_1 = 10^{-7}$ and $\varepsilon_2 = 10^{-10}$ are good choices for fitting typical bulk scattering properties of cloud and aerosol particles.

The original δ -fit method resamples the phase function at equal scattering angle intervals, but some other investigators use an equal sampling with respect to the cosine of scattering angles. The present numerical simulations show that the fitting results are better when equal $\mu = \cos \Theta$ intervals are used, or w_i are taken proportional to the difference of μ if other intervals are chosen.

7. Numerical validation of the theory

To demonstrate the performance of the vectorized δ -fit method, reflectivity and transmissivity of an ice cloud layer are computed by the adding-doubling radiative transfer model [11, 14]. A moderately roughened hexagonal column shape is selected from the scattering property library [15], and weighted over a gamma-like particle size distribution. The effective variance of the distribution is 0.1 and the effective diameter is $D_{eff} = 30 \mu\text{m}$. The cloud optical thickness is 5. Simulations are conducted at $0.865 \mu\text{m}$, and no contributions from background aerosol scattering and molecular Rayleigh scattering are considered.

The original phase matrix is fully expanded with 700 expansion coefficients for each scattering matrix element. The radiative transfer simulation result with 700 expansion coefficients is therefore used as a reference. The simulation results with scattering matrices truncated at 50 coefficients are compared with the reference. For the δ -fit method, the truncation angle is set to 5° . The original and reconstructed scattering phase matrix elements are shown in Fig. 1.

Fig. 2 shows the result for the reflected radiance in the principal plane. The top panel is the intensity of the reference calculation, and the middle and bottom panels show relative errors of truncated simulations. The δ -fit method which has no TMS correction performs as well as the δ -M method with TMS correction. The amplitude of oscillation in the reflected radiance is smallest when the δ -fit method is used, but the bias is close to zero with the δ -M plus TMS method. These results agree with previous studies [7, 8]. The transmissivity of the same cloud layer is presented in Fig. 3. The combination of the δ -M and TMS methods results in a significant error

in the forward direction. This is because the TMS method introduces a spurious source term in the forward direction.

Figures 4 and 5 shows the second element (Q) of the Stokes vector in the reflected and transmitted directions. The polarized reflectivity calculation with the δ -fit method shows a significant improvement over the δ -M method. The overall errors of δ -M + TMS and δ -fit methods are comparable, but the δ -M + TMS method shows smaller biases. The transmission calculation indicates that the δ -fit method performs worse, even compared to the δ -M method without TMS correction except near the forward direction. Since the δ -fit method improves scattering matrix consistency in side- to back-scattering directions at the expense of accuracy in forward scattering directions, the result is not surprising.

8. Conclusions

This short communication interprets the δ -fit method as a correction to the source function by adapting the similarity transformation to be mathematically exact. With this theoretical framework, the traditional δ -fit method is extended for phase matrix expansion. The vectorized δ -fit method is consistent with the traditional δ -fit method for the first scattering matrix element a_1 . Some adjustments to the traditional δ -fit method are applied to cope with a problem that is specific to phase matrix expansion.

The numerical experiment with an ice cloud phase matrix shows that the vectorized δ -fit method performs as well as the δ -M plus TMS method for reflectivity and polarized reflectivity calculations in the principal plane. The transmitted radiance calculation by the δ -fit method is also comparable to the δ -M plus TMS

method, but achieves better accuracy in the forward directions. The polarized transmitted radiance by the δ -fit method suffers from larger error than the δ -M method without TMS correction, especially in the forward direction. This is presumably because of the design of the δ -fit method.

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Fig. 1. Original and reconstructed scattering phase matrix elements. The reconstruction is from 50 coefficients computed by the δ -fit method. The scattering phase matrix elements are identical except in the forward direction.

Fig. 2. Reflected radiance in the principal plane by an untruncated scattering matrix with 700 expansion coefficients (top) and relative errors of radiative transfer simulations with scattering matrices truncated at 50 coefficients (middle, bottom). The bottom panel expands around zero error. The solar zenith angle is $\theta_0 = 60^\circ$, and the result for relative azimuth angle $\phi = 0^\circ$ is plotted with positive viewing zenith angles, and the result for relative azimuth angle $\phi = 180^\circ$ is plotted with negative viewing zenith angles. The peak in the error at -60° corresponds to the glory direction.

Fig. 3. The same as Fig. 2, but for transmitted radiance.

Fig. 4. The same as Fig. 2, but for the second element of the Stokes vector in the reflected direction. Note that the third element is zero in the principal plane. In the vicinity of neutral points, data points are removed from relative error plots (middle, bottom)

Fig. 5. The same as Fig. 3, but for the second element of the Stokes vector in the transmission direction.