cc

Radiative Transfer Single Scattering Albedo
Estimation With A SuperPadé Approximation Of
Chandrasekhar's H-Function

Eric Steinfelds and Mark A. Samuel
Department of Physics, Oklahoma State University
Stillwater, Oklahoma 74078

N. J. McCormick
Department of Mechanical Engineering, University of Washington
Seattle, Washington 98195-2600

James H. Reid
L. H. Lanzl Institute of Medical Physics
3600 15th Avenue W, Seattle, Washington 98119

Abstract

Three algorithms for evaluating the single scattering albedo within an isotropically scattering semi-infinite medium from measurements external to the medium are developed. Two of the algorithms require the computation of the Chandrasekhar H -function, which is done by means of a new SuperPadé approximation technique.

1. Introduction

The objective of this work is two-fold: a) to solve an inverse radiative transfer problem for a large (effectively semi-infinite) isotropic scattering medium that is illuminated uniformly over its surface, and b) to introduce a new way of approximately evaluating the Chandrasekhar¹ H -function.

The application of the H -function calculation to an inverse problem presented here involves the estimation of the single scattering albedo, ϖ . For a set of prescribed incident illumination conditions Siewert² developed a very succinct set of equations for determining ϖ from measured values of one (or in all other cases two) directionally-integrated moments of the outgoing radiance; his paper appears to be the first to show the potential for estimating the scattering properties of a multiple-scattering medium by using a detector located only outside the medium. His algorithm, however, requires that the incident illumination be distributed over the hemisphere of incident directions either in an isotropic (or in all other cases a prescribed anisotropic) manner.

Here we will show that by requiring that the incident illumination be normally incident, which is more typical of a laser beam experiment, for example, and measuring only the normally-directed backscattered radiance with a narrow field-of-view (FOV) detector, then

SW96 28

ϖ can be estimated from an algorithm involving the H -function evaluated at the normally-inward direction. On the other hand, if only a flat-surface (hemispherical FOV) detector is available, ϖ can be estimated with a different algorithm and the same H -function. By combining the two algorithms then the H -function need not even be computed, but this requires the use of both detectors.

Several approximate methods have been used to evaluate the H -function,³⁻⁷ including a low-level Padé approximation.⁴ The numerical approximation method for the computation of the H -function used here relies on the use of Padé approximants to solve the nonlinear integral equation

$$H(z) = 1 + \frac{\varpi z}{2} H(z) \int_0^1 \frac{H(\mu)}{z + \mu} d\mu, \quad z \notin [-1, 0], \quad (1)$$

where ϖ is the single-scattering albedo and z is a complex variable. An important constraint on $H(z)$ is that $H^{-1}(-\nu_0) = 0$, where $\nu_0 > 1$ is the positive discrete eigenvalue of the homogeneous radiative transport equation, as given by the positive root of

$$\frac{\varpi z}{2} \ln \left[\frac{z+1}{z-1} \right] = 1, \quad z \notin [-1, 1]. \quad (2)$$

In the method of Padé approximants^{3,9} a function is approximated by a ratio of two polynomials. For a given power series

$$S(z) = S_0(z) + S_1(z)\varpi + \dots + S_J(z)\varpi^J, \quad (3)$$

where $J = N + M$, a Padé approximant (PA) is written as

$$[N/M] = \frac{a_0(z) + a_1(z)\varpi + \dots + a_N(z)\varpi^N}{1 + b_1(z)\varpi + \dots + b_M(z)\varpi^M} \quad (4)$$

where $[N/M] = S(z) + O(\varpi^{J+1})$. Once the coefficients $a_i(z)$ and $b_i(z)$ have been determined, a Padé approximant prediction (PAP) for the next coefficient in the power series $S_{J+1}(z)$ follows from the PA. Also, an estimate of the sum of the series, i.e., the full Padé summation (FPS), can be obtained. The PAP and FPS have been applied with remarkable success to the perturbation expansions of quantum field theory and statistical mechanics by Samuel *et al.*^{10,11}

One of us (Steinfelds¹²) has proposed using the method of PA to accelerate the convergence of iterative solutions of Fredholm-type integral equations. The nonlinear integral equation for the H -function in Eq. (1) is of a type to which this method can be applied. In this instance, the power series expansion is taken in terms of the albedo ϖ .

Siewert's algorithm² and three algorithms for solving the inverse problem are in Sec. 2. Section 3 contains a detailed exposition of the numerical algorithms used to evaluate the H -function with SuperPadé approximations and Sec. 4 provides some numerical results.

2. Inverse Albedo Estimation Algorithms

The radiation intensity $I(x, \mu)$ for $x \geq 0$ is taken to be a function of the direction cosine μ measured with respect to the (dimensionless) mean-free-path distance x from the surface into the semi-infinite medium. For isotropic scattering the radiative transfer equation for the semi-infinite medium is

$$\mu \frac{\partial}{\partial x} I(x, \mu) + I(x, \mu) = \frac{\varpi}{2} \int_{-1}^1 I(x, \mu') d\mu', \quad x > 0, \quad (5)$$

for $\varpi < 1$, where

$$I(x, \mu) = \int_0^{2\pi} I(x, \mu, \phi) d\phi \quad (6)$$

and ϕ is the azimuthal angle measured in the plane perpendicular to the x -axis. The half-space problem is defined by the incident illumination

$$I(0, \mu) = F(\mu), \quad \mu > 0, \quad (7)$$

and the constraint that $I(x, \mu) \rightarrow 0$ as $x \rightarrow \infty$. Chandrasekhar¹ has shown that the radiation emerging from the half-space is given by

$$I(0, -\mu) = \frac{\varpi}{2} H(\mu) \int_0^1 \frac{H(\mu') F(\mu') \mu'}{\mu' + \mu} d\mu', \quad \mu > 0, \quad (8)$$

where $H(\mu)$ satisfies Eq. (1).

Siewert² showed for the general class of “ β -moment” boundary conditions $F(\mu) = K\mu^\beta$, $\mu > 0$, that if various angular moments of the emerging radiance $I^{(\beta)}(0, -\mu)$ were measured, as defined by

$$E_\alpha^{(\beta)} = \int_0^1 I^{(\beta)}(0, -\mu) \mu^\alpha d\mu, \quad (9)$$

then ϖ can be estimated from any of the set of equations

$$\varpi = 4 \frac{K^{-1} E_\beta^{(\beta)}}{[K^{-1} E_0^{(\beta)} + (\beta + 1)^{-1}]^2}, \quad \beta = 0, 1, 2, \dots \quad (10)$$

A major limitation in using this equation, however, is that the $F(\mu) = K\mu^\beta$ incident illumination is difficult to experimentally achieve, and because only the measurement of $E_1^{(\beta)}$ can be conveniently done with a flat-surface hemispherical FOV detector.

Because of these limitations we instead force the incident illumination to satisfy the normally-incident, “ δ ”-boundary condition $F(\mu) = K\delta(\mu - 1)$, $\mu > 0$, and observe from Eq. (8) that

$$I^{(\delta)}(0, -\mu) = K \frac{\varpi H(1)}{2} \frac{H(\mu)}{\mu + 1}, \quad \mu > 0. \quad (11)$$

Thus with the use of a normally-directed, narrow FOV detector that measures $I^{(\delta)}(0, -1)$,

$$\varpi H^2(1) = 4K^{-1}I^{(\delta)}(0, -1) . \quad (12)$$

This is an algorithm for implicitly estimating ϖ from $\varpi H^2(1)$, which can be easily done with the SuperPadé results of Sec. 3.

Another algorithm that could be conveniently implemented is to use a flat-surface hemispherical FOV detector and then measure $E_1^{(\delta)}$, defined similarly to Eq. (9) with $F(\mu) = K\delta(\mu - 1)$, $\mu > 0$. From Eq. (11) it then follows that

$$E_1^{(\delta)} = K \frac{\varpi H(1)}{2} \int_0^1 \frac{H(\mu)\mu}{\mu + 1} d\mu . \quad (13)$$

But use of a partial fraction expansion and Eq. (1) shows that

$$\frac{\varpi H(1)}{2} \int_0^1 \frac{H(\mu)\mu}{\mu + 1} d\mu = 1 - \left(1 - \frac{\varpi\alpha_0}{2}\right) H(1) , \quad (14)$$

where $\alpha_k = \int_0^1 \mu^k H(\mu) d\mu$. For isotropic scattering¹

$$1 - \frac{\varpi\alpha_0}{2} = (1 - \varpi)^{1/2} , \quad (15)$$

so it follows from the last three equations that a second algorithm for estimating ϖ is

$$(1 - \varpi)H^2(1) = (1 - K^{-1}E_1^{(\delta)})^2 . \quad (16)$$

Finally, from the ratio of Eqs. (12) and (16) it follows that

$$\left(\frac{1 - \varpi}{\varpi}\right) = \frac{(1 - K^{-1}E_1^{(\delta)})^2}{4K^{-1}I^{(\delta)}(0, -1)} . \quad (17)$$

This third algorithm is an explicit algorithm that does not require computation of $H(1)$, but measurements are needed with both the normally-directed narrow FOV and the flat-surface hemispherical FOV detectors. The result also can be obtained as a special case, for monodirectional illumination and isotropic scattering of a half-space, from an inverse radiative transfer equation derived in a different way.¹³

While the primary application of Eqs. (10), (12), (16), and (17) is to estimate ϖ , the equations also could be used in a different manner. If ϖ is known and the measurement errors for the radiation field can be neglected, then the difference between the left-hand and right-hand sides of these four equations could give an indirect indication of the degree of scattering anisotropy.

3. Approximants For The H -Function

The PA method has been applied in a variety of disciplines. For quantum electrodynamics and quantum chromodynamics, for example, the perturbation series are divergent and may not even be Borel summable and the coefficients in the power series are believed to diverge strongly like $S_n = n!k^n n^\gamma$, where k and γ are constants that depend on the problem under consideration.¹⁴ Yet the PAP works well for QED and QCD and also for series generated in statistical mechanics.^{10,11} Perhaps the ability of a sufficiently complicated rational function to imitate the analytic structure of some given function accounts for this success. For large enough N and M , zeros and poles of any function can be exactly reproduced, and branch points and essential singularities approximated by a set of poles.

Steinfelds¹² has suggested an application of the PA method to the solution of Fredholm integral equations of the second kind. To apply the PA method to Eq. (1) suggests that we rewrite the equation as

$$H(z) = 1 + \varpi H(z) \int_0^1 G(z, \mu) H(\mu) d\mu . \quad (18)$$

Here ϖ can be viewed as the power series expansion parameter. Let the n th iterate in the Neumann series solution to this equation be $H_n(z)$ and define

$$S_n(z) = \frac{H_{n+1}(z) - H_n(z)}{\varpi^n} . \quad (19)$$

Once the $S_n(z)$ have been computed for $n = 1$ to J we construct the PA of Eq. (4). Then the PA method predicts the next term $S_{J+1}(z)$. In particular,

$$\begin{aligned} S_0(z) &= 1 , \\ S_1(z) &= \int_0^1 G(z, \mu) d\mu , & (a) \\ S_2(z) &= \int_0^1 G(z, \mu) d\mu \int_0^1 G(z, \mu') d\mu' , & (b) \\ &+ \int_0^1 \int_0^1 G(z, \mu) G(\mu, \mu') d\mu' d\mu , & (c) \\ S_3(z) &= \int_0^1 G(z, \mu) d\mu \int_0^1 G(z, \mu') d\mu' \int_0^1 G(z, \mu'') d\mu'' , & (d) \\ &+ \int_0^1 G(z, \mu'') d\mu'' \int_0^1 \int_0^1 G(z, \mu) G(\mu, \mu') d\mu' d\mu , & (e) \\ &+ \int_0^1 \int_0^1 G(z, \mu) G(\mu, \mu') d\mu' d\mu \int_0^1 G(z, \mu'') d\mu'' , & (f) \\ &+ \int_0^1 G(z, \mu) \int_0^1 G(\mu, \mu') d\mu' \int_0^1 G(\mu, \mu'') d\mu'' d\mu , & (g) \\ &+ \int_0^1 G(z, \mu) \int_0^1 G(\mu, \mu') \int_0^1 G(\mu', \mu'') d\mu'' d\mu' d\mu , & (h) \end{aligned} \quad (20)$$

etc. The nesting of the integrals in these terms can be represented by diagrams that resemble uncrossed corrections to a propagator in quantum field theory. Figure 1 illustrates the diagrams for the terms (a) through (h) in the preceding equation.

Since we have the means to estimate the next term PAP, and we also have error formulas (that include the sign) for the PAP, we can correct the PAP to obtain a more precise estimate that we call the SuperPadé approximant prediction (SPAP) defined by

$$\hat{S}_{N+M+1} = \frac{S_{N+M+1}}{1 + r} , \quad (21)$$

where S_{N+M+1} is the PAP of Eq. (3) and $\hat{S}_{N+M+1}$ is the SPAP. For the H -function for $z = 1$, the formula for r for the N/M PAP in Eq. (21) is¹⁰

$$r = -M!B(B+1)\dots(B+M-1)/L^{2M} , \quad (22)$$

where r is the relative error (i.e., the estimate minus the exact, all divided by the exact) and¹⁰

$$L = N + M + aM + b . \quad (23)$$

In our case the constants B , a , and b were determined by first examining the numerical values of $S_1(1)$ to $S_7(1)$ and comparing the results to those in the following equations¹¹

$$S_{n+2} = S_{n+1}^2/S_n , \quad [n/1]\text{PAP} , \quad (24)$$

$$S_{n+3} = \frac{2S_n S_{n+1} S_{n+2} - S_{n-1} S_{n+2}^2 - S_{n+1}^3}{S_n^2 - S_{n-1} S_{n+1}} , \quad [n/2]\text{PAP} , \quad (25)$$

with $S_j = 0$ for $j < 0$. (Formulas for S_n for $M = 3$ and 4 are also given in Ref. 11. For general N and M the PAPs are constructed numerically.) We then calculated r for the PAPs for small N and M and determined that r is given by the error formula in Eq. (22) with $B = 1.34$, $a = -0.5$, and $b = 1.6$. We then used $\hat{S}_{N+M+1}$, applied the PAP again to obtain S_{N+M+2} , and then applied the correction again and after using Eq. (21) obtained the SPAP $\hat{S}_{N+M+2}$; the process can be continued indefinitely.

4. Numerical Results For The H -Function

Our results for the number of terms in $S_n(z)$ (i.e., diagrams of Fig. 1) versus n needed for the H -function for $n = 1$ to $n = 11$ are 1, 2, 5, 14, 42, 132, 429, 1430, 4862, 16796, 58786, etc. For the number of terms indicated we checked our predictions by direct counting for $n = 1$ to $n = 9$. The SPAP agrees with the direct counting exactly; in fact, when they initially disagreed for $n = 7$ a check revealed an error in the direct counting. Later a direct calculation of $S_9(1)$ agreed with our estimate to within 0.014%.

In Table 1 we give the FPS results for the 3/4, 4/3, and the 4/4. The ordinary partial sum (PS) results, given by Eq. (3), are also given. It can be seen that in all cases the Padé results are more precise than the corresponding PS results, up to $n = 7$. It should be emphasized that the FPS results use the same input as the PS.

Table 2 contains the coefficients from $n = 0$ to $n = 15$. The results for $n = 0$ to 5 were used along with the SPAP to obtain the results for $n = 6$ and 7 , which agreed with the

direct calculation to within $< 0.1\%$. The results for $n = 0$ to 7 were then used to obtain the coefficients for n up to 15 by repeated application of the SuperPadé method.

Table 3 gives results for the percent error for the $H(1)$ -function when compared with the “exact” results of Stibbs and Weir.¹⁵ The SuperPadé evaluation of $H(1)$ is a more severe test of the method than for $H(\mu)$, $0 \leq \mu < 1$, since in general the full Padé summation (FPS) for smaller values of μ are more precise. The FPS is compared with the PS results in Table 3 for the same number of $S_n(1)$ coefficients, $n = 0$ to 7. It can be seen that in all cases the FPS results are much more precise than the PS results.

5. Concluding Comments

A concise way of estimating the single scattering albedo ϖ has been developed, along with an approximate method of computing the Chandrasekhar H -function needed for two of the inverse algorithms. Although in this paper we have focused on evaluating algorithms for a normally incident illumination ($\mu = 1$), the algorithms also can be extended to non-normally incident illumination ($\mu < 1$) but require azimuthally-dependent measurements; in such cases, our numerical results for $\mu < 1$ are even better than shown here. We believe that the methods used here may be of great practical utility in solving linear integral equations as well as other nonlinear integral equations.

Acknowledgments

This work was supported in part by the U.S. Department of Energy under grant DE-FG05-84ER40215. The authors appreciate the initiative of David Jette and the Lanzl Institute in bringing our research team together.

Figure caption

Fig. 1. Diagrams of $S_n(z)$ terms in Eq. (20) for $n = 1$ to 3

REFERENCES

1. S. Chandrasekhar, *Radiative Transfer* (Dover, New York, 1960).
2. C. E. Siewert, J. Math. Phys. **19**, 1587-1588 (1978).
3. I. Abu-Shumays, Nucl. Sci. Eng. **26**, 430-431 (1966).
4. I. Abu-Shumays, Nucl. Sci. Eng. **27**, 607-608 (1967).
5. C. T. Kelley, J. Math. Phys. **19**, 500-51 (1978).
6. C. T. Kelley, J. Math. Phys. **21**, 1625-1628 (1980).
7. C. T. Kelley, J. Math. Phys. **23**, 2097-2100 (1982).
8. G. A. Baker, Jr., *Essentials of Padé Approximants* (Academic, New York, 1975).
9. C. Bender and S. Orszag, *Advanced Mathematical Methods for Scientists and Engineers* (McGraw-Hill, New York, 1978).
10. M. A. Samuel, J. Ellis, and M. Karliner, Phys. Rev. Lett. **74**, 4380-4383 (1995); J. Ellis, E. Gardi, M. Karliner, and M. A. Samuel, Phys. Lett. **B366**, 268-27??? (1996).
11. M. A. Samuel, G. Li, and E. Steinfelds, Phys. Rev. E **51**, 3911-3933 (1995).
12. E. Steinfelds, Oklahoma State Univ. (private communication, 1995).
13. C. E. Siewert, J. Appl. Math. Phys. (ZAMP) **30**, 522 (1979).
14. A. I. Vainshtein and V. I. Zakharov, Phys. Rev. Lett. **73**, 1207 (1994).
15. D. W. N. Stibbs and R. E. Weir, Mon. Not. Roy. Astronom. Soc. **119**, 512 (1959).

Table 1. $H(1)$ functions obtained with Padé approximants and from partial sums with 7th order iterations

π	Pade34	Pade43	Pade44	Prtl Sum (PS)	"Exact"
0.3	1.1268438	1.1268438	1.126844	1.126843	1.126844
0.5	1.251255	1.251254	1.251257	1.250940	1.251259
0.8	1.597526	1.597457	1.597945	1.571937	1.598219
0.9	1.842901	1.842344	1.846299	1.748239	1.850098
0.95	2.045295	2.043641	2.056968	1.857371	2.077123
0.975	2.189267	2.1861712	2.212264	1.918297	2.270984
0.99	2.299123	2.294248	2.334419	1.957090	2.472792
0.995	2.340862	2.335252	2.382079	1.970430	2.587346
1.0	2.385145	2.378988	2.434109	1.983958	2.907809

Table 2. Coefficients $S_n(1)$ for $H(1)$ functions obtained directly from Eq. (21) up to $n = 7$ and from the SuperPadé Approximant Prediction for $n \geq 8$.

n	$S_n(1)$	n	$S_n(1)$	n	$S_n(1)$
1	0.693147	10	35.257	19	7224.31
2	0.804054	11	62.263	20	13300.4
3	1.096628	12	110.84	21	24549.8
4	1.626989	13	198.62	22	45434.9
5	2.544145	14	357.89	23	84357.1
6	4.125346	15	647.94	24	157341.
7	6.870243	16	1177.9	25	295683.
8	11.6787	17	2149.3	26	563063.
9	20.164	18	3934.6		

Table 3. $H(1)$ functions obtained from the SuperPadé Approximant Prediction (SPAP) and Partial Sum (PS) methods.

ϖ	(SPAP)	(PS)	"exact"
0.1	1.03682	1.03682	1.036815
0.2	1.07864	1.07861	1.078644
0.3	1.12684	1.12684	1.126844
0.4	1.18337	1.18325	1.183380
0.5	1.25126	1.25094	1.251259
0.6	1.33540	1.33379	1.335406
0.7	1.44469	1.43790	1.444745
0.8	1.59797	1.57195	1.598219
0.85	1.70433	1.65388	1.704991
0.9	1.84833	1.74826	1.850098
0.925	1.94522	1.80082	1.947955
0.95	2.07339	1.85740	2.077123
0.975	2.26728	1.91833	2.270984
0.99	2.46309	1.95713	2.472792
0.995	2.55935	1.97046	2.587346
1.0	2.68543	1.98399	2.907809

$S_1(z)$

$S_2(z)$

$S_3(z)$

(c)

(e)

(f)

(g)

(h)

S1(z)

S2(z)

S3(z)