

# Chapter 8

## Theory of Differential Approximations of Radiative Transfer Equation

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**Abstract** The radiative transfer equation (RTE) arises in a variety of applications. The equation is challenging to solve numerically for a couple of reasons: high dimensionality, integro-differential form, highly forward-peaked scattering in application. In the literature, various approximations of RTE have been proposed in the literature. In an earlier publication, we explored a family of differential approximations to RTE, to be called RT/DA equations. In this paper, we study the RT/DA equations and investigate numerically the closeness of solutions of the RT/DA equations to that of the RTE.

### 8.1 Introduction

The radiative transfer equation (RTE) arises in a variety of applications, such as neutron transport, heat transfer, stellar atmospheres, optical molecular imaging, infrared and visible light in space and the atmosphere, and so on. We refer the reader to [1, 14, 15, 19, 20]. Recently, there is much interest in analysis and numerical simulation of the RTE and its related inverse problems, motivated by applications in biomedical optics [4, 7, 8].

We proceed to give a brief description of RTE as follows. Let  $X$  be a domain in  $\mathbb{R}^3$  with a Lipschitz boundary  $\partial X$ . The unit outward normal  $n(x)$  exists a.e. on  $\partial X$ . Denote by  $\Omega$  the unit sphere in  $\mathbb{R}^3$ . For each fixed direction  $\omega \in \Omega$ , introduce a new Cartesian coordinate system  $(z_1, z_2, s)$  by the relations

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$$x = z + s\omega, \quad z = z_1\omega_1 + z_2\omega_2,$$

where  $(\omega_1, \omega_2, \omega)$  is an orthonormal basis of  $\mathbb{R}^3$ ,  $z_1, z_2, s \in \mathbb{R}$ . With respect to this new coordinate system, we denote by  $X_\omega$  the projection of  $X$  on the plane  $s = 0$  in  $\mathbb{R}^3$  and by  $X_{\omega,z}$  ( $z \in X_\omega$ ) the intersection of the straight line  $\{z + s\omega \mid s \in \mathbb{R}\}$  with  $X$ . We assume that the domain  $X$  is such that for any  $(\omega, z)$  with  $z \in X_\omega$ ,  $X_{\omega,z}$  is the union of a finite number of line segments:

$$X_{\omega,z} = \bigcup_{i=1}^{N(\omega,z)} \{z + s\omega \mid s \in (s_{i,-}, s_{i,+})\}.$$

Here  $s_{i,\pm} = s_{i,\pm}(\omega, z)$  depend on  $\omega$  and  $z$ , and  $x_{i,\pm} := z + s_{i,\pm}\omega$  are the intersection points of the line  $\{z + s\omega \mid s \in \mathbb{R}\}$  with  $\partial X$ . We further assume  $\sup_{\omega,z} N(\omega, z) < \infty$ , known as a generalized convexity condition. As an example, for a convex domain  $X$ ,  $\sup_{\omega,z} N(\omega, z) = 1$ . We then introduce the following subsets of  $\partial X$ :

$$\partial X_{\omega,-} = \{z + s_{i,-}\omega \mid 1 \leq i \leq N(\omega, z), z \in X_\omega\},$$

$$\partial X_{\omega,+} = \{z + s_{i,+}\omega \mid 1 \leq i \leq N(\omega, z), z \in X_\omega\}.$$

It can be shown that for a.e.  $z \in X_\omega$ ,  $n(z + s_{i,-}\omega) \cdot \omega \leq 0$ ; if  $x \in \partial X$  and  $n(x) \cdot \omega < 0$ , then  $x \in \partial X_{\omega,-}$ . Likewise, for a.e.  $z \in X_\omega$ ,  $n(z + s_{i,+}\omega) \cdot \omega \geq 0$ ; if  $x \in \partial X$  and  $n(x) \cdot \omega > 0$ , then  $x \in \partial X_{\omega,+}$ . Then the incoming boundary  $\Gamma_-$  and outgoing boundary  $\Gamma_+$  are

$$\Gamma_- = \{(x, \omega) \mid x \in \partial X_{\omega,-}, \omega \in \Omega\}, \quad \Gamma_+ = \{(x, \omega) \mid x \in \partial X_{\omega,+}, \omega \in \Omega\}.$$

Denote by  $d\sigma(\omega)$  the infinitesimal area element on the unit sphere  $\Omega$ . For the spherical coordinate system

$$\omega = (\sin \theta \cos \psi, \sin \theta \sin \psi, \cos \theta)^T, \quad 0 \leq \theta \leq \pi, \quad 0 \leq \psi \leq 2\pi, \quad (8.1)$$

$d\sigma(\omega) = \sin \theta d\theta d\psi$ . We will need an integral operator  $S$  defined by

$$(Su)(x, \omega) = \int_{\Omega} k(\omega \cdot \hat{\omega}) u(x, \hat{\omega}) d\sigma(\hat{\omega}) \quad (8.2)$$

with  $k$  a nonnegative normalized phase function:

$$\int_{\Omega} k(\omega \cdot \hat{\omega}) d\sigma(\hat{\omega}) = 1 \quad \forall \omega \in \Omega. \quad (8.3)$$

One well-known example is the Henyey–Greenstein phase function (cf. [10])

$$k(t) = \frac{1 - g^2}{4\pi(1 + g^2 - 2gt)^{3/2}}, \quad t \in [-1, 1], \quad (8.4)$$

where the parameter  $g \in (-1, 1)$  is the anisotropy factor of the scattering medium. Note that  $g = 0$  for isotropic scattering,  $g > 0$  for forward scattering, and  $g < 0$  for backward scattering.

With the above notation, a boundary value problem of the RTE reads (cf. [1, 13])

$$\omega \cdot \nabla u(x, \omega) + \sigma_t(x) u(x, \omega) = \sigma_s(x) (Su)(x, \omega) + f(x, \omega), \quad (x, \omega) \in X \times \Omega, \quad (8.5)$$

$$u(x, \omega) = u_{\text{in}}(x, \omega), \quad (x, \omega) \in \Gamma_-. \quad (8.6)$$

Here  $\sigma_t = \sigma_a + \sigma_s$ ,  $\sigma_a$  is the macroscopic absorption cross section,  $\sigma_s$  is the macroscopic scattering cross section, and  $f$  and  $u_{\text{in}}$  are source functions in  $X$  and on  $\Gamma_-$ , respectively. We assume that these given functions satisfy

$$\sigma_t, \sigma_s \in L^\infty(X), \quad \sigma_s \geq 0 \text{ and } \sigma_t - \sigma_s \geq c_0 \text{ in } X \text{ for some constant } c_0 > 0, \quad (8.7)$$

$$f \in L^2(X \times \Omega), \quad u_{\text{in}} \in L^2(\Gamma_-). \quad (8.8)$$

These assumptions are naturally valid in applications; the last part of (8.7) means that the absorption effect is not negligible. For a vacuum setting around  $X$ , the incoming flux boundary condition  $u_{\text{in}}(x, \omega) = 0$  on  $\Gamma_-$ .

It can be shown [1] that the problem (8.5)–(8.6) has a unique solution  $u \in H_2^1(X \times \Omega)$ , where

$$H_2^1(X \times \Omega) := \{v \in L^2(X \times \Omega) \mid \omega \cdot \nabla v \in L^2(X \times \Omega)\}$$

with  $\omega \cdot \nabla v$  denoting the generalized directional derivative of  $v$  in the direction  $\omega$ .

It is challenging to solve the RTE problem numerically for a couple of reasons. First, it is a high-dimensional problem. The spatial domain is three dimensional and the region for the angular variable is two dimensional. Second, when the RTE is discretized by the popular discrete-ordinate method, the integral term  $Su(x, \omega)$  on the right side of the equation is approximated by a summation that involves all the numerical integration points on the unit sphere. Consequently, for the resulting discrete system, the desired locality property is not valid, and many of the solution techniques for solving sparse systems from discretization of partial differential equations cannot be applied efficiently to solve the discrete systems of RTE. Moreover, in applications involving highly forward-peaked media, which are typical in biomedical imaging, the phase function tends to be numerically singular. Take the Henyey–Greenstein phase function (8.4) as an example:  $k(1) = (1 + g)/[4\pi(1 - g)^2]$  blows up as  $g \rightarrow 1^-$ . In such applications, it is even more difficult to solve RTE since accurate numerical solutions require a high resolution of the direction variable, leading to prohibitively large amount of computations. For these reasons, various approximations of RTE have been proposed in the literature, e.g., the delta-Eddington approximation [11], the Fokker–Planck approximation [16, 17], the Boltzmann–Fokker–Planck approximation [5, 18], the generalized Fokker–Planck approximation [12], the Fokker–Planck–Eddington approximation, and the generalized Fokker–Planck–Eddington approximation [6]. In [9], we provided a preliminary study of a family of differential approximations of the RTE. For convenience, we will call these approximation equations as RT/DA (radiative transfer/differential approximation) equations. An RT/DA equation with  $j$  terms for the approximation of the integral operator will be called an RT/DA $_j$  equation.

This paper is devoted to a mathematical study of the RT/DA equations, as well as numerical experiments on how accurate are the RT/DA equations as approximations of the RTE. We prove the well posedness of the RT/DA equations and provide numerical examples to show the increased improvement in solution accuracy when the number of terms,  $j$ , increases in RT/DA $_j$  equations.

## 8.2 Differential Approximation of the Integral Operator

The idea of the derivation of the RT/DA equations is based on the approximation of the integral operator  $S$  by a sequence of linear combinations of the inverse of linear elliptic differential operators on the unit sphere [9]. The point of departure of the approach is the knowledge of eigenvalues and eigenfunctions of the operator  $S$ . Specifically, for a spherical harmonic of order  $n$ ,  $Y_n(\omega)$  (cf. [3] for an introduction and spherical harmonics),

$$(SY_n)(\omega) = k_n Y_n(\omega), \quad (8.9)$$

$$k_n = 2\pi \int_{-1}^1 k(s) P_n(s) ds, \quad P_n : \text{Legendre polynomial of deg. } n. \quad (8.10)$$

In other words,  $k_n$  is an eigenvalue of  $S$  with spherical harmonics of order  $n$  as corresponding eigenfunctions. The eigenvalues have the property that

$$\{k_n\} \text{ is bounded and } k_n \rightarrow 0 \text{ as } n \rightarrow \infty. \quad (8.11)$$

Denote by  $\Delta^*$  the Laplace–Beltrami operator on the unit sphere  $\Omega$ . Then,

$$-(\Delta^* Y_n)(\omega) = n(n+1) Y_n(\omega).$$

Let  $\{Y_{n,m} \mid -n \leq m \leq n, n \geq 0\}$  be an orthonormalized basis in  $L^2(\Omega)$ . We have the expansion

$$u(\omega) = \sum_{n=0}^{\infty} \sum_{m=-n}^n u_{n,m} Y_{n,m}(\omega) \text{ in } L^2(\Omega), \quad u_{n,m} = \int_{\Omega} u(\omega) Y_{n,m}(\omega) d\sigma(\omega).$$

With such an expansion of  $u \in L^2(\Omega)$ , we have an expansion for  $Su$ :

$$Su(\omega) = \sum_{n=0}^{\infty} k_n \sum_{m=-n}^n u_{n,m} Y_{n,m}(\omega) \text{ in } L^2(\Omega).$$

Suppose there are real numbers  $\{\lambda_i, \alpha_i\}_{i \geq 1}$  such that

$$\sum_{i=1}^{\infty} \frac{\lambda_i}{1 + n(n+1)\alpha_i} = k_n, \quad n = 0, 1, \dots. \quad (8.12)$$

Then formally,

$$S = \sum_{i=1}^{\infty} \lambda_i (I - \alpha_i \Delta^*)^{-1}. \quad (8.13)$$

The formal equality (8.13) motivates us to consider approximating  $S$  by

$$S_j = \sum_{i=1}^j \lambda_{j,i} (I - \alpha_{j,i} \Delta^*)^{-1}, \quad j = 1, 2, \dots \quad (8.14)$$

The eigenvalues of  $S_j$  are  $\sum_{i=1}^j \lambda_{j,i} (1 + n(n+1) \alpha_{j,i})^{-1}$  with associated eigenfunctions the spherical harmonics of order  $n$ :

$$(S_j Y_n)(\omega) = \left[ \sum_{i=1}^j \frac{\lambda_{j,i}}{1 + n(n+1) \alpha_{j,i}} \right] Y_n(\omega).$$

Note that for a fixed  $j$ ,

$$\sum_{i=1}^j \frac{\lambda_{j,i}}{1 + n(n+1) \alpha_{j,i}} \rightarrow 0 \quad \text{as } n \rightarrow \infty.$$

Thus, the eigenvalue sequence of  $S_j$  has a unique accumulation point 0, a property for the operator  $S$  [cf. (8.11)]. Hence, we choose the parameters  $\{\lambda_{j,i}, \alpha_{j,i}\}_{i=1}^j$  so that for some integer  $n_j$  depending on  $j$ ,

$$\sum_{i=1}^j \frac{\lambda_{j,i}}{1 + n(n+1) \alpha_{j,i}} = k_n, \quad n = 0, 1, \dots, n_j - 1. \quad (8.15)$$

We require  $n_j \rightarrow \infty$  as  $j \rightarrow \infty$ .

The following results are shown in [9]:

**Theorem 8.1.** *Under the assumption (8.15) and*

$$\sup_{n \geq n_j} \left| \sum_{i=1}^j \lambda_{j,i} (1 + n(n+1) \alpha_{j,i})^{-1} \right| \rightarrow 0 \quad \text{as } j \rightarrow \infty, \quad (8.16)$$

*we have the convergence*  $\|S_j - S\|_{\mathcal{L}(L^2(\Omega), L^2(\Omega))} \rightarrow 0$  *as*  $j \rightarrow \infty$ .

A sufficient condition for (8.16) is that all  $\lambda_{j,i}$  and  $\alpha_{j,i}$  are positive.

**Theorem 8.2.** *Assume (8.15) and  $\lambda_{j,i} > 0$  and  $\alpha_{j,i} > 0$  for  $i = 1, \dots, j$ . Then (8.16) holds.*

Notice that  $\alpha_{j,i} > 0$  is needed to ensure ellipticity of the differential operator  $(I - \alpha_{j,i} \Delta^*)$ . When we discretize the operator  $S_j$ , the positivity of  $\{\lambda_{j,i}\}_{i=1}^j$  is desirable for numerical stability in computing approximations of  $S_j$ .

Consider an operator  $S_j$  of the form (8.14) to approximate  $S$ . From now on, we drop the letter  $j$  in the subscripts for  $\lambda_{j,i}$  and  $\alpha_{j,i}$ . As noted after Theorem 8.2, to

maintain ellipticity of the differential operator  $(I - \alpha_i \Delta^*)$  and for stable numerical approximation of the operator  $S_j$ , we require

$$\alpha_i > 0, \lambda_i > 0, \quad 1 \leq i \leq j. \quad (8.17)$$

Recall the property (8.11); for the numbers  $\{k_n\}$  defined in (8.10), we assume  $k_0 \geq k_1 \geq \dots$ . This assumption is quite reasonable and is valid for phase functions in practical use.

To get some idea about the operators  $S_j$ , we consider the special cases  $j = 1$  and 2 next. For  $j = 1$ , we have

$$S_1 Y_n(\omega) = k_{1,n} Y_n(\omega), \quad k_{1,n} = \frac{\lambda_1}{1 + \alpha_1 n(n+1)}. \quad (8.18)$$

Equating the first two eigenvalues of  $S$  and  $S_1$ , we can find

$$\lambda_1 = k_0, \quad \alpha_1 = \frac{1}{2} \left( \frac{k_0}{k_1} - 1 \right). \quad (8.19)$$

Observe that (8.17) is satisfied.

For  $j = 2$ ,  $S_2 = \lambda_1(I - \alpha_1 \Delta^*)^{-1} + \lambda_2(I - \alpha_2 \Delta^*)^{-1}$  with the parameters satisfying  $\lambda_1 > 0$ ,  $\lambda_2 > 0$ ,  $\alpha_1 > 0$ ,  $\alpha_2 > 0$ , and  $\alpha_1 \neq \alpha_2$ . We have

$$S_2 Y_n(\omega) = k_{2,n} Y_n(\omega), \quad k_{2,n} = \frac{\lambda_1}{1 + \alpha_1 n(n+1)} + \frac{\lambda_2}{1 + \alpha_2 n(n+1)}. \quad (8.20)$$

Require the parameters to match the first three eigenvalues  $k_{2,i} = k_i$ ,  $i = 0, 1, 2$ , i.e.,

$$\lambda_1 + \lambda_2 = k_0, \quad (8.21)$$

$$\frac{\lambda_1}{1 + 2\alpha_1} + \frac{\lambda_2}{1 + 2\alpha_2} = k_1, \quad (8.22)$$

$$\frac{\lambda_1}{1 + 6\alpha_1} + \frac{\lambda_2}{1 + 6\alpha_2} = k_2. \quad (8.23)$$

Consider the system (8.21)–(8.23) for a general form solution. Use  $\alpha_1$  as the parameter for the solution. It is shown in [9] that

$$\alpha_2 = \frac{1}{6} \cdot \frac{(3k_1 - 2k_0 - k_2) + 6(k_1 - k_2)\alpha_1}{(k_2 - k_1) + 2(3k_2 - k_1)\alpha_1}, \quad (8.24)$$

$$\lambda_2 = \frac{2[(k_1 - k_0) + 2k_1\alpha_1][(k_2 - k_0) + 6k_2\alpha_1]}{(2k_0 + k_2 - 3k_1) + 12(k_2 - k_1)\alpha_1 + 12(3k_2 - k_1)\alpha_1^2}, \quad (8.25)$$

$$\lambda_1 = 1 - \lambda_2. \quad (8.26)$$

The issue of positivity of the solution  $(\alpha_1, \alpha_2, \lambda_1, \lambda_2)$  is also discussed in [9].

Next, we take the Henyey–Greenstein phase function as an example; in this case,

$$k_n = g^n, \quad n = 0, 1, \dots$$

For the one-term approximation  $S_1 = \lambda_1(I - \alpha_1 \Delta^*)^{-1}$ , from (8.19), we have

$$\lambda_1 = 1, \quad \alpha_1 = \frac{1-g}{2g}. \quad (8.27)$$

For the two-term approximation  $S_2 = \lambda_1(I - \alpha_1 \Delta^*)^{-1} + \lambda_2(I - \alpha_2 \Delta^*)^{-1}$ , we have

$$\alpha_2 = \frac{1-g}{6g} \cdot \frac{g-2+6g\alpha_1}{g-1+2(3g-1)\alpha_1}, \quad (8.28)$$

$$\lambda_2 = \frac{2(g-1+2g\alpha_1)(g^2-1+6g^2\alpha_1)}{(1-g)(2-g)+12g(g-1)\alpha_1+12g(3g-1)\alpha_1^2}, \quad (8.29)$$

$$\lambda_1 = \frac{g(1-g)(2g-1)(1+8\alpha_1+12\alpha_1^2)}{(1-g)(2-g)+12g(g-1)\alpha_1+12g(3g-1)\alpha_1^2}. \quad (8.30)$$

On the issue of positivity of the one parameter solution  $(\alpha_1, \alpha_2, \lambda_1, \lambda_2)$  given by the formulas (8.28)–(8.30), with  $\alpha_1 > 0$ , it is shown in [9] that under the assumption  $g > 1/2$ , valid in applications with highly forward-peaked scattering, the condition for a positive solution  $(\alpha_1, \alpha_2, \lambda_1, \lambda_2)$  is

$$\alpha_1 > \frac{2-g}{6g}. \quad (8.31)$$

Since  $\alpha_1 = 1/2$  satisfies (8.31), one solution is

$$\alpha_1 = \frac{1}{2}, \quad \alpha_2 = \frac{1-g}{6g}, \quad \lambda_1 = \frac{4g(1-g)}{4g-1}, \quad \lambda_2 = \frac{4g^2-1}{4g-1}. \quad (8.32)$$

Now consider the case  $j = 3$ :

$$S_3 = \lambda_1(I - \alpha_1 \Delta^*)^{-1} + \lambda_2(I - \alpha_2 \Delta^*)^{-1} + \lambda_3(I - \alpha_3 \Delta^*)^{-1} \quad (8.33)$$

with the parameters  $\alpha_1, \alpha_2$ , and  $\alpha_3$  pairwise distinct. We want to match the first four eigenvalues

$$k_{3,0} = k_0, \quad k_{3,1} = k_1, \quad k_{3,2} = k_2, \quad k_{3,3} = k_3,$$

i.e., for the special case of the Henyey–Greenstein phase function,

$$\lambda_1 + \lambda_2 + \lambda_3 = 1, \quad (8.34)$$

$$\frac{\lambda_1}{1+2\alpha_1} + \frac{\lambda_2}{1+2\alpha_2} + \frac{\lambda_3}{1+2\alpha_3} = g, \quad (8.35)$$

$$\frac{\lambda_1}{1+6\alpha_1} + \frac{\lambda_2}{1+6\alpha_2} + \frac{\lambda_3}{1+6\alpha_3} = g^2, \quad (8.36)$$

$$\frac{\lambda_1}{1+12\alpha_1} + \frac{\lambda_2}{1+12\alpha_2} + \frac{\lambda_3}{1+12\alpha_3} = g^3. \quad (8.37)$$

We choose  $\alpha_1$  and  $\alpha_2$ , positive and distinct, as the parameters and express the other quantities in terms of them. There are many positive solution sets to the system (8.34)–(8.37) with positive parameters  $\alpha_1$  and  $\alpha_2$ . For the numerical examples in Sect. 8.6, we use parameter sets so that overall the eigenvalues of  $S_3$  are close to those of  $S$ . In particular, for  $g = 0.9$ , we choose

$$\begin{aligned}\alpha_1 &= 0.00957621, & \alpha_2 &= 0.08, & \alpha_3 &= 0.712, \\ \lambda_1 &= 0.660947, & \lambda_2 &= 0.248262, & \lambda_3 &= 0.0907913;\end{aligned}$$

for  $g = 0.95$ , we choose

$$\begin{aligned}\alpha_1 &= 0.00325598, & \alpha_2 &= 0.06, & \alpha_3 &= 0.701, \\ \lambda_1 &= 0.78042, & \lambda_2 &= 0.174622, & \lambda_3 &= 0.0449584;\end{aligned}$$

and for  $g = 0.99$ , we choose

$$\begin{aligned}\alpha_1 &= 0.000306188, & \alpha_2 &= 0.05, & \alpha_3 &= 0.95, \\ \lambda_1 &= 0.940247, & \lambda_2 &= 0.0526772, & \lambda_3 &= 0.00707558.\end{aligned}$$

For  $g = 0.9$ , we compare the eigenvalues of  $S_j$  for  $j = 1, 2, 3$  with those of  $S$  in Figs. 8.1, 8.2, and 8.3, respectively. From these figures, we can tell that the approximation of  $S_3$  should be more accurate than that of  $S_2$ , which should be in turn more accurate than  $S_1$ . This observation is valid for other values of  $g$  below.

For  $g = 0.95$ , the eigenvalues of  $S_1$ ,  $S_2$ , and  $S_3$  are shown in Figs. 8.4–8.6.

For  $g = 0.99$ , the eigenvalues of  $S$ ,  $S_1$ ,  $S_2$ , and  $S_3$  are shown in Fig. 8.7. Evidently, because of the strong singular nature of the phase function for  $g = 0.99$ , a higher value  $j$  will be needed for  $S_j$  to be a good approximation of  $S$ .

### 8.3 Analysis of the RT/DA Problems

We use  $S_j$  of (8.14) for the approximation of the integral operator  $S$ . In the following, we drop the subscript  $j$  in the parameters  $\lambda_{j,i}$  and  $\alpha_{j,i}$  for  $S_j$  and write

$$S_j u(x, \omega) = \sum_{i=1}^j \lambda_i (I - \alpha_i \Delta^*)^{-1} u(x, \omega).$$

Then the RT/DA $_j$  problem is

$$\omega \cdot \nabla u(x, \omega) + \sigma_t(x) u(x, \omega) = \sigma_s(x) S_j u(x, \omega) + f(x, \omega), \quad (x, \omega) \in X \times \Omega, \quad (8.38)$$

$$u(x, \omega) = u_{\text{in}}(x, \omega), \quad (x, \omega) \in \Gamma_-. \quad (8.39)$$



Let us consider the well posedness of (8.38)–(8.39). Introduce

$$w_i(x, \omega) = (I - \alpha_i \Delta^*)^{-1} u(x, \omega), \quad 1 \leq i \leq j, \quad (8.40)$$

$$w(x, \omega) = \sum_{i=1}^j \lambda_i w_i(x, \omega). \quad (8.41)$$

Then (8.38) can be rewritten as

$$\omega \cdot \nabla u(x, \omega) + \sigma_t(x) u(x, \omega) = \sigma_s(x) w(x, \omega) + f(x, \omega), \quad (x, \omega) \in X \times \Omega. \quad (8.42)$$

For simplicity we limit the analysis to the case where  $X$  is a convex domain in  $\mathbb{R}^3$ . The argument can be extended to a domain  $X$  satisfying the generalized convexity condition without problem [1]. Then for each  $\omega \in \Omega$  and each  $z \in X_\omega$ ,  $X_{\omega, z}$  is the line segment

$$X_{\omega, z} = \{z + s\omega \mid s \in (s_-, s_+)\},$$

where  $s_\pm = s_\pm(\omega, z)$  depend on  $\omega$  and  $z$  and  $x_\pm := z + s_\pm \omega$  are the intersection points of the line  $\{z + s\omega \mid s \in \mathbb{R}\}$  with  $\partial X$ .

In the following, we write  $s_\pm$  instead of  $s_\pm(\omega, z)$  wherever there is no danger for confusion. We write (8.42) as

$$\frac{\partial}{\partial s} u(z + s\omega, \omega) + \sigma_t(z + s\omega) u(z + s\omega, \omega) = \sigma_s(z + s\omega) w(z + s\omega, \omega) + f(z + s\omega, \omega)$$

and multiply it by  $\exp(\int_{s_-}^s \sigma_t(z + s\omega) ds)$  to obtain

$$\begin{aligned} & \frac{\partial}{\partial s} \left( e^{\int_{s_-}^s \sigma_t(z + s\omega) ds} u(z + s\omega, \omega) \right) \\ & = e^{\int_{s_-}^s \sigma_t(z + s\omega) ds} (\sigma_s(z + s\omega) w(z + s\omega, \omega) + f(z + s\omega, \omega)). \end{aligned}$$

Integrate this equation from  $s_-$  to  $s$ :

$$\begin{aligned} & e^{\int_{s_-}^s \sigma_t(z + s\omega) ds} u(z + s\omega, \omega) - u_{\text{in}}(z + s_-\omega, \omega) \\ & = \int_{s_-}^s e^{\int_{s_-}^t \sigma_t(z + s\omega) ds} (\sigma_s(z + t\omega) w(z + t\omega, \omega) + f(z + t\omega, \omega)) dt. \end{aligned}$$

Thus, (8.38) and (8.39) is converted to a fixed-point problem

$$u = Au + F, \quad (8.43)$$

where

$$\begin{aligned} Au(z + s\omega, \omega) &= \int_{s_-}^s e^{-\int_t^s \sigma_t(z + s\omega) ds} \sigma_s(z + t\omega) w(z + t\omega, \omega) dt, \\ F(z + s\omega, \omega) &= e^{-\int_{s_-}^s \sigma_t(z + s\omega) ds} u_{\text{in}}(z + s_-\omega, \omega) \\ &+ \int_{s_-}^s e^{-\int_t^s \sigma_t(z + s\omega) ds} f(z + t\omega, \omega) dt. \end{aligned}$$

We will show that  $A$  is a contractive mapping in a weighted  $L^2(X \times \Omega)$  space. Denote  $\kappa = \sup\{\sigma_s(x)/\sigma_t(x) \mid x \in X\}$ . By (8.7), we know that  $\kappa < 1$ . Consider

$$\begin{aligned} & \int_{s_-}^{s_+} \sigma_t(z+s\omega) |Au(z+s\omega, \omega)|^2 ds \\ &= \int_{s_-}^{s_+} \sigma_t(z+s\omega) \left| \int_{s_-}^s e^{-\int_t^s \sigma_r(z+s\omega) ds} \sigma_s(z+t\omega) w(z+t\omega, \omega) dt \right|^2 ds \\ &\leq \int_{s_-}^{s_+} \sigma_t(z+s\omega) \left( \int_{s_-}^s e^{-\int_t^s \sigma_r(z+s\omega) ds} \sigma_s(z+t\omega) dt \right) \\ &\quad \cdot \left( \int_{s_-}^s e^{-\int_t^s \sigma_r(z+s\omega) ds} \sigma_s(z+t\omega) |w(z+t\omega, \omega)|^2 dt \right) ds. \end{aligned}$$

Since

$$\begin{aligned} \int_{s_-}^s e^{-\int_t^s \sigma_r(z+s\omega) ds} \sigma_s(z+t\omega) dt &\leq \kappa \int_{s_-}^s e^{-\int_t^s \sigma_r(z+s\omega) ds} \sigma_t(z+t\omega) dt \\ &= \kappa \left( 1 - e^{-\int_{s_-}^s \sigma_r(z+s\omega) ds} \right) < \kappa, \end{aligned}$$

we have

$$\begin{aligned} & \int_{s_-}^{s_+} \sigma_t(z+s\omega) |Au(z+s\omega, \omega)|^2 ds \\ &\leq \kappa \int_{s_-}^{s_+} \sigma_t(z+s\omega) \int_{s_-}^s e^{-\int_t^s \sigma_r(z+s\omega) ds} \sigma_s(z+t\omega) |w(z+t\omega, \omega)|^2 dt ds \\ &= \kappa \int_{s_-}^{s_+} \sigma_s(z+t\omega) |w(z+t\omega, \omega)|^2 \left( \int_t^{s_+} e^{-\int_t^s \sigma_r(z+s\omega) ds} \sigma_t(z+s\omega) ds \right) dt. \end{aligned}$$

Now

$$\int_t^{s_+} e^{-\int_t^s \sigma_r(z+s\omega) ds} \sigma_t(z+s\omega) ds = 1 - e^{-\int_t^{s_+} \sigma_r(z+s\omega) ds} < 1,$$

we obtain

$$\begin{aligned} \int_{s_-}^{s_+} \sigma_t(z+s\omega) |Au(z+s\omega, \omega)|^2 ds &\leq \kappa \int_{s_-}^{s_+} \sigma_s(z+t\omega) |w(z+t\omega, \omega)|^2 dt \\ &\leq \kappa^2 \int_{s_-}^{s_+} \sigma_t(z+t\omega) |w(z+t\omega, \omega)|^2 dt. \end{aligned}$$

Thus, we have proved the inequality

$$\|\sigma_t^{1/2} Au\|_{L^2(X \times \Omega)} \leq \kappa \|\sigma_t^{1/2} w\|_{L^2(X \times \Omega)}. \quad (8.44)$$

Returning to the definition (8.40), we have, equivalently,

$$(I - \alpha_i \Delta^*) w_i = u \quad \text{in } X \times \Omega.$$

For a.e.  $x \in X$ ,  $w_i(x, \cdot) \in H^1(\Omega)$  and

$$\int_{\Omega} (w_i v + \alpha_i \nabla^* w_i \cdot \nabla^* v) d\sigma(\omega) = \int_{\Omega} u v d\sigma(\omega) \quad \forall v \in H^1(\Omega). \quad (8.45)$$

Since  $\alpha_i > 0$ , this problem has a unique solution by the Lax–Milgram Lemma. Take  $v(\omega) = w_i(x, \omega)$  in (8.45):

$$\int_{\Omega} (|w_i|^2 + \alpha_i |\nabla^* w_i|^2) d\sigma(\omega) = \int_{\Omega} u w_i d\sigma(\omega).$$

Thus,

$$\int_{\Omega} (|w_i|^2 + 2\alpha_i |\nabla^* w_i|^2) d\sigma(\omega) \leq \int_{\Omega} |u|^2 d\sigma(\omega). \quad (8.46)$$

In particular,

$$\int_{\Omega} |w_i|^2 d\sigma(\omega) \leq \int_{\Omega} |u|^2 d\sigma(\omega).$$

Therefore,

$$\|\sigma_i^{1/2} w_i\|_{L^2(X \times \Omega)} \leq \|\sigma_i^{1/2} u\|_{L^2(X \times \Omega)}. \quad (8.47)$$

Since  $\lambda_i > 0$  and  $\sum_{i=1}^j \lambda_i = 1$ , from the definitions (8.41) and (8.47), we get

$$\|\sigma_i^{1/2} w\|_{L^2(X \times \Omega)} \leq \|\sigma_i^{1/2} u\|_{L^2(X \times \Omega)}. \quad (8.48)$$

Combining (8.44) and (8.48), we see that the operator  $A : L^2(X \times \Omega) \rightarrow L^2(X \times \Omega)$  is contractive with respect to the weighted norm  $\|\sigma_i^{1/2} v\|_{L^2(X \times \Omega)}$ :

$$\|\sigma_i^{1/2} A u\|_{L^2(X \times \Omega)} \leq \kappa \|\sigma_i^{1/2} u\|_{L^2(X \times \Omega)}. \quad (8.49)$$

By an application of the Banach fixed-point theorem, we conclude that (8.43) has a unique solution  $u \in L^2(X \times \Omega)$ . By (8.42), we also have  $\omega \cdot \nabla u(x, \omega) \in L^2(X \times \Omega)$ . Therefore, the solution  $u \in H_2^1(X \times \Omega)$ .

In summary, we have shown the following existence and uniqueness result:

**Theorem 8.3.** *Under the assumptions (8.7), (8.8), (8.15), and (8.17), the problem (8.38) and (8.39) has a unique solution  $u \in H_2^1(X \times \Omega)$ .*

Next we show a positivity property required for the model (8.38) and (8.39) to be physically meaningful.

**Theorem 8.4.** *Under the assumptions of Theorem 8.3,*

$$f \geq 0 \text{ in } X \times \Omega, \quad u_{\text{in}} \geq 0 \text{ on } \Gamma_- \quad \implies \quad u \geq 0 \text{ in } X \times \Omega. \quad (8.50)$$

*Proof.* From (8.43),

$$u = (I - A)^{-1} F = \sum_{j=0}^{\infty} A^j F.$$

By the given condition,  $F \geq 0$ . So the proof is done if we can show that  $u \geq 0$  implies  $Au \geq 0$ . This property follows from the implication  $u \geq 0 \implies w_i \geq 0$  for the solution  $w_i$  of the problem (8.45). In (8.45), take  $v = w_i^- = \min(w_i, 0)$  to obtain

$$\int_{\Omega} (|w_i^-|^2 + \alpha_i |\nabla^* w_i^-|^2) d\sigma(\omega) = \int_{\Omega} u w_i^- d\sigma(\omega) \leq 0.$$

Hence,  $w_i^- = 0$ , i.e.,  $w_i \geq 0$ .  $\square$

We now derive an error estimate for the approximation (8.38)–(8.39) of the RTE problem (8.5)–(8.6). Denote the solution of the problem (8.38)–(8.39) by  $u_j$  and consider the error  $e := u - u_j$ . From (8.38)–(8.39) and (8.5)–(8.6), we obtain the following problem for the error:

$$\omega \cdot \nabla e + \sigma_t e = \sigma_s e_0 + \sigma_s \sum_{i=1}^j \lambda_i (I - \alpha_i \Delta^*)^{-1} e \quad \text{in } X \times \Omega, \quad (8.51)$$

$$e = 0 \quad \text{in } \Gamma_-, \quad (8.52)$$

where

$$e_0 = Su - \sum_{i=1}^j \lambda_i (I - \alpha_i \Delta^*)^{-1} u. \quad (8.53)$$

Since  $\lambda_i > 0$  and  $\sum_{i=1}^j \lambda_i = 1$ , we obtain from (8.51) to (8.52) that, as in (8.43),

$$e = Ae + E$$

with

$$E(z + s\omega, \omega) = \int_{s_-}^s e^{-\int_t^s \sigma_t(z+s\omega) ds} (\sigma_s e_0)(z + t\omega, \omega) dt.$$

Thus,

$$\begin{aligned} \|\sigma_t^{1/2} e\|_{L^2(X \times \Omega)} &\leq \|\sigma_t^{1/2} Ae\|_{L^2(X \times \Omega)} + \|\sigma_t^{1/2} E\|_{L^2(X \times \Omega)} \\ &\leq \kappa \|\sigma_t^{1/2} e\|_{L^2(X \times \Omega)} + \|\sigma_t^{1/2} E\|_{L^2(X \times \Omega)}. \end{aligned}$$

Therefore,

$$\|\sigma_t^{1/2} e\|_{L^2(X \times \Omega)} \leq \frac{1}{1 - \kappa} \|\sigma_t^{1/2} E\|_{L^2(X \times \Omega)} \leq c \|e_0\|_{L^2(X \times \Omega)}. \quad (8.54)$$

By expanding functions in terms of the spherical harmonics, we have

$$\|e_0\|_{L^2(X \times \Omega)} \leq c_j \|u\|_{L^2(X \times \Omega)}, \quad c_j = \max_n \left| k_n - \sum_{i=1}^j \frac{\lambda_i}{1 + \alpha_i n(n+1)} \right|. \quad (8.55)$$

Hence, from (8.54), we get the error bound

$$\|\sigma_t^{1/2}(u - u_j)\|_{L^2(X \times \Omega)} \leq c c_j \|u\|_{L^2(X \times \Omega)}. \quad (8.56)$$

**Theorem 8.5.** *Under the assumptions of Theorem 8.3, we have the error bound (8.56) with  $c_j$  given in (8.55).*

## 8.4 An Iteration Method

We now consider the convergence of an iteration method for solving the problem defined by (8.42) and (8.39)–(8.41). Let  $w^{(0)}$  be an initial guess, e.g., we may take  $w^{(0)} = 0$ . Then, for  $n = 1, 2, \dots$ , define  $u^{(n)}$  and  $w^{(n)}$  as follows:

$$\omega \cdot \nabla u^{(n)} + \sigma_t u^{(n)} = \sigma_s w^{(n-1)} + f \quad \text{in } X \times \Omega, \quad (8.57)$$

$$u^{(n)} = u_{\text{in}} \quad \text{on } \Gamma_-, \quad (8.58)$$

$$w_i^{(n)} = (I - \alpha_i \Delta^*)^{-1} u^{(n)}, \quad 1 \leq i \leq j, \quad (8.59)$$

$$w^{(n)} = \sum_{i=1}^j \lambda_i w_i^{(n)}. \quad (8.60)$$

Denote the iteration errors  $e_u^{(n)} := u - u^{(n)}$ ,  $e_w^{(n)} = w - w^{(n)}$ . Then we have the error relations

$$\begin{aligned} \omega \cdot \nabla e_u^{(n)} + \sigma_t e_u^{(n)} &= \sigma_s e_w^{(n-1)} \quad \text{in } X \times \Omega, \\ e_u^{(n)} &= 0 \quad \text{on } \Gamma_-, \\ e_{w_i}^{(n)} &= (I - \alpha_i \Delta^*)^{-1} e_u^{(n)}, \quad 1 \leq i \leq j, \\ e_w^{(n)} &= \sum_{i=1}^j \lambda_i e_{w_i}^{(n)}. \end{aligned}$$

Similar to (8.44) and (8.48), we have

$$\begin{aligned} \|\sigma_t^{1/2} e_u^{(n)}\|_{L^2(X \times \Omega)} &\leq \kappa \|\sigma_t^{1/2} e_w^{(n-1)}\|_{L^2(X \times \Omega)}, \\ \|\sigma_t^{1/2} e_w^{(n-1)}\|_{L^2(X \times \Omega)} &\leq \|\sigma_t^{1/2} e_u^{(n-1)}\|_{L^2(X \times \Omega)}. \end{aligned}$$

Thus,

$$\|\sigma_t^{1/2} e_u^{(n)}\|_{L^2(X \times \Omega)} \leq \kappa \|\sigma_t^{1/2} e_u^{(n-1)}\|_{L^2(X \times \Omega)},$$

and so we have

$$\|\sigma_t^{1/2} e_u^{(n)}\|_{L^2(X \times \Omega)} \leq \kappa^n \|\sigma_t^{1/2} e_u^{(0)}\|_{L^2(X \times \Omega)} \rightarrow 0 \quad \text{as } n \rightarrow \infty.$$

Moreover, we also have the convergence of the sequence  $\{w^{(n)}\}$ :

$$\|\sigma_t^{1/2} e_w^{(n)}\|_{L^2(X \times \Omega)} \leq \|\sigma_t^{1/2} e_u^{(n)}\|_{L^2(X \times \Omega)} \rightarrow 0 \quad \text{as } n \rightarrow \infty.$$

## 8.5 Error Analysis of a Hybrid Analytic/Finite Element Method

To focus on the main idea, in this section, we perform the analysis for the case of solving an RT/DA<sub>1</sub> equation with  $u_{\text{in}} = 0$ . The same argument can be extended straightforward to an RT/DA<sub>j</sub> equation for an arbitrary  $j \geq 1$ . Thus, consider the problem

$$\omega \cdot \nabla u(x, \omega) + \sigma_t(x) u(x, \omega) = \sigma_s(x) w(x, \omega) + f(x, \omega), \quad (x, \omega) \in X \times \Omega, \quad (8.61)$$

$$u(x, \omega) = 0, \quad (x, \omega) \in \Gamma_-, \quad (8.62)$$

$$(I - \alpha \Delta^*) w(x, \omega) = u(x, \omega), \quad (x, \omega) \in X \times \Omega. \quad (8.63)$$

A weak formulation of (8.63) is  $w(x, \cdot) \in H^1(\Omega)$  and

$$\int_{\Omega} (wv + \alpha \nabla^* w \cdot \nabla^* v) d\sigma(\omega) = \int_{\Omega} uv d\sigma(\omega) \quad \forall v \in H^1(\Omega) \quad (8.64)$$

for a.e.  $x \in X$ , where  $\nabla^*$  is the first-order Beltrami operator. Let  $V_{\omega}^h$  be a finite element subspace of  $H^1(\Omega)$ . Then a finite element approximation of (8.64) is to find  $w_h(x, \cdot) \in V_{\omega}^h$  such that

$$\int_{\Omega} (w_h v_h + \alpha \nabla^* w_h \cdot \nabla^* v_h) d\sigma(\omega) = \int_{\Omega} u_h v_h d\sigma(\omega) \quad \forall v_h \in V_{\omega}^h, \quad (8.65)$$

where the numerical solution  $u_h$  is defined by (8.61) with  $w$  replaced with  $w_h$  and (8.62). We have, similar to (8.43),

$$\begin{aligned} u_h(z + s\omega, \omega) &= \int_{s_-}^s e^{-\int_t^s \sigma_t(z+s\omega) ds} \sigma_s(z+t\omega) w_h(z+t\omega, \omega) dt \\ &\quad + \int_{s_-}^s e^{-\int_t^s \sigma_t(z+s\omega) ds} f(z+t\omega, \omega) dt. \end{aligned} \quad (8.66)$$

Denote the error functions

$$e_{u,h}(x, \omega) = u(x, \omega) - u_h(x, \omega), \quad e_{w,h}(x, \omega) = w(x, \omega) - w_h(x, \omega). \quad (8.67)$$

Subtract (8.66) from (8.43):

$$e_{u,h}(z + s\omega, \omega) = \int_{s_-}^s e^{-\int_t^s \sigma_t(z+s\omega) ds} \sigma_s(z+t\omega) e_{w,h}(z+t\omega, \omega) dt. \quad (8.68)$$

Similar to derivation of (8.44), we then deduce from (8.68) that

$$\int_{s_-}^{s_+} \sigma_t(z+s\omega) |e_{u,h}(z+s\omega, \omega)|^2 ds \leq \kappa^2 \int_{s_-}^{s_+} \sigma_t(z+s\omega) |e_{w,h}(z+s\omega, \omega)|^2 ds. \quad (8.69)$$

To bound the error  $e_{w,h}$ , we subtract (8.65) from (8.64) with  $v = v_h$ :

$$\int_{\Omega} (e_{w,h} v_h + \alpha \nabla^* e_{w,h} \cdot \nabla^* v_h) d\sigma(\omega) = \int_{\Omega} e_{u,h} v_h d\sigma(\omega) \quad \forall v_h \in V_{\omega}^h. \quad (8.70)$$

Thus,

$$\begin{aligned} \int_{\Omega} (|e_{w,h}|^2 + \alpha |\nabla^* e_{w,h}|^2) d\sigma(\omega) &= \int_{\Omega} [e_{w,h}(w - v_h) + \alpha \nabla^* e_{w,h} \cdot \nabla^*(w - v_h)] d\sigma(\omega) \\ &\quad + \int_{\Omega} e_{u,h}(v_h - w + e_{w,h}) d\sigma(\omega). \end{aligned}$$

For any  $\varepsilon > 0$ , we have positive constants  $C_1(\varepsilon)$  and  $C_2(\varepsilon)$  such that

$$\begin{aligned} \int_{\Omega} e_{w,h}(w - v_h) d\sigma(\omega) &\leq \varepsilon \int_{\Omega} |e_{w,h}|^2 d\sigma(\omega) + C_1(\varepsilon) \int_{\Omega} |w - v_h|^2 d\sigma(\omega), \\ \int_{\Omega} e_{u,h}(v_h - w + e_{w,h}) d\sigma(\omega) &\leq \frac{1}{2} \int_{\Omega} |e_{u,h}|^2 d\sigma(\omega) + \frac{1+\varepsilon}{2} \int_{\Omega} |e_{w,h}|^2 d\sigma(\omega) \\ &\quad + C_2(\varepsilon) \int_{\Omega} |w - v_h|^2 d\sigma(\omega). \end{aligned}$$

Moreover,

$$\int_{\Omega} \nabla^* e_{w,h} \cdot \nabla^*(w - v_h) d\sigma(\omega) \leq \frac{1}{2} \int_{\Omega} |\nabla^* e_{w,h}|^2 d\sigma(\omega) + \frac{1}{2} \int_{\Omega} |\nabla^*(w - v_h)|^2 d\sigma(\omega).$$

Then,

$$\begin{aligned} \int_{\Omega} (|e_{w,h}|^2 + \alpha |\nabla^* e_{w,h}|^2) d\sigma(\omega) &\leq (1+\varepsilon) \int_{\Omega} |e_{u,h}|^2 d\sigma(\omega) + C_3(\varepsilon) \int_{\Omega} |w - v_h|^2 d\sigma(\omega) \\ &\quad + \alpha \int_{\Omega} |\nabla^*(w - v_h)|^2 d\sigma(\omega) \\ &\leq (1+\varepsilon) \int_{\Omega} |e_{u,h}|^2 d\sigma(\omega) + C(\varepsilon) \|w - v_h\|_{H^1(\Omega)}^2. \end{aligned}$$

Since  $v_h \in V_{\omega}^h$  is arbitrary, we have

$$\int_{\Omega} (|e_{w,h}|^2 + \alpha |\nabla^* e_{w,h}|^2) d\sigma(\omega) \leq (1+\varepsilon) \int_{\Omega} |e_{u,h}|^2 d\sigma(\omega) + C(\varepsilon) \inf_{v_h \in V_{\omega}^h} \|w - v_h\|_{H^1(\Omega)}^2. \quad (8.71)$$

We now integrate (8.69) and apply (8.71):

$$\begin{aligned} \|\sigma_t^{1/2} e_{u,h}\|_{L^2(X \times \Omega)}^2 &\leq \kappa^2 \|\sigma_t^{1/2} e_{w,h}\|_{L^2(X \times \Omega)}^2 \\ &= \kappa^2 \int_X \sigma_t(x) dx \int_{\Omega} |e_{w,h}(x, \omega)|^2 d\sigma(\omega) \\ &\leq (1+\varepsilon) \kappa^2 \|\sigma_t^{1/2} e_{u,h}\|_{L^2(X \times \Omega)}^2 + C(\varepsilon) \int_X \left[ \inf_{v_h \in V_{\omega}^h} \|w - v_h\|_{H^1(\Omega)}^2 \right] dx. \end{aligned}$$

Choose  $\varepsilon > 0$  small enough to obtain

$$\|\sigma_t^{1/2} e_{u,h}\|_{L^2(X \times \Omega)}^2 \leq C \int_X \left[ \inf_{v_h \in V_{\omega}^h} \|w - v_h\|_{H^1(\Omega)}^2 \right] dx. \quad (8.72)$$

In a typical error estimate, if  $w \in L^2(X, H^{k+1}(\Omega))$  and piecewise polynomials of degree less than or equal to  $k$  are used for the finite element space  $V_\omega^h$ , then

$$\int_X \left[ \inf_{v_h \in V_\omega^h} \|w - v_h\|_{H^1(\Omega)}^2 \right] dx \leq ch^{2k} \|w\|_{L^2(X, H^{k+1}(\Omega))}^2. \quad (8.73)$$

From (8.72), we then have the error bound

$$\|e_{u,h}\|_{L^2(X \times \Omega)} \leq ch^k \|w\|_{L^2(X, H^{k+1}(\Omega))}. \quad (8.74)$$

## 8.6 Numerical Experiments

Here we report some numerical results on the differences between numerical solutions of RTE and those of RT/DA equations. For definiteness, we use the Henyey–Greenstein phase function and consider the approximations  $S_j$ ,  $1 \leq j \leq 3$ , specified in Sect. 8.2.

For the discretization of the unit sphere  $\Omega$  for the direction variable  $\omega$ , we use the finite element method described in [2]. The angular discretizations used all have  $n_\phi = 8$  and have various values of  $n_\theta$ . For reference, the total number of angular nodes in each discretization is listed in Table 8.1.

Table 8.1: Number of angular nodes

$n_\theta$	Nodes
4	26
8	98
16	386
32	1538
64	6146
128	24578

**Experiment 8.6.1.** We first make sure that the numerical methods behave as expected. Let us comment on the discretization of  $S$  used in approximating the RTE. For ease, we compare the numerical solution of the RTE with the numerical solutions to the RT/DA<sub>1</sub> equation calculated on the same mesh. This leaves us with a choice of weights when solving the RTE. Initially, the choice was made that  $w_i = \frac{4\pi}{N}$  where  $N$  is the number of angular nodes. However, this is not a good quadrature rule, as the nodes are not quite evenly spaced on the sphere. This point is illustrated in Table 8.2. In this table, we numerically integrate

$$\int_\Omega Y_1(\omega') k_{.5}(\omega_0 \cdot \omega') d\sigma(\omega')$$



using both uniform weights and the weights introduced below. Here  $k_s$  is the HG phase function with anisotropy factor  $g = 0.5$ ,  $\omega_0$  is rather arbitrarily chosen to be  $\frac{1}{\sqrt{3}}(1, 1, 1)^T$ , and  $Y_1(\omega)$  is the order 1 spherical harmonic:

$$Y_1(\omega) = \frac{1}{2} \sqrt{\frac{3}{\pi}} \cos(\theta).$$

The true value of this integral is  $.5Y_1(\omega_0) \approx 0.14105$ .

When solving the approximation to the RT/DA<sub>1</sub> equation, a matrix  $A$  is formed with the property that

$$f^T A g = \int_{\Omega} f(\omega) g(\omega) d\sigma(\omega)$$

if  $f$  is a vector containing function values of  $f$  at the nodes  $\omega_i$  and  $f, g$  are elements of the finite element space associated with the angular mesh. We choose the weight vector  $w$  to be  $w = Ae$ , where  $e$  is the vector with all components 1. This quadrature rule will be exact for all functions in the finite element space associated with the angular mesh. Since this rule will correctly integrate any piecewise linear function in the finite element space, it may be thought of as an analogue of the trapezoidal rule for the sphere. Quick investigation shows that for the example integral above, this method is order 2 in terms of  $n_{\theta}$ , which makes it order 1 in terms of the number of nodes. It seems likely that this is true in general.

Table 8.2: Comparison of trapezoidal weights vs. uniform weights in evaluating  $\int_{\Omega} Y_1(\omega') k_s(\omega_0 \cdot \omega') d\sigma(\omega')$  for specific choice of  $\omega_0$

$n_{\theta}$	Trapezoidal rule	Trapezoidal error	Uniform rule	Uniform error
4	1.51038e-01	9.99030e-03	1.29518e-01	1.15298e-02
8	1.42538e-01	1.49073e-03	1.28156e-01	1.28914e-02
16	1.41424e-01	3.76434e-04	1.28242e-01	1.28050e-02
32	1.41141e-01	9.39943e-05	1.28244e-01	1.28030e-02
64	1.41071e-01	2.34917e-05	1.28244e-01	1.28035e-02

We take  $\mu_t(x) = 2$ ,  $\mu_s(x) = 1$ ,  $g = 0.9$ , and  $f = (\mu_t - g\mu_s)Y_1(\omega)$ . Under these choices and with appropriate choice of boundary conditions, the solution to both the RTE and RT/DA<sub>1</sub> equation is  $Y_1$ . We report the errors

$$e_S := \left\{ \sum_i w_i \int_X (u_S(x, \omega_i) - Y_1(\omega_i))^2 dx \right\}^{1/2} \quad (8.75)$$

$$e_{S_1} := \left\{ \sum_i w_i \int_X (u_{S_1}(x, \omega_i) - Y_1(\omega_i))^2 dx \right\}^{1/2} \quad (8.76)$$

in Tables 8.3 and 8.4. We see that both methods converge in the above norm. We report the maximum difference between  $u_S$  and  $u_{S_1}$  in Table 8.5. Unless specified otherwise, all meshes have 96 space elements. A “–” in the tables reflects the fact that the iteration algorithm used to solve the discrete systems does not converge within a fixed (large) number of iterations.

Table 8.3: Experiment 8.6.1: error between  $u_S$ ,  $u_{S_1}$ , and  $Y_1$ 

$n_\theta$	$e_S$	$e_{S_1}$
4	–	0.301621
8	–	0.236104
16	0.227244	0.172195
32	0.129529	0.123071
64	0.088994	0.087421

Table 8.4: Experiment 8.6.1: different errors

$n_\theta$	$\max  u_S - Y_1 $	$\text{Mean}  u_S - Y_1 $	$\max  u_{S_1} - Y_1 $	$\text{Mean}  u_{S_1} - Y_1 $
4	–	–	6.070e-03	8.433e-04
8	–	–	3.363e-03	1.668e-04
16	1.077e-01	1.275e-02	1.306e-03	3.851e-05
32	1.558e-02	3.707e-04	4.410e-04	9.002e-06
64	4.315e-03	4.332e-05	1.381e-04	2.212e-06

Table 8.5: Experiment 8.6.1: maximum error at the nodes of the mesh between  $u_S$  and  $u_{S_1}$ 

$n_\theta$	$\max  u_S - u_{S_1} $
16	0.127953
32	0.019912
64	0.007467

To investigate the relative error, we introduce new notation. Define the set of all nodes as

$$\mathcal{N} = \{(x, \omega) \mid x \text{ is a node of the spatial mesh, } \omega \text{ is a node of the angular mesh}\}.$$

For a given relative error level  $e$ , define

$$\mathcal{N}_e = \{(x, \omega) \in \mathcal{N} \mid |u_S(x, \omega) - u_{S_1}(x, \omega)| / |u_S(x, \omega)| < e\}.$$

Finally, define  $f(e) = |\mathcal{N}_e| / |\mathcal{N}|$  for the fraction of nodes at which the solution to the RT/DA<sub>1</sub> equation agrees with the RTE within relative error  $e$ . Here we use the convention that  $|\cdot|$  applied to a set denotes cardinality.

We plot  $f(e)$  in Fig. 8.8. Note that there is no logical upper bound on the domain  $e$ . However, we will only plot  $0 < e < 1$ , as it makes the graphs more readable.  $\square$

**Experiment 8.6.2.** The spatial domain is  $X = [0, 1]^3$ . We choose  $\mu_t = 2$ ,  $\mu_s = 1$ , and the Henyey–Greenstein phase function with several different choices of scattering parameter  $g$ . The source function  $f$  is taken to be

$$f(x, \omega) = \begin{cases} 1 & \text{if } x \in R \\ 0 & \text{otherwise} \end{cases}$$

where  $R$  is approximately a sphere of radius  $1/4$  centered at  $(0.5, 0.5, 0.5)$ . To do the numerical simulations the domain  $X$  is partitioned into 324 tetrahedrons and we use various angular discretizations to investigate the effect of angular discretization.

Again let  $\mathcal{N}$  be the set of all nodes of the mesh. Let  $u_S^h$  be the numerical solution to the RTE and let  $u_{S_j}^h$  be the numerical solution to the RT/DA $_j$  equation. For a given relative error level,  $e$ , define the set of all nodes on which the numerical solution to the RT/DA $_j$  equation agrees with the RTE within relative error  $e$ . That is,

$$\mathcal{N}_{e,j} = \{(x, \omega) \in \mathcal{N} \mid |u_S^h(x, \omega) - u_{S_j}^h(x, \omega)| < e|u_S^h(x, \omega)|\}.$$

Define  $f_j(e) = |\mathcal{N}_{e,j}|/|\mathcal{N}|$ , giving the fraction of nodes at which the solution to the RT/DA $_j$  equation agrees with the RTE within relative error  $e$ . Obviously, we would like  $f(e) \approx 1$  for as small  $e$  as possible.

Plots of  $f_j(e)$  are shown with scattering parameter  $\eta = 0.9, 0.95$ , and  $0.99$  for the RT/DA $_j$  ( $j = 1, 2, 3$ ) equations in Figs. 8.9–8.16. We observe that (1) as  $j$  increases, the RT/DA $_j$  equation with properly chosen parameter values provides increasingly accurate solution to the RTE, and (2) as  $g$  gets close to  $1-$ , higher value of  $j$  will be needed for the RT/DA $_j$  equation to be a good approximation of the RTE.  $\square$

## Acknowledgement

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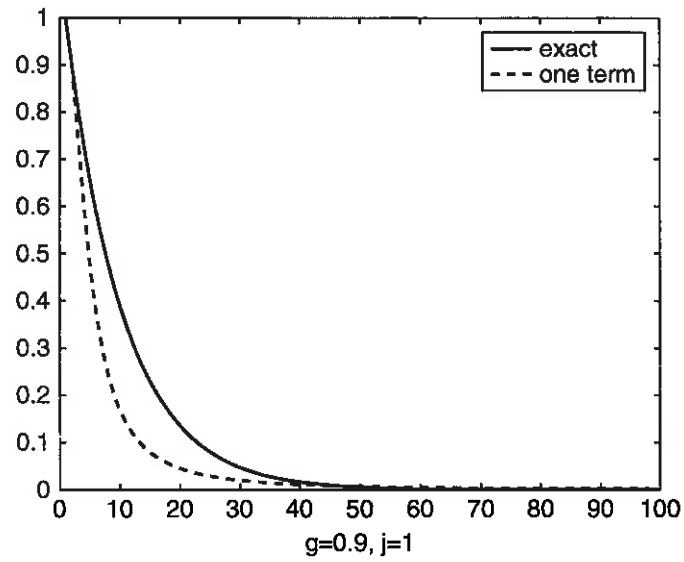


Fig. 8.1: Eigenvalues of  $S$  (solid line) and  $S_1$  (broken line)

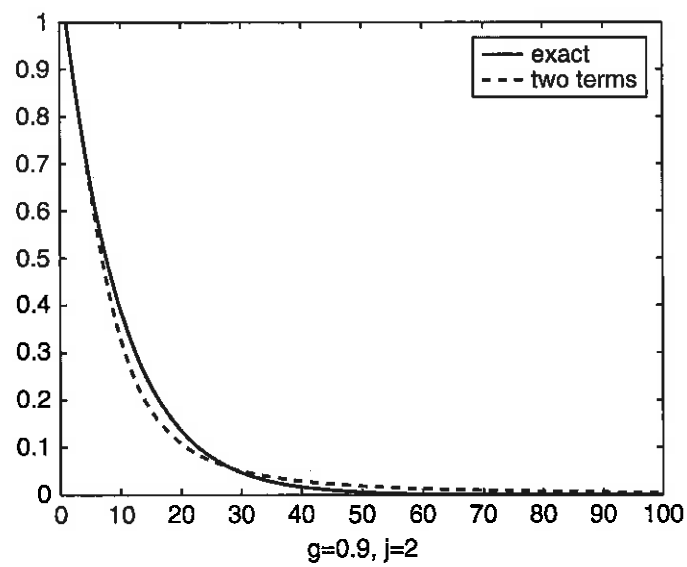


Fig. 8.2: Eigenvalues of  $S$  (solid line) and  $S_2$  with the choice (8.32) (broken line)

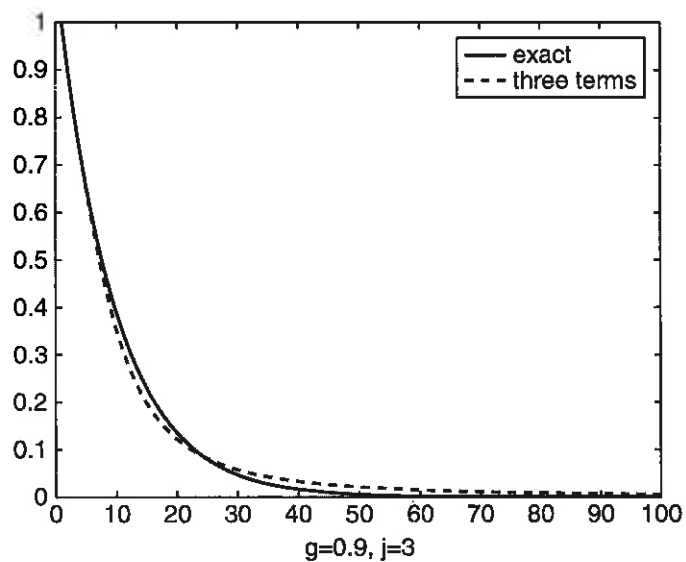


Fig. 8.3: Eigenvalues of  $S$  (solid line) and  $S_3$  (broken line)

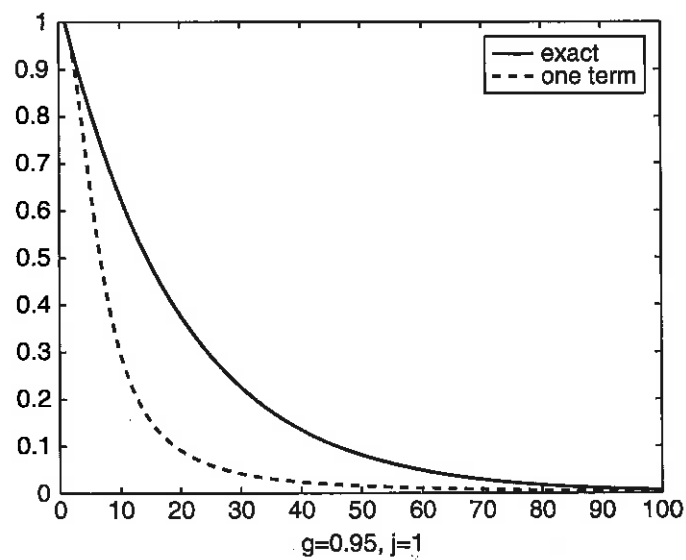
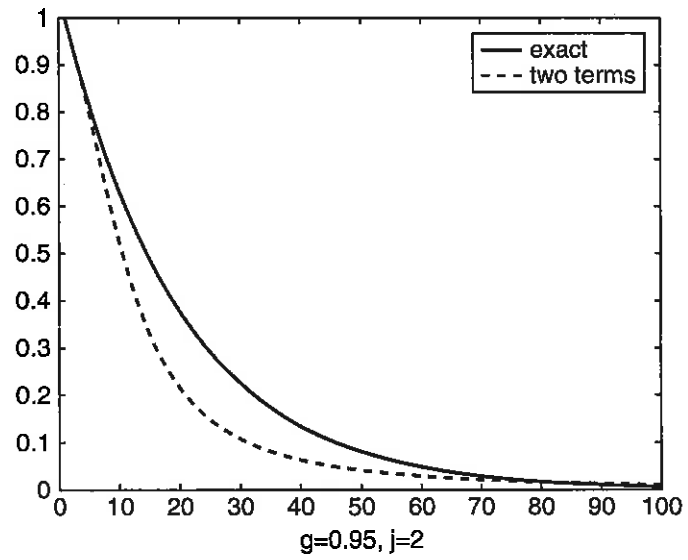
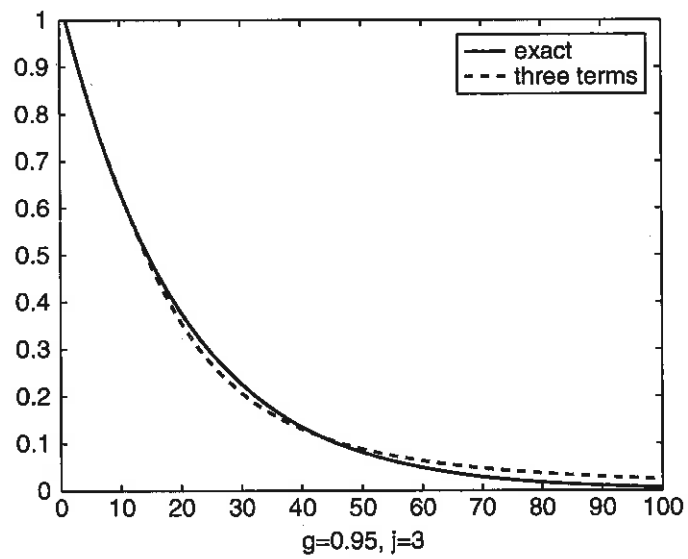
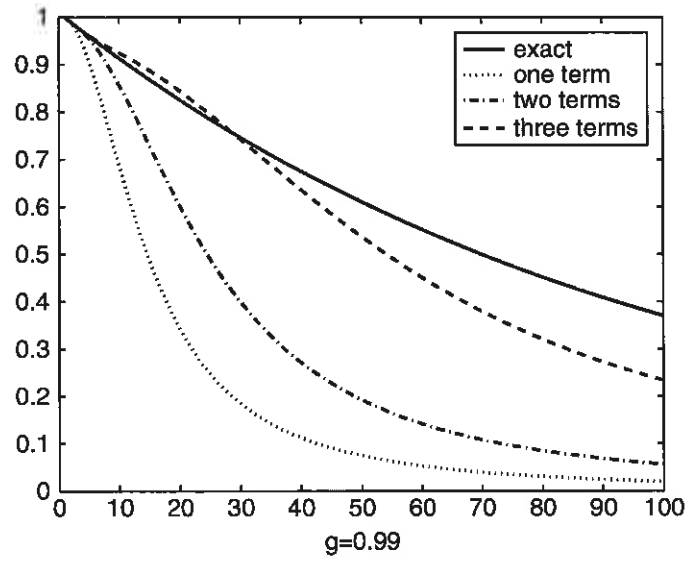
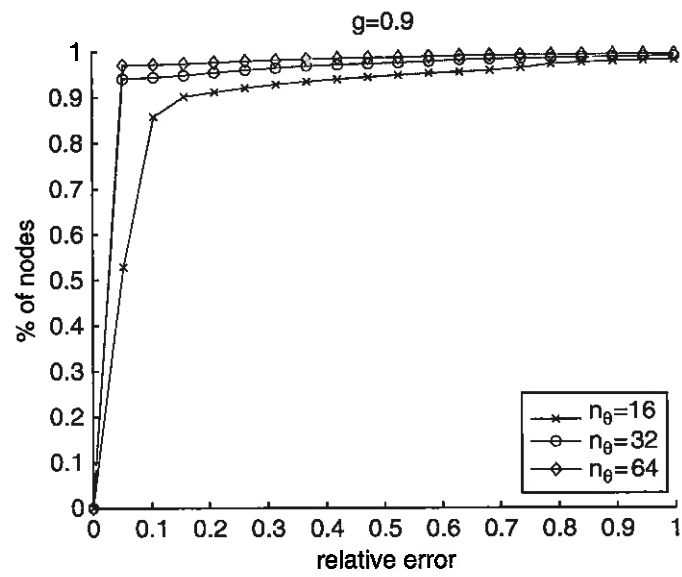
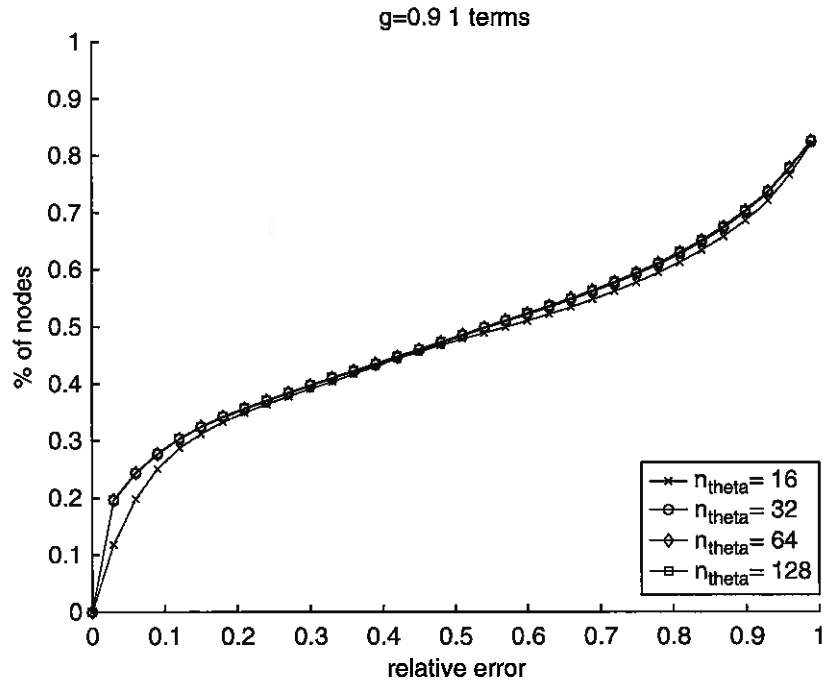
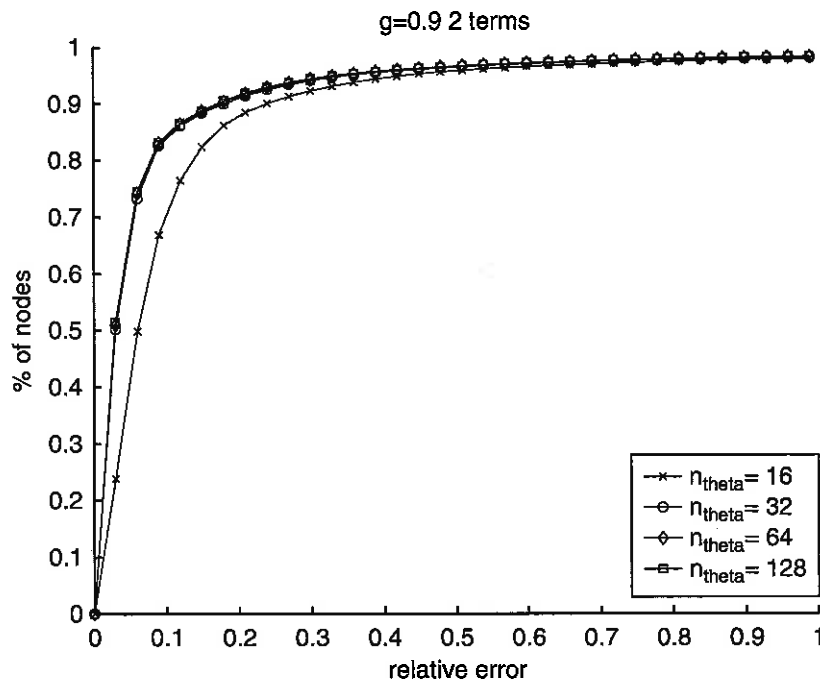


Fig. 8.4: Eigenvalues of  $S$  (solid line) and  $S_1$  (broken line)

Fig. 8.5: Eigenvalues of  $S$  (solid line) and  $S_2$  (broken line)Fig. 8.6: Eigenvalues of  $S$  (solid line) and  $S_3$  (broken line)

Fig. 8.7: Eigenvalues of  $S$ ,  $S_1$ ,  $S_2$ , and  $S_3$ Fig. 8.8:  $f$  vs  $e$  for Experiment 8.6.1



Fig. 8.9: Experiment 8.6.2:  $f$  vs.  $e$  for  $g = 0.9$  using one-term approximation  $S_1$ Fig. 8.10: Experiment 8.6.2:  $f$  vs.  $e$  for  $g = 0.9$  using two-term approximation  $S_2$

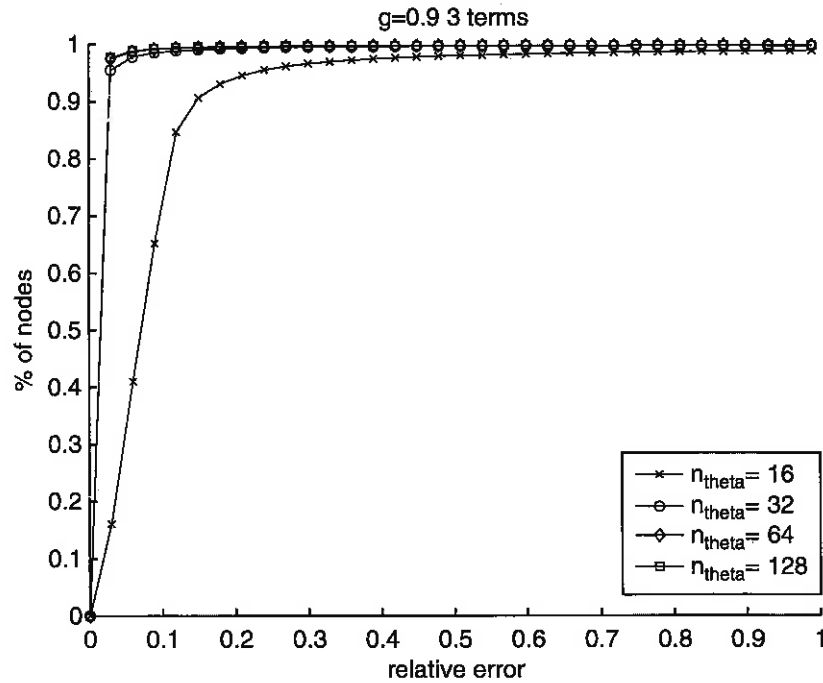


Fig. 8.11: Experiment 8.6.2:  $f$  vs.  $e$  for  $g = 0.9$  using three term approximation  $S_3$

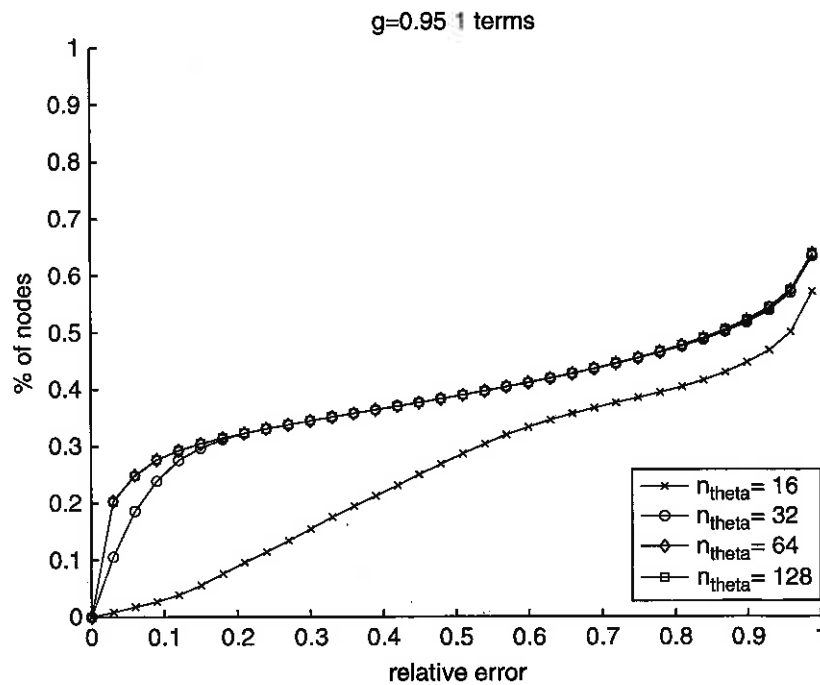
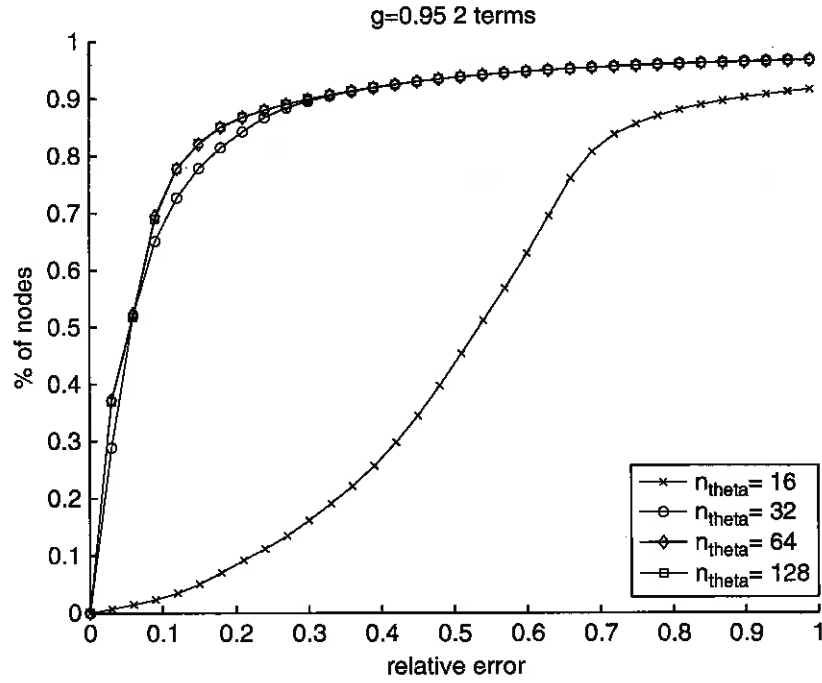
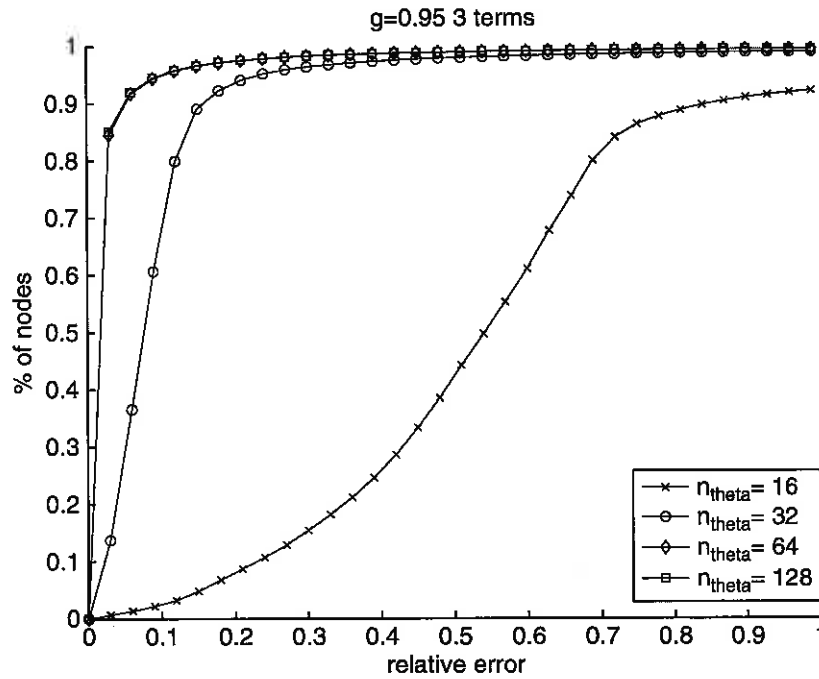


Fig. 8.12: Experiment 8.6.2:  $f$  vs.  $e$  for  $g = 0.95$  using one-term approximation  $S_1$

Fig. 8.13: Experiment 8.6.2:  $f$  vs.  $e$  for  $g = 0.95$  using two-term approximation  $S_2$ Fig. 8.14: Experiment 8.6.2:  $f$  vs.  $e$  for  $g = 0.95$  using three term approximation  $S_3$

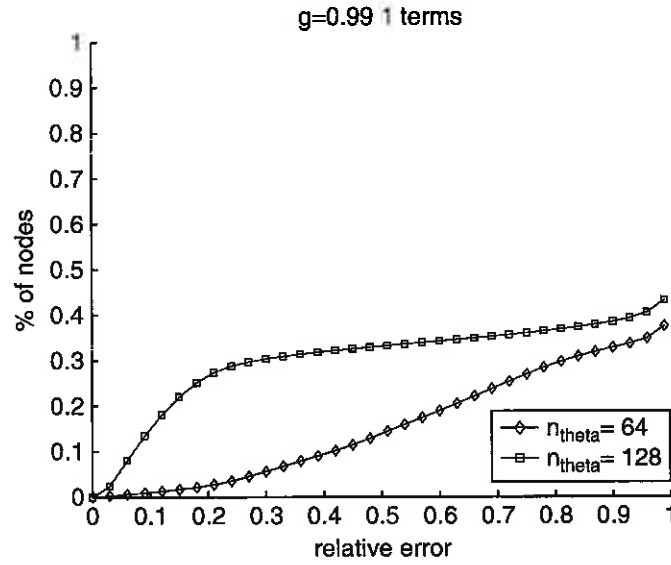


Fig. 8.15: Experiment 8.6.2:  $f$  vs.  $e$  for  $g = 0.99$  using one-term approximation  $S_1$

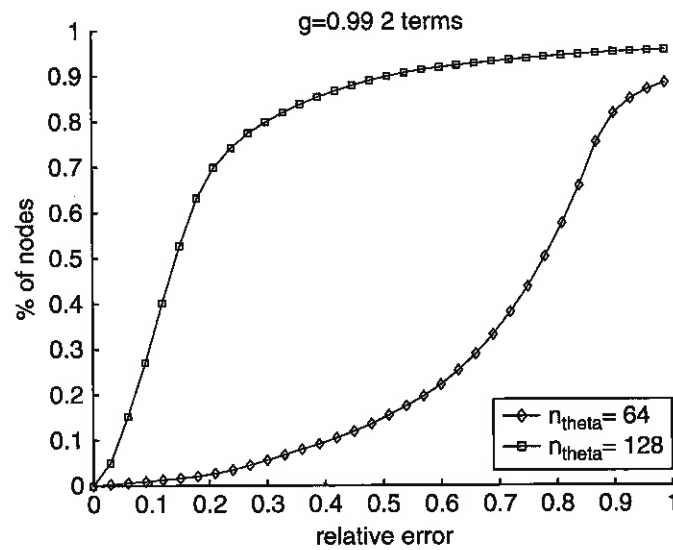


Fig. 8.16: Experiment 8.6.2:  $f$  vs.  $e$  for  $g = 0.99$  using two-term approximation  $S_2$