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ORIGINAL PAPER

On simplified spherical harmonics equations for the radiative transfer equation

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Abstract The radiative transfer equation (RTE) arises in a wide range of applications in sciences and engineering. Due to the high dimension and complicated form of the RTE, it is challenging to solve the equation directly. In the literature, several approximation methods were developed for the RTE. One approximation method, the simplified spherical harmonics (SP_N) method, provides an efficient way to generate good approximate solutions of the RTE with high absorption and small geometries. The main purpose of the paper is to study well-posedness of the simplified spherical harmonics system. The weak formulation used in the proof of the solution existence and uniqueness provides a starting point for developing the Galerkin finite element method to solve the simplified spherical harmonics system.

Keywords Radiative transfer equation · Simplified spherical harmonics (SP_N) method · Solution existence · Uniqueness

1 Introduction

The radiative transfer equation (RTE) arises in a wide range of applications of physics, chemistry, and other areas of sciences and engineering; see, e.g., [4–6,13,16–18,20].

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In the stationary monoenergetic case, the radiative transfer equation (RTE) is (cf. [1, 15]):

$$\boldsymbol{\omega}\cdot\nabla\phi(\boldsymbol{x},\boldsymbol{\omega}) + \mu_t(\boldsymbol{x})\,\phi(\boldsymbol{x},\boldsymbol{\omega}) = \mu_s(\boldsymbol{x})\int_{\Omega}\eta(\boldsymbol{x},\boldsymbol{\omega}\cdot\hat{\boldsymbol{\omega}})\,\phi(\boldsymbol{x},\hat{\boldsymbol{\omega}})\,d\sigma(\hat{\boldsymbol{\omega}}) + Q(\boldsymbol{x}). \quad (1)$$

Here the unknown function ϕ depends on a spatial variable $\boldsymbol{x}$ in a Lipschitz domain X of the three dimensional space and on an angular variable $\boldsymbol{\omega} \in \Omega$, Ω being the unit sphere in $\mathbb{R}^3$, $\mu_t = \mu_a + \mu_s$, μ_a is an absorption parameter, μ_s is a scattering parameter, η is a scattering phase function, and Q is a source function. The phase function η is non-negative and is normalized,

$$\int_{\Omega}\eta(\boldsymbol{x},\boldsymbol{\omega}\cdot\hat{\boldsymbol{\omega}})\,d\sigma(\hat{\boldsymbol{\omega}}) = 1 \quad \forall\boldsymbol{x}\in X,\ \boldsymbol{\omega}\in\Omega.$$

In many applications, the function η is independent of $\boldsymbol{x}$. One well-known example is the Henyey-Greenstein phase function (cf. [10])

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

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.

For the data $\mu_a,\ \mu_s$ and Q, we assume

$$\mu_a, \mu_s \in L^\infty(X), \quad \mu_s \ge 0 \text{ a.e. in } X, \quad \mu_a \ge c_0 > 0 \text{ a.e. in } X, \quad (3)$$

$$Q \in L^2(X). \quad (4)$$

These assumptions are naturally valid in applications; the last part of (3) means that the absorption effect is not negligible. Under these assumptions, it is possible to show that the RTE (1) together with some suitable boundary condition has a unique solution ([1]).

The RTE is complicated and it is not possible to find closed form solution for applications. Numerical methods are needed to solve the RTE. However, it is challenging to develop efficient and effective numerical methods to solve the RTE for applications, since it is an integro-differential equation involving both partial derivatives and integrals and is of high dimension with five independent variables. Because it is difficult to solve the RTE, various approximation methods have been proposed for the RTE, e.g., the discrete-ordinates (S_N) method ([5]), spherical harmonics (P_N) expansion method ([4]), the zonal method ([11,12]). The P_N approximation method has been shown to provide increasingly improved results as the order N increases ([19]). However, the P_N approximation method requires solving a set of $(N+1)^2$ coupled partial differential equations in the spatial variable $\boldsymbol{x}$, and even for a moderately small value of N, it is rather expensive to use the method. In [14], a simplified spherical harmonics

(SP_N) method is developed that requires solving only $(N+1)/2$ partial differential equations for an odd order N. The SP_N method is shown to produce good approximate solutions of the RTE with high absorption and small geometries (see also [7]). In the literature, there has been no mathematical study on the SP_N method. This paper is intended as an initial step for such a study.

We recall the equations derived in [14] for the SP_N method for $N = 7$. Introduce

$$\begin{aligned}\varphi_1 &= \phi_0 + 2\,\phi_2,\\ \varphi_2 &= 3\,\phi_2 + 4\,\phi_4,\\ \varphi_3 &= 5\,\phi_4 + 6\,\phi_6,\\ \varphi_4 &= 7\,\phi_6.\end{aligned}$$

Then the function

$$\phi_0 = \varphi_1 - \frac{2}{3}\,\varphi_2 + \frac{8}{15}\,\varphi_3 - \frac{16}{35}\,\varphi_4$$

approximates the quantity

$$\int_\Omega \phi(\boldsymbol{x},\boldsymbol{\omega})\,d\sigma(\boldsymbol{\omega})$$

where ϕ is the solution of the RTE problem. The three dimensional SP_7 equations are

$$-\nabla\cdot\frac{1}{3\,\mu_{a1}}\nabla\varphi_1 + \mu_a\varphi_1 = Q_1 + \frac{2\,\mu_a}{3}\,\varphi_2 - \frac{8\,\mu_a}{15}\,\varphi_3 + \frac{16\,\mu_a}{35}\,\varphi_4, \tag{5}$$

$$\begin{aligned}&-\nabla\cdot\frac{1}{7\,\mu_{a3}}\nabla\varphi_2 + \left(\frac{4\,\mu_a}{9} + \frac{5\,\mu_{a2}}{9}\right)\varphi_2\\ &= Q_2 + \frac{2\,\mu_a}{3}\,\varphi_1 + \left(\frac{16\,\mu_a}{45} + \frac{4\,\mu_{a2}}{9}\right)\varphi_3 - \left(\frac{32\,\mu_a}{105} + \frac{8\,\mu_{a2}}{21}\right)\varphi_4,\end{aligned} \tag{6}$$

$$\begin{aligned}&-\nabla\cdot\frac{1}{11\,\mu_{a5}}\nabla\varphi_3 + \left(\frac{64\,\mu_a}{225} + \frac{16\,\mu_{a2}}{45} + \frac{9\,\mu_{a4}}{25}\right)\varphi_3\\ &= Q_3 - \frac{8\,\mu_a}{15}\,\varphi_1 + \left(\frac{16\,\mu_a}{45} + \frac{4\,\mu_{a2}}{9}\right)\varphi_2 + \left(\frac{128\,\mu_a}{525} + \frac{32\,\mu_{a2}}{105} + \frac{54\,\mu_{a4}}{175}\right)\varphi_4,\end{aligned} \tag{7}$$

$$\begin{aligned}&-\nabla\cdot\frac{1}{15\,\mu_{a7}}\nabla\varphi_4 + \left(\frac{256\,\mu_a}{1225} + \frac{64\,\mu_{a2}}{245} + \frac{324\,\mu_{a4}}{1225} + \frac{13\,\mu_{a6}}{49}\right)\varphi_4\\ &= Q_4 + \frac{16\,\mu_a}{35}\,\varphi_1 - \left(\frac{32\,\mu_a}{105} + \frac{8\,\mu_{a2}}{21}\right)\varphi_2 + \left(\frac{128\,\mu_a}{525} + \frac{32\,\mu_{a2}}{105} + \frac{54\,\mu_{a4}}{175}\right)\varphi_3,\end{aligned} \tag{8}$$

where

$$Q_1 = Q,\quad Q_2 = -\frac{2\,Q}{3},\quad Q_3 = \frac{8\,Q}{15},\quad Q_4 = -\frac{16\,Q}{35}, \tag{9}$$

and $\mu_{an} = \mu_{an}(\boldsymbol{x})$ is the nth-order absorption parameter:

$$\mu_{an}(\boldsymbol{x}) := \mu_t(\boldsymbol{x}) - \mu_s(\boldsymbol{x})\, g^n = \mu_a(\boldsymbol{x}) + \mu_s(\boldsymbol{x})\left(1 - g^n\right), \quad n = 1, 2, \ldots. \tag{10}$$

For convenience in later use, we also introduce the nth-order reduced scattering parameter:

$$\mu_{sn}(\boldsymbol{x}) := \mu_s(\boldsymbol{x})\left(1 - g^n\right), \quad n = 1, 2, \ldots. \tag{11}$$

Note that by the assumption (3),

$$\mu_{an}, \mu_{sn} \in L^\infty(X), \quad \mu_{an} \geq c_0, \ \mu_{sn} \geq 0 \text{ a.e. in } X, \quad n = 1, 2, \ldots. \tag{12}$$

To focus on the essential part of mathematical argument, we will mainly limit ourselves to the case of a perfect reflecting boundary condition, i.e., the case where the reflectivity coefficient is 1 (but see Remark 3 at the end of Sect. 3 for the case of partly-reflecting boundary condition). Then the boundary conditions are ([14]):

$$\frac{1}{3\,\mu_{a1}} \frac{\partial \varphi_1}{\partial n} = S_1(\boldsymbol{x}), \quad \boldsymbol{x} \in \partial X, \tag{13}$$

$$\frac{1}{7\,\mu_{a3}} \frac{\partial \varphi_2}{\partial n} = S_2(\boldsymbol{x}), \quad \boldsymbol{x} \in \partial X, \tag{14}$$

$$\frac{1}{11\,\mu_{a5}} \frac{\partial \varphi_3}{\partial n} = S_3(\boldsymbol{x}), \quad \boldsymbol{x} \in \partial X, \tag{15}$$

$$\frac{1}{15\,\mu_{a7}} \frac{\partial \varphi_4}{\partial n} = S_4(\boldsymbol{x}), \quad \boldsymbol{x} \in \partial X, \tag{16}$$

where $\partial/\partial n$ denotes the normal differentiation and for a given source function $S(\boldsymbol{x}, \boldsymbol{\omega})$, with $\boldsymbol{n}(\boldsymbol{x})$ the unit outward normal vector at $\boldsymbol{x}$ on the boundary ∂X,

$$S_1(\boldsymbol{x}) = \int_{\boldsymbol{\omega}\cdot\boldsymbol{n}(\boldsymbol{x})<0} S(\boldsymbol{x}, \boldsymbol{\omega})\, |\boldsymbol{\omega}\cdot\boldsymbol{n}(\boldsymbol{x})|\, d\sigma(\boldsymbol{\omega}), \tag{17}$$

$$S_2(\boldsymbol{x}) = \frac{1}{2} \int_{\boldsymbol{\omega}\cdot\boldsymbol{n}(\boldsymbol{x})<0} S(\boldsymbol{x}, \boldsymbol{\omega}) \left(5\, |\boldsymbol{\omega}\cdot\boldsymbol{n}(\boldsymbol{x})|^3 - 3\, |\boldsymbol{\omega}\cdot\boldsymbol{n}(\boldsymbol{x})|\right) d\sigma(\boldsymbol{\omega}), \tag{18}$$

$$S_3(\boldsymbol{x}) = \frac{1}{8} \int_{\boldsymbol{\omega}\cdot\boldsymbol{n}(\boldsymbol{x})<0} S(\boldsymbol{x}, \boldsymbol{\omega}) \left(63\, |\boldsymbol{\omega}\cdot\boldsymbol{n}(\boldsymbol{x})|^5 - 70\, |\boldsymbol{\omega}\cdot\boldsymbol{n}(\boldsymbol{x})|^3 + 15\, |\boldsymbol{\omega}\cdot\boldsymbol{n}(\boldsymbol{x})|\right) d\sigma(\boldsymbol{\omega}), \tag{19}$$

$$S_4(\boldsymbol{x}) = \frac{1}{16} \int_{\boldsymbol{\omega}\cdot\boldsymbol{n}(\boldsymbol{x})<0} S(\boldsymbol{x}, \boldsymbol{\omega}) \left(429\, |\boldsymbol{\omega}\cdot\boldsymbol{n}(\boldsymbol{x})|^7 - 693\, |\boldsymbol{\omega}\cdot\boldsymbol{n}(\boldsymbol{x})|^5 + 315\, |\boldsymbol{\omega}\cdot\boldsymbol{n}(\boldsymbol{x})|^3 - 35\, |\boldsymbol{\omega}\cdot\boldsymbol{n}(\boldsymbol{x})|\right) d\sigma(\boldsymbol{\omega}). \tag{20}$$

The simplified spherical harmonics system SP_7 consists of the partial differential equation (5)–(8) and the boundary conditions (13)–(16). To obtain the simplified spherical harmonics system SP_5, we drop (8) and (16), and set $\varphi_4 = 0$ in (5)–(7) and (13)–(15). To obtain the simplified spherical harmonics system SP_3, we drop (7)–(8) and (15)–(16), and set $\varphi_4 = \varphi_3 = 0$ in (5)–(6) and (13)–(14). To obtain the simplified spherical harmonics system SP_1, we drop (6)–(8) and (14)–(16), and set $\varphi_4 = \varphi_3 = \varphi_2 = 0$ in (5) and (13). The differential equation for SP_1 is known as the diffusion equation:

$$-\nabla\cdot\frac{1}{3\,\mu_{a1}}\nabla\varphi_1 + \mu_a\varphi_1 = Q_1 \quad \text{in } X.$$

This paper is devoted to a study of well-posedness of the simplified spherical harmonics systems. In Sect. 2, we recall some mathematical knowledge useful in the study of well-posedness of elliptic boundary value problems. In Sect. 3, we introduce a weak formulation of the simplified spherical harmonics system SP_7 and show the existence of its unique solution. The results proved for SP_7 are valid also for SP_N with $N = 1, 3, 5$. In Sect. 4, we provide a few concluding remarks regarding the numerical solution of the simplified spherical harmonics systems.

2 Mathematical preliminary

We first state the well-known Lax-Milgram Lemma (see, e.g., [2, Sect. 8.3] or [9]), which is widely applied in the study of well-posedness of linear elliptic boundary value problems. Some explanations are given afterwards.

Theorem 1 *Assume V is a Hilbert space, $a(\cdot,\cdot) : V \times V \to \mathbb{R}$ is a bounded, V-elliptic bilinear form, $\ell : V \to \mathbb{R}$ is a continuous linear form. Then there is a unique solution of the problem*

$$u \in V, \quad a(u, v) = \ell(v) \quad \forall\, v \in V. \tag{21}$$

We recall that a function space V is called a Hilbert space if there is an inner product $(\cdot,\cdot)$ defined over the space such that V is complete with respect to the corresponding norm induced by the inner product. As an example, the space $L^2(X)$ of square integrable functions over X is a Hilbert space with the canonical inner product

$$(u, v)_{L^2(X)} = \int_X u(\boldsymbol{x})\, v(\boldsymbol{x})\, dx.$$

The corresponding norm in $L^2(X)$ is

$$\|v\|_{L^2(X)} = (v, v)^{1/2}_{L^2(X)} = \left[\int_X |v(\boldsymbol{x})|^2 dx\right]^{1/2}.$$

The completeness of $L^2(X)$ refers to the property that if $\{v_n\}_{n\ge 1} \subset L^2(X)$ is a Cauchy sequence in the sense that $\lim_{m,n\to\infty} \|v_m - v_n\|_{L^2(X)} \to 0$, then the sequence has a limit function $v \in L^2(X)$: $\lim_{n\to\infty} \|v_n - v\|_{L^2(X)} = 0$. In the study of the simplified spherical harmonics system, we will need the following Sobolev space

$$H^1(X) = \left\{\psi \in L^2(X) \mid \nabla\psi \in L^2(X)^3\right\}, \tag{22}$$

i.e., V consists of all square integrable functions ψ whose first order partial derivatives $\partial_{x_1}\psi,\ \partial_{x_2}\psi$, and $\partial_{x_3}\psi$ are all square integrable. Here, ∇ is the gradient operator, $\nabla\psi := (\partial_{x_1}\psi, \partial_{x_2}\psi, \partial_{x_3}\psi)^T$. For some detail on the Sobolev space $H^1(X)$, see, e.g., [2, Chap. 7] or [9]. $H^1(X)$ is a Hilbert space with the inner product

$$(u, v)_{H^1(X)} = \int_X [u(\boldsymbol{x})\, v(\boldsymbol{x}) + \nabla u(\boldsymbol{x})\cdot\nabla v(\boldsymbol{x})]\, dx$$

and the corresponding norm

$$\|v\|_{H^1(X)} = \left\{\int_X \left[|v(\boldsymbol{x})|^2 + |\nabla v(\boldsymbol{x})|^2\right] dx\right\}^{1/2}.$$

For a function $v \in H^1(X)$, its value (trace) on the boundary ∂X is well-defined and we have the inequality

$$\|v\|_{L^2(\partial X)} \le c\, \|v\|_{H^1(X)} \quad \forall\, v \in H^1(X) \tag{23}$$

for some constant $c > 0$ depending only on X.

A form $a : V \times V \to \mathbb{R}$ is said to be bilinear if it is linear with respect to each of the two arguments:

$$a(c_1u_1 + c_2u_2, v) = c_1a(u_1, v) + c_2a(u_2, v) \quad \forall\, u_1, u_2, v \in V,\ c_1, c_2 \in \mathbb{R},$$
$$a(u, c_1v_1 + c_2v_2) = c_1a(u, v_1) + c_2a(u, v_2) \quad \forall\, u, v_1, v_2 \in V,\ c_1, c_2 \in \mathbb{R}.$$

The bilinear form $a(\cdot, \cdot)$ is said to be bounded (or continuous) if

$$|a(u, v)| \le c\, \|u\|_V \|v\|_V \quad \forall\, u, v \in V$$

for some constant $c > 0$ independent of u and v. It is V-elliptic if there is a constant $m > 0$ such that

$$a(v, v) \ge m\, \|v\|_V^2 \quad \forall\, v \in V.$$

The form $\ell : V \to \mathbb{R}$ is said to be linear if

$$\ell(c_1v_1 + c_2v_2) = c_1\ell(v_1) + c_2\ell(v_2) \quad \forall\, v_1, v_2 \in V,\ c_1, c_2 \in \mathbb{R},$$

and is continuous if for some constant $c > 0$,

$$|\ell(v)| \le c\,\|v\|_V \quad \forall\, v \in V.$$

Theorem 1 is applied in Sect. 3 where a concrete example is provided for the space V, the bilinear form $a(\cdot,\cdot)$, the linear form $\ell(\cdot)$ and the verification of the assumptions stated in Theorem 1.

3 Well-posedness of the simplified spherical harmonics system

To study the existence and uniqueness of a solution to the simplified spherical harmonics system of (5)–(8) and (13)–(16), we start with a weak formulation of the system. We need the vector-valued function space

$$\boldsymbol{V} := H^1(X)^4, \tag{24}$$

where the Sobolev space $H^1(X)$ is introduced in Sect. 2. Functions in the space $\boldsymbol{V}$ have four component functions in V, e.g., $\boldsymbol{\psi} = (\psi_1, \psi_2, \psi_3, \psi_4)^T$, $\boldsymbol{\psi} \in \boldsymbol{V}$ if and only if $\psi_i \in H^1(X)$, $1 \le i \le 4$. Suppose the system has a smooth solution $\boldsymbol{\varphi} = (\varphi_1, \varphi_2, \varphi_3, \varphi_4)^T$. We multiply (5) by $\psi_1 \in V$, integrate over X and apply the boundary condition (13). The result is an integral equality

$$a_1(\boldsymbol{\varphi}, \psi_1) = \ell_1(\psi_1) \quad \forall\, \psi_1 \in H^1(X), \tag{25}$$

where the bilinear form $a_1(\cdot,\cdot)$ and the linear form $\ell_1(\cdot)$ are defined by

$$a_1(\boldsymbol{\varphi}, \psi_1) = \int_X \left[\frac{1}{3\,\mu_{a1}} \nabla\varphi_1 \cdot \nabla\psi_1 + \mu_a \left(\varphi_1 - \frac{2}{3}\varphi_2 + \frac{8}{15}\varphi_3 - \frac{16}{35}\varphi_4\right)\psi_1\right] dx, \tag{26}$$

$$\ell_1(\psi_1) = \int_X Q_1 \psi_1 dx + \int_{\partial X} S_1 \psi_1 ds. \tag{27}$$

Similarly, we derive from the Eq. (6) and the boundary condition (14), from the Eq. (7) and the boundary condition (15), and from the Eq. (8) and the boundary condition (16), the following equalities:

$$a_2(\boldsymbol{\varphi}, \psi_2) = \ell_2(\psi_2) \quad \forall\, \psi_2 \in H^1(X), \tag{28}$$

$$a_3(\boldsymbol{\varphi}, \psi_3) = \ell_3(\psi_3) \quad \forall\, \psi_3 \in H^1(X), \tag{29}$$

$$a_4(\boldsymbol{\varphi}, \psi_4) = \ell_4(\psi_4) \quad \forall\, \psi_4 \in H^1(X), \tag{30}$$

where for the bilinear forms,

$$a_2(\boldsymbol{\varphi}, \psi_2) = \int_X \left[\frac{1}{7\,\mu_{a3}} \nabla\varphi_2 \cdot \nabla\psi_2 + \mu_a \left(\frac{4}{9}\varphi_2 - \frac{2}{3}\varphi_1 - \frac{16}{45}\varphi_3 + \frac{32}{105}\varphi_4 \right) \psi_2 \right.$$
$$\left. + \mu_{a2} \left(\frac{5}{9}\varphi_2 - \frac{4}{9}\varphi_3 + \frac{8}{21}\varphi_4 \right) \psi_2 \right] dx, \tag{31}$$

$$a_3(\boldsymbol{\varphi}, \psi_3) = \int_X \left[\frac{1}{11\,\mu_{a5}} \nabla\varphi_3 \cdot \nabla\psi_3 + \mu_a \left(\frac{64}{225}\varphi_3 + \frac{8}{15}\varphi_1 - \frac{16}{45}\varphi_2 - \frac{128}{525}\varphi_4 \right) \psi_3 \right.$$
$$\left. + \mu_{a2} \left(\frac{16}{45}\varphi_3 - \frac{4}{9}\varphi_2 - \frac{32}{105}\varphi_4 \right) \psi_3 + \mu_{a4} \left(\frac{9}{25}\varphi_3 - \frac{54}{175}\varphi_4 \right) \psi_3 \right] dx, \tag{32}$$

$$a_4(\boldsymbol{\varphi}, \psi_4) = \int_X \left[\frac{1}{15\,\mu_{a7}} \nabla\varphi_4 \cdot \nabla\psi_4 + \mu_a \left(\frac{256}{1225}\varphi_4 - \frac{16}{35}\varphi_1 + \frac{32}{105}\varphi_2 - \frac{128}{525}\varphi_3 \right) \psi_4 \right.$$
$$+ \mu_{a2} \left(\frac{64}{245}\varphi_4 + \frac{8}{21}\varphi_2 - \frac{32}{105}\varphi_3 \right) \psi_4 + \mu_{a4} \left(\frac{324}{1225}\varphi_4 - \frac{54}{175}\varphi_3 \right) \psi_4$$
$$\left. + \mu_{a6} \frac{13}{49} \varphi_4 \psi_4 \right] dx, \tag{33}$$

and for the linear forms,

$$\ell_2(\psi_2) = \int_X Q_2 \psi_2 dx + \int_{\partial X} S_2 \psi_2 ds, \tag{34}$$

$$\ell_3(\psi_3) = \int_X Q_3 \psi_3 dx + \int_{\partial X} S_3 \psi_3 ds, \tag{35}$$

$$\ell_4(\psi_4) = \int_X Q_4 \psi_4 dx + \int_{\partial X} S_4 \psi_4 ds. \tag{36}$$

Adding the equalities (25), (28)–(30), we obtain the weak formulation of the system

$$\boldsymbol{\varphi} \in \boldsymbol{V}, \quad a(\boldsymbol{\varphi}, \boldsymbol{\psi}) = \ell(\boldsymbol{\psi}) \quad \forall\, \boldsymbol{\psi} \in \boldsymbol{V}, \tag{37}$$

where

$$a(\boldsymbol{\varphi}, \boldsymbol{\psi}) := \sum_{i=1}^{4} a_i(\boldsymbol{\varphi}, \psi_i), \tag{38}$$

$$\ell(\boldsymbol{\psi}) := \sum_{i=1}^{4} \ell_i(\psi_i). \tag{39}$$

For the well-posedness, we apply the Lax-Milgram Lemma. The most difficult condition to verify is the $\boldsymbol{V}$-ellipticity of the bilinear form $a(\cdot,\cdot)$. We note from the definitions (38), (26) and (31)–(33) that

$$a(\boldsymbol{\psi},\boldsymbol{\psi}) = \int_X \left(\frac{1}{3\,\mu_{a1}} |\nabla\psi_1|^2 + \frac{1}{7\,\mu_{a3}} |\nabla\psi_2|^2 + \frac{1}{11\,\mu_{a5}} |\nabla\psi_3|^2 + \frac{1}{15\,\mu_{a7}} |\nabla\psi_4|^2 + \mu_a \boldsymbol{\psi}^T A \boldsymbol{\psi} + \mu_{s,2} \boldsymbol{\psi}^T A_2 \boldsymbol{\psi} + \mu_{s,4} \boldsymbol{\psi}^T A_4 \boldsymbol{\psi} + \mu_{s,6} \boldsymbol{\psi}^T A_6 \boldsymbol{\psi} \right) dx, \qquad (40)$$

where

$$A = A_0 + A_2 + A_4 + A_6$$

and

$$A_0 = \begin{pmatrix} 1 & -\frac{2}{3} & \frac{8}{15} & -\frac{16}{35} \\ -\frac{2}{3} & \frac{4}{9} & -\frac{16}{45} & \frac{32}{105} \\ \frac{8}{15} & -\frac{16}{45} & \frac{64}{225} & -\frac{128}{525} \\ -\frac{16}{35} & \frac{32}{105} & -\frac{128}{525} & \frac{256}{1225} \end{pmatrix}, \quad A_2 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & \frac{5}{9} & -\frac{4}{9} & \frac{8}{21} \\ 0 & -\frac{4}{9} & \frac{16}{45} & -\frac{32}{105} \\ 0 & \frac{8}{21} & -\frac{32}{105} & \frac{64}{245} \end{pmatrix},$$

$$A_4 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{9}{25} & -\frac{54}{175} \\ 0 & 0 & -\frac{54}{175} & \frac{324}{1225} \end{pmatrix}, \quad A_6 = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & \frac{13}{49} \end{pmatrix}.$$

Note that for $i = 0, 2, 4, 6$, the matrix A_i counts for contribution from the term involving μ_{ai}, where $\mu_{a0} \equiv \mu_a$. Also note that all the matrices $A,\ A_0,\ A_2,\ A_4$, and A_6 are symmetric.

The eigenvalues of the matrix A are all positive:

$$\lambda_1 \doteq 0.1151929871184648,$$
$$\lambda_2 \doteq 0.2455018429016393,$$
$$\lambda_3 \doteq 0.6217959073051715,$$
$$\lambda_4 \doteq 3.017509262674723.$$

So the matrix A is positive definite. Also, it is easy to verify that the matrices $A_0,\ A_2,\ A_4$, and A_6 are positive semi-definite.

Now we apply Theorem 1 to the weak formulation (37) of the simplified spherical harmonics systems.

Theorem 2 *Assume* (3), (4) *and* $S \in L^2(\partial X \times \Omega)$. *Then the problem* (37) *has a unique solution* $\boldsymbol{\varphi} \in \boldsymbol{V}$.

Proof Note that the assumption (4) implies $Q_i \in L^2(X)$ for the Q_i, $1 \le i \le 4$, defined in (9), and the assumption $S \in L^2(\partial X \times \Omega)$ implies $S_i \in L^2(\partial X)$ for S_i, $1 \le i \le 4$, defined in (17)–(20).

Now we verify all the assumptions of Theorem 1. The space $\boldsymbol{V}$ is a Hilbert space since $H^1(X)$ is a Hilbert space. From the definitions (38) and (39), it is obvious that $a(\boldsymbol{\varphi}, \boldsymbol{\psi})$ is a bilinear form and $\ell(\boldsymbol{\psi})$ is a linear form. Applying the Cauchy-Schwarz inequalities

$$\left| \int_X u(\boldsymbol{x})\, v(\boldsymbol{x})\, dx \right| \le \|u\|_{L^2(X)} \|v\|_{L^2(X)},$$

$$\left| \int_{\partial X} u(\boldsymbol{x})\, v(\boldsymbol{x})\, dx \right| \le \|u\|_{L^2(\partial X)} \|v\|_{L^2(\partial X)}$$

together with the condition (12), the trace inequality (23), $Q_i \in L^2(X)$ and $S_i \in L^2(\partial X)$ for $1 \le i \le 4$, we see that $a(\boldsymbol{\varphi}, \boldsymbol{\psi})$ is bounded and $\ell(\boldsymbol{\psi})$ is continuous. So the only remaining condition to verify is the $\boldsymbol{V}$-ellipticity of the bilinear form $a(\cdot, \cdot)$. From (40), positiveness of the parameter μ_a, non-negativeness of the parameters μ_{s2}, μ_{s4}, μ_{s6}, and properties of the matrices A_0, A_2, A_4, and A_6, we have

$$a(\boldsymbol{\psi}, \boldsymbol{\psi}) \ge \int_X \left(\frac{1}{3\,\mu_{a1}} |\nabla \psi_1|^2 + \frac{1}{7\,\mu_{a3}} |\nabla \psi_2|^2 + \frac{1}{11\,\mu_{a5}} |\nabla \psi_3|^2 + \frac{1}{15\,\mu_{a7}} |\nabla \psi_4|^2 + \mu_a \lambda_1 |\boldsymbol{\psi}|^2 \right) dx.$$

Using (12) again, we then deduce that for some constant $c > 0$,

$$a(\boldsymbol{\psi}, \boldsymbol{\psi}) \ge c\, \|\boldsymbol{\psi}\|_{\boldsymbol{V}}^2 \quad \forall\, \boldsymbol{\psi} \in \boldsymbol{V}.$$

Thus, $a(\boldsymbol{\varphi}, \boldsymbol{\psi})$ is $\boldsymbol{V}$-elliptic. Therefore, we can apply Theorem 1 to conclude that the problem (37) has a unique solution $\boldsymbol{\varphi} \in \boldsymbol{V}$. □

Furthermore, the solution $\boldsymbol{\phi} \in \boldsymbol{V}$ of the problem (37) can be shown to depend continuously on the data.

It is natural to ask if the components of the unique solution $\boldsymbol{\varphi} \in \boldsymbol{V}$ guaranteed in Theorem 2 satisfy the Eqs. (5)–(8) and the boundary conditions (13)–(16). To answer this question, we need to explore the smoothness properties of the solution $\boldsymbol{\varphi} \in \boldsymbol{V}$. In addition to the Sobolev space $H^1(X)$, for an integer $k \ge 1$, we need the notion of the Sobolev space $H^k(X)$ of square integrable functions whose partial derivatives of order less than or equal to k are square integrable. Assume $\mu_a, \mu_s \in C^1(\overline{X})$, i.e., μ_a and μ_s are continuously differentiable, and S_i are boundary values of $H^1(X)$ functions. Then following a standard argument in the solution regularity theory for elliptic boundary value problems ([9]), applied to each of the sub-problems (25) and (28)–(30), it is possible to show the solution components are smoother than $H^1(X)$:

$$\varphi_i \in H^2(X), \quad 1 \le i \le 4.$$

Therefore, again following a standard argument, we can show that the component functions $\{\varphi_i\}_{i=1}^4$ satisfy the Eqs. (5)–(8) almost everywhere in X and the boundary conditions (13)–(16) almost everywhere on ∂X. Generally, for an positive integer m, if $\mu_a, \mu_s \in C^{m+1}(\overline{X})$, and for $1 \le i \le 4$, $Q_i \in H^m(X)$ and S_i is the boundary value of an $H^{m+1}(X)$ function, then

$$\varphi_i \in H^{m+2}(X), \quad 1 \le i \le 4.$$

In particular, if $m \ge 2$, then by a so-called embedding theorem for Sobolev spaces ([2, Chap. 7]), we have

$$\varphi_i \in C^2(\overline{X}), \quad 1 \le i \le 4$$

and then the Eqs. (5)–(8) and the boundary conditions (13)–(16) are satisfied in the classical pointwise sense.

Remark 3 It is possible to extend the proof of Theorem 2 to account for partly-reflecting boundary condition. Here we illustrate such an extension for the SP_N method with $N = 1$. The discussion for other values of N is essentially the same, but involves lengthy formulas and expressions, and is hence omitted.

Denote by $R(\cdot)$ the reflectivity of the boundary ∂X; it is a measurable function with values in [0, 1]. A popular choice of $R(\cdot)$ is given in [14, (5)]. However, the well-posedness theory does not depend on the concrete form of this function. Then the boundary value problem is

$$-\nabla\cdot\frac{1}{3\,\mu_{a1}}\nabla\varphi_1 + \mu_a\varphi_1 = Q_1 \quad \text{in } X, \tag{41}$$

$$\frac{1}{3\,\mu_{a1}}\frac{\partial\varphi_1}{\partial n} + c_1\varphi_1 = \tilde{S}_1 \quad \text{on } \partial X. \tag{42}$$

Here,

$$c_1 = \frac{1/2 - R_1}{1 + 3\,R_2}, \qquad \tilde{S}_1(\boldsymbol{x}) = \frac{2}{1 + 3\,R_2}\,S_1(\boldsymbol{x})$$

in which,

$$R_1 = \int_0^1 R(\tau)\,\tau\,d\tau, \qquad R_2 = \int_0^1 R(\tau)\,\tau^2 d\tau.$$

Since $R(\cdot)$ takes on values in [0, 1], we know that $0 \le R_1 \le 1/2,\ 0 \le R_2 \le 1/3$ and therefore, $c_1 \ge 0$ (for a perfect reflecting boundary, $c_1 = 0$). The weak formulation of the boundary value problem (41)–(42) is

$$\varphi_1 \in H^1(X)\ :\ \int\limits_X \left(\frac{1}{3\,\mu_{a1}}\nabla\varphi_1\cdot\nabla\psi_1 + \mu_a\varphi_1\psi_1\right)dx + c_1\int\limits_{\partial X}\varphi_1\psi_1 ds$$
$$= \int\limits_X Q_1\psi_1 dx + \int\limits_{\partial X}\tilde{S}_1\psi_1 ds \quad \forall\,\psi_1 \in H^1(X). \tag{43}$$

Under the assumptions stated in Theorem 2, similar to the proof of Theorem 2, we can apply the Lax-Milgram Lemma to conclude that the weak formulation (43) has a unique solution. The property $c_1 \geq 0$ is needed in proving the $H^1(X)$-ellipticity of the bilinear form defined by the left side of (43).

4 Concluding remarks

The radiative transfer equation (RTE) is difficult to solve numerically due to its high dimension and integro-differential form. The simplified spherical harmonics (SP_N) method provides an efficient way to generate good approximate solutions of the RTE in the case of high absorption and small geometries. In this paper, we study the well-posedness of the simplified spherical harmonics system. This is achieved through the introduction and analysis of the weak formulation (37). The solution existence and uniqueness result, Theorem 2, is shown for SP_7. As explained near the end of Sect. 1, the result proved for SP_7 is valid also for SP_N with $N = 1, 3, 5$.

The weak formulation (37) provides a starting point for developing the Galerkin finite element method to solve the simplified spherical harmonics system. We briefly comment on this point here. Let $\{\mathcal{T}^h\}$ be a regular family of finite element partitions of the domain $\overline{X}$ (see, e.g., [2,3,8]), where the meshsize h stands for the maximal element side length in the mesh $\mathcal{T}^h$. Corresponding to the mesh $\mathcal{T}^h$, we introduce a finite element space $V^h \subset H^1(X)$, consisting of continuous, piecewise polynomials of certain degree (say, of degree 1, 2, etc.). Let $\boldsymbol{V}^h = (V^h)^4$. Then the finite element method for solving the problem (37) is

$$\boldsymbol{\varphi}^h \in \boldsymbol{V}^h, \quad a(\boldsymbol{\varphi}^h, \boldsymbol{\psi}^h) = \ell(\boldsymbol{\psi}^h) \quad \forall\,\boldsymbol{\psi}^h \in \boldsymbol{V}^h. \tag{44}$$

Similar to Theorem 2, we can show that the discrete system (44) has a unique solution $\boldsymbol{\varphi}^h \in \boldsymbol{V}^h$ and for the error of this finite element solution, we have, for some constant c,

$$\|\boldsymbol{\varphi} - \boldsymbol{\varphi}^h\|_{\boldsymbol{V}} \leq c \inf_{\boldsymbol{\psi}\in\boldsymbol{V}^h} \|\boldsymbol{\varphi} - \boldsymbol{\psi}^h\|_{\boldsymbol{V}}. \tag{45}$$

Based on the inequality (45), we can then show the convergence of the finite element solution as the meshsize approaches zero,

$$\|\boldsymbol{\varphi} - \boldsymbol{\varphi}^h\|_{\boldsymbol{V}} \to 0 \quad \text{as } h \to 0,$$

and derive error bounds in terms of powers of h where the true solution $\boldsymbol{\varphi}$ has more regularity than being in $\boldsymbol{V}$. Discussions on a finite element system of the form (44) can be found in, e.g. [2, Chap. 10].

References

1. A. Agoshkov, *Boundary Value Problems for Transport Equations* (Birkhäuser, Boston, 1998)
2. K. Atkinson, W. Han, *Theoretical Numerical Analysis*: *A Functional Analysis Framework*, 3rd edn. (Springer, Berlin, 2009)
3. S.C. Brenner, L.R. Scott, *The Mathematical Theory of Finite Element Methods*, 3rd edn. (Springer, New York, 2008)
4. K.M. Case, P.F. Zweifel, *Linear Transport Theory* (Addison-Wesley, Reading, 1967)
5. S. Chandrasekhar, *Radiative Transfer* (Clarendon, London, 1950)
6. G.R. Choppin, J.-O. Liljenzin, J. Rydberg, *Radiochemistry and Nuclear Chemistry*, 3rd edn. (Butterworth-Heinemann, Woburn, 2002)
7. M. Chu, K. Vishwanath, A.D. Klose, H. Dehghani, Light transport in biological tissue using three-dimensional frequency-domain simplified spherical harmonics equations. Phys. Med. Biol. **54**, 2493–2509 (2009)
8. P.G. Ciarlet, *The Finite Element Method for Elliptic Problems* (North Holland, Amsterdam, 1978)
9. L.C. Evans, *Partial Differential Equations*. (American Mathematical Society, 1998)
10. L. Henyey, J. Greenstein, Diffuse radiation in the galaxy. Astrophys J. **93**, 70–83 (1941)
11. H.C. Hottel, E.S. Cohen, Radiant heat exchange in a gas-filled enclosure: allowance for nonuniformity of gas temperature. AIChE J. **4**, 3–14 (1958)
12. H.C. Hottel, A.F. Sarofim, *Radiative Transfer* (McGraw-Hill, New York, 1967)
13. C.E. Junge, *Air Chemistry and Radiochemistry* (Academic Press, New York, 1963)
14. A.D. Klose, E.W. Larsen, Light transport in biological tissue based on the simplified spherical harmonics equations. J. Comput. Phys. **220**, 441–470 (2006)
15. E.E. Lewis, W.F. Miller, *Computational Methods of Neutron Transport* (Wiley, New York, 1984)
16. M.F. Modest, *Radiative Heat Transfer*, 2nd edn. (Academic Press, NewYork, 2003)
17. F. Natterer, F. Wübbeling, *Mathematical Methods in Image Reconstruction* (SIAM, Philadelphia, 2001)
18. G.E. Thomas, K. Stamnes, *Radiative Transfer in the Atmosphere and Ocean* (Cambridge University Press, Cambridge, 1999)
19. S. Wright, M. Schweiger, S.R. Arridge, Reconstruction in optical tomography using the P_N approximations. Meas. Sci. Technol. **18**, 79–86 (2007)
20. W. Zdunkowski, T. Trautmann, A. Bott, *Radiation in the Atmosphere: A Course in Theoretical Meteorology* (Cambridge University Press, Cambridge, 2007)