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Energy dependent radiative transfer equation and energy discretization

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ABSTRACT

The radiative transfer equation (RTE) arises in a wide variety of applications. In certain situations, the energy dependence is not negligible. In a series of two papers, we study the energy dependent RTE. In this first paper of the series, we focus on the well-posedness analysis and energy discretization. We use a mixed formulation so that the analysis covers both cases of non-vanishing absorption and vanishing absorption. We introduce a natural energy discretization scheme and derive an optimal order error estimate for the scheme. Angular discretization, spatial discretization and fully discrete schemes, as well as numerical simulation results, are the topics of the sequel.

1. Introduction

The radiative transfer equation (RTE) is an integro-differential equation which describes the propagation of radiation within a participating medium. Its applications are extremely diverse, ranging from applications in biomedical imaging [1,2] to the investigation of stellar phenomena [3]. The energy dependent form occurs frequently in neutron transport [4,5] and has recently been applied in proton radiation therapy treatment planning [6].

The RTE is notoriously difficult to solve in many real-world applications. Analytical solutions for the equation are known only for a small subset of situations, which necessitates its numerical solution. Yet numerically, due to the high dimension and the integro-differential form of the equation, the computational demands are significant, and there has been much investigation within each field of applications (cf. [5,7–10]). Some techniques employed include approximations to the equation itself [11,12], numerical techniques [13,14], and high performance implementations [10,15].

However, compared to the numerical analysis of the ordinary monoenergetic RTE, relatively little work has been done with the energy dependent form and cases which contain void regions where the absorption is considered negligible. In this paper, we consider the well-posedness of the boundary value problem of the RTE in a mixed formulation that covers both cases of non-vanishing absorption and vanishing absorption. In addition, an energy discretization is introduced alongside a rigorous analysis of the semi-discretization. Recently, the monoenergetic form of the RTE under conditions permitting vanishing absorption has been analyzed using a mixed variational framework [16]. In this paper, we show that this approach can be extended to establish the existence and uniqueness of the energy dependent problem. Further, the monoenergetic theory is applied to the proposed energy discretization to establish well-posedness of the resulting semi-discretization. An optimal order error estimate is derived for the energy discretization.

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Let $X \subset \mathbb{R}^3$ be a bounded domain with a boundary $\partial X \in C^1$, let Ω be the unit sphere in $\mathbb{R}^3$, and let $E = [e_{\min}, e_{\max}]$ be a closed bounded interval in $\mathbb{R}$ for the energy domain. Denote $U = X \times \Omega \times E$ and $\Gamma = \partial X \times \Omega \times E$. We define the inflow and outflow portions of Γ by

$$\Gamma_- = \{(\mathbf{x}, \boldsymbol{\omega}, e) \in \Gamma \mid \boldsymbol{\omega} \cdot \boldsymbol{\nu}(\mathbf{x}) < 0\} \quad \text{and} \quad \Gamma_+ = \{(\mathbf{x}, \boldsymbol{\omega}, e) \in \Gamma \mid \boldsymbol{\omega} \cdot \boldsymbol{\nu}(\mathbf{x}) > 0\}, \tag{1}$$

respectively; here $\boldsymbol{\nu}(\mathbf{x})$ denotes the unit outward normal at the spatial variable $\mathbf{x} \in \partial X$. We consider the following boundary value problem (BVP) of the RTE (cf. [4,17])

$$\boldsymbol{\omega} \cdot \nabla_x u(\mathbf{x}, \boldsymbol{\omega}, e) + \sigma_t(\mathbf{x}, e) u(\mathbf{x}, \boldsymbol{\omega}, e) - Su(\mathbf{x}, \boldsymbol{\omega}, e) = f(\mathbf{x}, \boldsymbol{\omega}, e) \quad \text{in } U, \tag{2}$$

$$u(\mathbf{x}, \boldsymbol{\omega}, e) = g(\mathbf{x}, \boldsymbol{\omega}, e) \quad \text{on } \Gamma_-, \tag{3}$$

where ∇_x denotes the gradient with respect to the spatial variable $\mathbf{x} \in X$ and

$$Su(\mathbf{x}, \boldsymbol{\omega}, e) := \int_E \int_\Omega \sigma_s(\mathbf{x}, e') \mathcal{P}(\mathbf{x}, \boldsymbol{\omega} \cdot \boldsymbol{\omega}', e, e') u(\mathbf{x}, \boldsymbol{\omega}', e') d\boldsymbol{\omega}' de'. \tag{4}$$

Here, σ_t denotes the total cross section which reflects the probability of a collision occurring. It can be written as $\sigma_t = \sigma_a + \sigma_s$, where σ_a and σ_s denote the absorption and scattering cross sections, respectively. The functions f and g reflect the source term and boundary data, respectively. The function $\mathcal{P}$ reflects the probability that particles scatter from direction $\boldsymbol{\omega}'$ with energy e' into direction $\boldsymbol{\omega}$ with energy e. The scattering term overall then reflects scattering from all directions and energies into direction $\boldsymbol{\omega}$ and energy e. It will be useful to define the quantity

$$\sigma_s'(\mathbf{x}, e) := \int_E \int_\Omega \sigma_s(\mathbf{x}, e') \mathcal{P}(\mathbf{x}, \boldsymbol{\omega} \cdot \boldsymbol{\omega}', e, e') d\boldsymbol{\omega}' de'.$$

We remark that at various times we will suppress a function's dependence on certain variables for ease of presentation. We let $I_0 := [-1, 1]$ be the range of the expression $\boldsymbol{\omega} \cdot \boldsymbol{\omega}'$. In the study of the boundary value problem (2)–(3), we make the following assumptions:

$$\sigma_t, \sigma_s \in L^\infty(X \times E), \quad \sigma_t \geq \sigma_s \geq 0, \text{ and } \sigma_t \geq \sigma_s'. \tag{5}$$

$$\mathcal{P} \in L^\infty(X \times I_0 \times E^2) \text{ is non-negative and } \mathcal{P}(\mathbf{x}, \boldsymbol{\omega} \cdot \boldsymbol{\omega}', e, e') = 0 \quad \text{for } e' < e. \tag{6}$$

$$\mathcal{P} \text{ is normalized such that } \int_E \int_\Omega \mathcal{P}(\mathbf{x}, \boldsymbol{\omega} \cdot \boldsymbol{\omega}', e, e') d\boldsymbol{\omega} de = 1. \tag{7}$$

The non-negativity of the cross sections in (5) is appropriate because these quantities represent the likelihood of a scattering or absorption event. Note that $\sigma_t - \sigma_s = \sigma_a \geq 0$. We again note that the condition allowing σ_a equality with zero is not often considered in the literature due to stability issues. In particular, the constant in a priori bounds is often dependent on the lower bound of σ_a. As a result, the estimates tend to infinity as the minimum value of σ_a approaches zero. One of the main contributions of [16] is in providing an a priori estimate independent of the lower bound of σ_a. The assumption $\sigma_t \geq \sigma_s'$ is necessary for establishing the positivity condition required by Brezzi's theorem which is used in establishing existence and uniqueness of the original BVP. The no-upscatter condition is given by the second part of (6). It states that a particle cannot gain energy due to a collision with an atomic nuclei. Because $\mathcal{P}$ denotes the probability that a particle scatters from an energy e' to energy e, assumption (6) ensures that particles scatter from lower energies to higher energies with probability zero.

In a series of two papers, we study the energy dependent RTE, theoretically and numerically. In this first paper, we focus on the well-posedness analysis and energy discretization, whereas angular discretization, spatial discretization and fully discrete schemes, as well as numerical simulation results, are the topics of the sequel. This paper is organized as follows: In Section 2 some function spaces are introduced. Section 3 provides the existence and uniqueness proof for the BVP (2)–(3). In Section 4 an approximation of the energy variable in (2)–(3) is introduced alongside a rigorous analysis of the obtained semi-discretization; after which, an optimal order error estimate is derived. We conclude in Section 5 and elaborate on the extensions of this work provided in the sequel.

2. Function spaces

We introduce function spaces needed for a discussion of the well-posedness of the BVP (2)–(3). Our well-posedness analysis is an extension of the monoenergetic arguments of [16] to include the energy domain. As a result, the function spaces are also the natural extension of those used in the monoenergetic case.

Define $Q = L^2(U)$ and

$$W := \left\{u \in L^2(U) \mid \boldsymbol{\omega} \cdot \nabla_x u \in L^2(U) \text{ and } u|_\Gamma \in L^2_w(\Gamma)\right\},$$

where $L^2_w(\Gamma)$ is the Hilbert space with the inner product

$$(u, v)_{L^2_w(\Gamma)} := \int_\Gamma uv|\boldsymbol{\omega} \cdot \boldsymbol{\nu}| ds d\boldsymbol{\omega} de.$$