On Spherical Harmonics and a Semi-discrete Finite Element Approximation for the Transport Equation

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ON SPHERICAL HARMONICS AND A SEMIDISCRETE FINITE ELEMENT APPROXIMATION FOR THE TRANSPORT EQUATION

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Abstract. This work is the first part in a series of two papers, where the objective is to construct, analyze and implement realistic particle transport models relevant in applications in radiation cancer therapy. Here we use spherical harmonics and derive an energy dependent model problem for the transport equation. Then we show stability and derive optimal convergence rates for semidiscrete (discretization in energy) finite element approximations of this model problem. The fully discrete problem, that considers the study of finite element discretizations in radial and spatial domains as well, is the subject of a forthcoming paper.

1. Introduction

This study concerns the mathematical modeling and numerical approximations of charged particle beams of interest in radiation therapy. We, primarily, assume the study of energy dependent radiation particle beams (electrons and ions) under the continuous slowing down approximation (CSDA). Roughly speaking, in this approximation, it is assumed that the particle loses its energy continuously along the length of its trajectory.

Our objective is two-fold: First we wish to derive a convection-diffusion model for the charged particle transport. Inspired by the classical idea of using asymptotic expansions to replace the scattering integral in the transport equation by a diffusion term, as, e.g. in Pomraning’s approach in [14], we employ spherical harmonic expansions and derive a more general and, mathematically, rigorous system of convection-diffusion-absorption equations for the coefficient vectors/matrices. Next, we focus on a canonical equation in the system and discretize it in the energy variable using the finite element method. Hence, we obtain a semidiscrete problem, for which we have derived stability estimates and optimal convergence rates.

Former approaches in this regard are considering forward-peaked beams. In, e.g. [15] where Prinja and Pomraning are considering asymptotic scaling for forward-peaked transport, [4] where Börgers and Larsen derive Fermi pencil beam equation, [2] where Asadzadeh, Brahme and Xin study Galerkin methods for broad beam transport, [1] where Asadzadeh, Brahme and Kempe extends the bipartition model for high energy electrons by Luo and Brahme in [12] to high energy ions and inhomogeneous media, and finally Brahme and Kempe [8] who studied solution of the Boltzmann equation for light ions. In all these studies ion particles are considered to be normally incident at the boundary of a semi infinite medium.

Key words and phrases. spherical harmonics, transport equation, finite element method, charged particle beams.

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In a previous study [1] we considered a detailed study of the bipartition model for ion transport. A related approach, based on a split of the scattering cross-section into the hard and soft parts is given by Larsen and Liang in [9].

An outline of this paper is as follows: In Section 2 we start with a transport equation model under continuously slowing down assumption (CSDA) and expand the solution function in spherical harmonics. In the subsequent Sections 3 and 4, we continue the spherical harmonic expansions procedure for the convection term and the collision integral, respectively. Section 5 is devoted to the extension of the source term for secondary particles. In Section 6 we state the system of equations and finally in our concluding Section 7 we prove stability estimates and derive optimal convergence rates for a semidiscrete scheme for the discretization in the energy variable.

2. The transport equation

Our objective is to solve the transport equation for the fluence differential \( f(x, r, \Omega, E) \) of charged particles symmetrically distributed around the \( x \)-axis at distance \( r \) from the same axis, traveling in direction \( \Omega \in S^2 \) with energy \( E \), using the continuous slowing down assumption (CSDA). We also define the angle \( \psi \) such that
\[
\begin{align*}
y &= r \cos \psi \\
z &= r \sin \psi
\end{align*}
\]
The equation is
\[
\Omega \cdot \nabla f - \frac{1}{2} \frac{\partial^2 \omega(E)f}{\partial E^2} - \frac{\partial S(E)f}{\partial E} = C_f(x, r, E) + Q(x, r, \Omega, E),
\]
where \( Q(x, r, \Omega, E) \) is a source term, either for incident primary electrons or for secondary electrons created in collisions between primary electrons and matter. Furthermore,
\[
C_f(x, r, \Omega, E) = \int_{4\pi} \sigma_s(E, \Omega \cdot \Omega') \left( f(x, r, \Omega', E) - f(x, r, \Omega, E) \right) d\Omega'
\]
is the collision factor, depending on the elastic scattering cross-section \( \sigma_s \).

Our first step will be to expand \( f \) into a series of spherical harmonics, using spherical coordinates \( \Omega = \Omega(\theta, \varphi) = (\cos \theta, \sin \theta \cos \varphi, \sin \theta \sin \varphi) \), where \( \theta \) is the angle from the \( x \)-axis,
\[
f(x, r, \Omega, E) = \sum_{n=0}^{\infty} \sum_{m=0}^{n} \frac{(n-m)!}{(n+m)!} \frac{2n+1}{4\pi} \alpha_m a_{n,m}(x, r, E) \cos(m\varphi) P_n^m(\cos \theta)
\]
\[
\equiv \sum_{n=0}^{\infty} \sum_{m=0}^{n} \tilde{a}_{n,m}(x, r, E) Y_n^m(\Omega),
\]
with
\[
\alpha_m = \begin{cases} 
1 & m = 0, \\
2 & m \geq 1,
\end{cases}
\]
where we have assumed that \( f \) is symmetric in \( \varphi \) so that the \( \sin(m\varphi) \) terms vanish (although the analysis below is essentially valid for \( \sin(m\varphi) \) terms too). The coefficients \( a_{n,m} \) are given by
\[
a_{n,m}(x, r, E) = \int_{-1}^{1} \int_{0}^{2\pi} f(x, r, \Omega, E) P_n^m(\cos \theta) \cos(m\varphi) \ d\varphi \ d(\cos \theta).
\]
We use the following definition for the associated Legendre polynomials

\begin{equation}
P^m_n(\mu) = (1 - \mu^2)^{m/2} \frac{d^m P_n(\mu)}{d\mu^m},
\end{equation}

\begin{equation}
P_n(\mu) = P^0_n(\mu) = 2^{-n} \sum_{k=0}^{\lfloor n/2 \rfloor} (-1)^k \binom{n}{k} \binom{2n-2k}{n} \mu^{n-2k}.
\end{equation}

Note that \( P^m_n(\mu) \equiv 0 \) if \( m > n \).

3. Expanding the convection term

To evaluate the term \( \Omega \cdot \nabla f \) in (2.1), we note that if \( f \) is rotationally symmetric (independent of \( \psi \)), then

\[ \Omega \cdot \nabla f(x, \Omega, E) = \cos \theta \frac{\partial f}{\partial x} + \sin \theta \cos \nu \frac{\partial f}{\partial r}, \]

where \( \nu = \varphi - \psi \), and hence we expand \( f = f(x, r, \theta, \nu, E) \) in spherical harmonics in the variables \( (\theta, \nu) \), and get a sum of terms of the kind

\[ \cos \theta Y^m_n(\theta, \nu) \quad \text{and} \quad \sin \theta \cos \nu Y^m_n(\theta, \nu). \]

We then wish to multiply the equation by \( Y^k_j(\theta, \nu) \) and integrate to get a system of equations for the coefficients \( a_{j,k}(x, r, E) \). We then end up with

\begin{equation}
\int_0^\pi \int_0^{2\pi} \left( \cos \theta \frac{\partial f}{\partial x} + \sin \theta \cos \nu \frac{\partial f}{\partial r} \right) P^k_j(\cos \theta) \cos(k\nu) \ d\nu \sin \theta \ d\theta
\end{equation}

\begin{equation}
= \sum_{n=0}^{\infty} \sum_{m=0}^{n} \frac{(n-m)!}{(n+m)!} \frac{2n+1}{4\pi} \alpha_m
\end{equation}

\begin{equation}
\int_0^\pi \int_0^{2\pi} \left( \cos \theta \frac{\partial a_{n,m}}{\partial x} + \sin \theta \cos \nu \frac{\partial a_{n,m}}{\partial r} \right) P^k_j(\cos \theta) \cos(k\nu) P^m_n(\cos \theta) \cos(m\nu) \ d\nu \sin \theta \ d\theta
\end{equation}

\begin{equation}
= \sum_{n \geq k-1} \left( A^k_{n,j} \frac{\partial a_{n,k}}{\partial x} + B^\pm_{n,j} \frac{\partial a_{n,k+1}}{\partial r} + B^-_{n,j} \frac{\partial a_{n,k-1}}{\partial r} \right),
\end{equation}

where

\begin{equation}
A^k_{n,j} = \frac{(n-k)!}{(n+k)!} \frac{2n+1}{2} \int_0^\pi \cos \theta P^k_j(\cos \theta) P^n_m(\cos \theta) \sin \theta \ d\theta,
\end{equation}

\begin{equation}
B^\pm_{n,j} = \frac{(n-(k \pm 1))!}{(n+(k \pm 1))!} \frac{2n+1}{4} \int_0^\pi \cos \theta P^k_j(\cos \theta) P^{n \pm 1}_m(\cos \theta) \sin \theta \ d\theta,
\end{equation}

since

\[ \int_0^{2\pi} \left\{ \frac{1}{\cos \nu} \right\} \cos(k\nu) \cos(m\nu) \ d\nu = \begin{cases}
\frac{2\pi\alpha_m^{-1} \delta_{mk}}{\pi \alpha_m}, & \text{if } \delta_{mk} = \delta_{m,k+1} + \delta_{m,k-1}
\end{cases}\]

where \( \delta_{mk} \) is the Kronecker delta.
3.1. The coefficients $A_{n,j}^k$. To evaluate the integral in (3.2), we set $\mu = \cos \theta$, and note that, see \cite{7}

\begin{equation}
(3.4) \quad \mu P_n^m(\mu) = \frac{n-m+1}{2n+1} P_{n+1}^m(\mu) + \frac{n+m}{2n+1} P_{n-1}^m(\mu),
\end{equation}

and since the associated Legendre polynomials are orthogonal, namely

$$
\int_{-1}^{1} P_j^m(\mu) P_n^m(\mu) \, d\mu = \frac{(j+m)!}{(j-m)!} \frac{2}{2j+1} \delta_{jn},
$$

the first part of the sum (3.1) becomes

\begin{equation}
(3.5) \quad \sum_{n \geq k} A_{n,j}^k \frac{\partial a_{n,k}}{\partial x} = \sum_{n \geq k} \left( \frac{n-k}{n+k} \frac{2n+1}{2} \frac{\partial a_{n,k}}{\partial x} \int_0^\pi \cos \theta P_j^k(\cos \theta) P_n^k(\cos \theta) \sin \theta \, d\theta \right)
\end{equation}

$$
= \sum_{n \geq k} \left( \frac{j+k}{j-k} \frac{2}{2j+1} \frac{n-k+1}{n+k+1} \frac{\partial a_{n,k}}{\partial x} \delta_{n+1,j} + \frac{n+k}{2n+1} \frac{\partial a_{n,k}}{\partial x} \delta_{n-1,j} \right)
\end{equation}

$$
= \frac{j+k}{2j+1} \frac{\partial a_{j-1,k}}{\partial x} + \frac{j-k+1}{2j+1} \frac{\partial a_{j+1,k}}{\partial x},
\end{equation}

for $k \leq j$, where the term with $a_{j-1,k}$ disappears if $k = j$.

3.2. The coefficients $B_{n,j}^{\pm k}$. Similarly, we wish to evaluate the sums

\begin{equation}
(3.6) \quad \sum_{n \geq k-1} B_{n,j}^{\pm k} \frac{\partial a_{n,k+1}}{\partial r} = \sum_{n \geq k+1} \left( \frac{n-(k+1)}{n+(k+1)} \frac{2n+1}{4} \frac{\partial a_{n,k+1}}{\partial r} \int_0^\pi \sin \theta P_j^k(\cos \theta) P_n^{k+1}(\cos \theta) \sin \theta \, d\theta \right),
\end{equation}

which turns out to be a bit more difficult. We may transform $\sin \theta P_n^m(\cos \theta)$, with $m = k \pm 1$ into a linear combination of “pure” Legendre polynomials $P_n^{m'}$ by repeatedly using the relation, see \cite{7}

\begin{equation}
(3.7) \quad \sin \theta P_n^m(\cos \theta) = 2(m-1) \cos \theta P_n^{m-1}(\cos \theta) - (n-m+2)(n+m-1) \sin \theta P_n^{m-2}(\cos \theta), \quad m \geq 2
\end{equation}

as well as (3.4), and finally the two relations

\begin{equation}
(3.8) \quad \sin \theta P_n^1(\cos \theta) = nP_{n-1}(\cos \theta) - n \cos \theta P_n(\cos \theta)
\end{equation}

\begin{equation}
(3.9) \quad \sin \theta P_n(\cos \theta) = \frac{1}{2n+1} \left( P_{n+1}^1(\cos \theta) - P_{n-1}^1(\cos \theta) \right).
\end{equation}
The final expressions are
\[(3.10)\]
\[
\sin \theta P_n^m(\mu) = \begin{cases} 
\frac{1}{2n+1} \left( P_{n+1}^1(\mu) - P_{n-1}^1(\mu) \right) & \text{if } m = 0 \\
\sum_{l=2}^{m/2} q_{n,m}(2l-1) R_{n,q}^{2l-1}(\mu) & \text{if } m \text{ even, } m > 0 \\
\sum_{l=1}^{(m-1)/2} q_{n,m}(2l) R_{n,q}^{2l}(\mu) & \text{if } m \text{ odd} \\
q_{n,m}(0) \frac{n(n+1)}{2n+1} (P_{n-1}(\mu) - P_{n+1}(\mu)) & \text{if } m \text{ even, } m = 0 \end{cases}
\]

with
\[(3.11)\]
\[P_n^m(\mu) = \frac{2m}{2n+1} \left( (n-m+1) P_{n+1}^m(\mu) + (n+m) P_{n-1}^m(\mu) \right)\]
\[(3.12)\]
\[q_{n,m}(l) = (-1)^{l+1} \frac{(n-l-1)! (n+m-1)!}{(n-m)! (n+l)!} \text{ if } m - l \text{ odd, } m \geq l + 1 \]

Here, \((\cdot)!!\) is the double factorial \((2n)!! = 2 \cdot 4 \cdot \ldots \cdot 2n, (2n+1)!! = 1 \cdot 3 \cdot \ldots \cdot (2n+1)\).

What now remains to evaluate \((3.6)\) is to evaluate the integrals
\[I_{j,q}^{k,p} = \int_{-1}^{1} P_j^k(\mu) P_q^p(\mu) \, d\mu,\]

with the special condition that \(k + p\) is even (as can be seen from \((3.10)\), with \(m = k \pm 1\), since if \(m\) is odd (even), then all \(P_n^m(\mu)\) in the sum \((3.10)\) will have \(p\) even (odd)). The integrals may be evaluated using the definition \((2.5)\) directly as
\[(3.13)\]
\[I_{j,q}^{k,p} = \int_0^\pi (\sin \theta)^{k+p+1} \left( \frac{d^k}{d\mu^k} P_j(\mu) \frac{d^p}{d\mu^p} P_q(\mu) \right) \bigg|_{\mu = \cos \theta} \, d\theta = 2^{-j+q} \sum_{\kappa=0}^{\left\lfloor \frac{k+1}{2} \right\rfloor} \sum_{\lambda=0}^{\kappa} (-1)^{\kappa+\lambda} \frac{(2j - 2\kappa)!}{\kappa!(j - \kappa)!(j - k - 2\kappa)!} \lambda! (q - \lambda)! (q - p - 2\lambda)! \cdot \int_0^\pi (\sin \theta)^{k+p+1} (\cos \theta)^{j+q-(p+k)-2(\kappa+\lambda)} \, d\theta.\]

Now, we note that the last integral is zero if \(j + q\) is odd, as we will then integrate an odd power of \(\cos \theta\) from 0 to \(\pi\). Otherwise, that is if \(k + p\) is even and \(j + q\) is even, we use the formula involving the \(\Gamma\) function
\[\int_0^{\pi/2} \sin^{2\alpha+1} \theta \cos^{2\beta+1} \theta \, d\theta = \frac{\Gamma(\alpha + 1)\Gamma(\beta + 1)}{2\Gamma(\alpha + \beta + 2)}\]
to end up with (using formula for $\Gamma$ function for the integers), see, e.g. [6] and [17],

\begin{equation}
I_{j,q}^{k,p} = 2^{-(j+q-(k+p)/2)} \left( \frac{k+p}{2} \right)! \sum_{\kappa=0}^{\left\lfloor \frac{k-p}{2} \right\rfloor} \sum_{\lambda=0}^{(2j-2\kappa)!} (-1)^{\kappa+\lambda} \frac{(2j-2\kappa)!}{\kappa!(j-\kappa)!(j-k-2\kappa)!} \frac{(2q-2\lambda)!}{\lambda!(q-\lambda)!(q-p-2\lambda)!} \cdot \frac{(j+q-(k+p)-2(\kappa+\lambda)-1)!!}{(j+q-2(\kappa+\lambda)+1)!!}.
\end{equation}

We note that both double-factorials contain only odd numbers.

Thus, we conclude

\[ B_{n,j}^{\pm,k} = \begin{cases} 0 & \text{if } n+j \text{ even} \\
\frac{1}{4} \left( I_{j,n+1}^{1,1}(\mu) - I_{j,n-1}^{1,1}(\mu) \right) & \text{if } n+j \text{ odd,} \\
\frac{1}{2} \sum_{l=2}^{(k+1)/2} \tilde{q}_{n,k\pm1}(2l-1) J_{j,n}^{k,2l-1} \text{ if } n+j \text{ odd,} \\
+ \frac{\tilde{q}_{n,k\pm1}(1)}{4} \left( (n+1)(n+2) I_{j,n-1}^{k,1} - n(n-1) I_{j,n+1}^{k,1} \right) & \text{if } n+j \text{ odd,}
\end{cases} \]

where

\begin{equation}
J_{j,n}^{k,m} = m \left( (n-m+1) I_{j,n+1}^{k,m} + (n+m) I_{j,n-1}^{k,m} \right)
\end{equation}

\begin{equation}
\tilde{q}_{n,m}(l) = \frac{(n-m)!}{(n+m)!} q_{n,m}(l) = (-1)^{\frac{m-1}{2}} \frac{(n-m-1)!!}{(n+m)!!} \frac{(n-l-1)!!}{(n+l)!!}.
\end{equation}

From (3.6) and (3.15) we see that the equation for the coefficient $a_{j,k}$ contains contributions from all coefficients $a_{n,m}$ with $m = k \pm 1$ and $n+j$ odd, in addition to the contribution from (3.5) when $m = k$ and $n = j \pm 1$.

4. Expanding the collision integral

Next, we wish to expand the collision integral into spherical harmonics, namely

\begin{equation}
C_f(x, r, \Omega, E) = \int_{4\pi} \sigma_s(E, \Omega' \cdot \Omega') \left( f(x, r, \Omega', E) - f(x, r, \Omega, E) \right) d\Omega'
\end{equation}

\begin{equation}
= \sum_{n=0}^{\infty} \sum_{m=0}^{n} C_{f,n,m}^{m}(x, r, E) Y_n^m(\Omega),
\end{equation}

where

\begin{equation}
C_{f,n,m}^{m}(x, r, E) = \frac{(n-m)!}{(n+m)!!} \left( \frac{2n+1}{2\pi} \right) \int_{4\pi} C_f(x, r, \Omega, E) Y_n^m(\Omega) d\Omega.
\end{equation}

By expanding $f$ in its spherical harmonics expansion with coefficients $a_{n,m}$, we may get a simple expression for the coefficients $C_{f,n,m}^{m}$. The second term in (4.1) is easy enough to
evaluate, and the first term may be evaluated by expanding $\sigma_s$ in Legendre polynomials in terms of $\mathbf{\Omega} \cdot \mathbf{\Omega}'$ and then using the addition formula for Legendre polynomials, see [7]. Due to orthogonality of spherical harmonics, the final result simplifies to

$$C_f^{m,n}(x, r, E) = 2\pi a_{n,m}(x, r, E) \int_{-1}^{1} \sigma_s(E, \mu) (P_n(\mu) - 1) \, d\mu. \quad (4.3)$$

5. Expanding the source term for secondary particles

Just as for the collision integral in the previous section, we can get a simple formula for the spherical harmonics coefficients of the source term for secondary particles. The source term is given by [11]

$$Q(x, r, \Omega, E) = \int_{4m}^{E_0} \sigma_c(E', \mu) \frac{1}{2\pi} \delta(\mathbf{\Omega} \cdot \mathbf{\Omega}' - \phi(E', E)) f_p(x, r, \Omega', E') \, dE' \, d\Omega', \quad (5.1)$$

where $f_p$ is the fluence of primary electrons, $\sigma_c$ is the collision cross-section, and

$$\phi(E', E) = \frac{(E(E' + 2m_0c^2))^{1/2}}{(E + 2m_0c^2)}$$

specifies the direction of motion of the secondary electron with kinetic energy $E'$ and direction $\Omega'$ given a primary electron with kinetic energy $E$ and direction $\Omega$, through $\mathbf{\Omega} \cdot \mathbf{\Omega}' = \phi(E', E)$. This follows from conservation of relativistic energy and momentum in a collision between the primary electron and a free electron.

By expanding $f_p$ in spherical harmonics with coefficients $a_{n,m}$, we get the following expression for the coefficients in the expansion for $Q$

$$Q^{n,m}(x, r, E) = \int_{2E}^{E_0} \sigma_c(E', E) P_n(\phi(E', E)) a_{n,m}(x, r, E') \, dE'. \quad (5.2)$$

Note that, in the derivation of this formula, although a Dirac function cannot be expanded in Legendre polynomials, we can use a sequence of smooth functions approaching the $\delta$-function, and go to the limit on both sides of the equation.

6. The system of equations

The transport equation (2.1) may now be written as a system of equations for the coefficients of the spherical harmonics expansion for the fluence $f$, see (2.3).

The equation for the coefficient $a_{j,k}(x, r, E)$ (with $j \geq k$) becomes

$$\sum_{n \geq k} \left( A_{n,j}^k \frac{\partial a_{n,k}}{\partial x} + B_{n,j}^k \frac{\partial a_{n,k}}{\partial r} \right) - \frac{1}{2} \frac{\partial^2 \omega(E) a_{j,k}}{\partial E^2} - \frac{\partial S(E) a_{j,k}}{\partial E} = C_{j}^{j,k}(x, r, E) + Q_{j}^{j,k}(x, r, E). \quad (6.1)$$

If we let the vector $a(x, r, E)$ contain the coefficients $a_{n,m}(x, r, E)$, we can write this as

$$A \frac{\partial a}{\partial x} + B \frac{\partial a}{\partial r} - \frac{1}{2} \frac{\partial^2 (\omega(E) a)}{\partial E^2} - \frac{\partial (S(E) a)}{\partial E} = C(E) a + q(x, r, E), \quad (6.2)$$

where $A$ and $B$ are matrices containing the coefficients $A_{n,j}^k$ and $B_{n,j}^k$, respectively, and $C(E)$ is a diagonal matrix.

The sparsity pattern for the matrices $A$ and $B$ can be seen in figure 1, with $n \leq N = 10$. The elements in each row and column are ordered in chunks of equal $m$, $m = 0, \ldots, N$, and within each chunk, $n$ runs from $m$ to $N$. 

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7. The Semidiscrete Problem: Discretization of $a_{j,i}(x,r,E)$ in the energy variable

In this section we discretize equation (6.1) in the energy variable $E$. In a forthcoming paper we shall study spatial discretization in $(x,r)$.

7.1. Notation. The equation (6.2) is a degenerate type convection-diffusion equation with variable coefficients. The source of degeneracy is the single-variable (energy) diffusion term related to considering the influence of secondary particles. Because of this structure it is more adequate, first, to study a semidiscrete approach for the energy variable using a mixed finite element method. To this end we reformulate the problem (6.2) as a first order system viz,

\[
\begin{aligned}
\frac{A}{\partial x} + B \frac{\partial u}{\partial r} - \frac{1}{2} \frac{\partial^2 (\omega(E)u)}{\partial E^2} - \frac{\partial (S(E)u)}{\partial E} &= C(E)u + q(x,r,E), \\
v &= \frac{\partial (\omega(E)u)}{\partial E}.
\end{aligned}
\]

We use a change of variable as $\tilde{E} = E_0 - E$ and supply the boundary condition as the energy from its peak $u(0)$ at $\tilde{E} = 0$ in the energy interval $\tilde{E} \in [0,E_0]$ corresponding to $E_0 \xrightarrow{E} 0$. 

**Figure 1.** The non-zero elements of the matrices $A$ and $B$ for $N = 10$. 

and \((x, r) = (0, 0)\). Then, evidently \(\frac{\partial G}{\partial E} = -\frac{2G}{\partial E}\) and \(\frac{\partial^2 G}{\partial E^2} = -\frac{2G}{\partial E^2}\). Further, to use the second relation in (7.1) we write

\[
S(E)u = \frac{S(E)}{\omega(E)} \omega(E)u \equiv \gamma(E)\omega(E)u.
\]

Thus

\[
\frac{\partial(S(E)u)}{\partial E} = \frac{\partial\gamma(E)}{\partial E} \omega(E)u + \gamma(E)\frac{\partial(\omega(E)u)}{\partial E}.
\]

Therefore, with the simplifying notation \(w_\beta = \frac{\partial w}{\partial \beta}\), (7.1) can be written as a first order PDE system

\[
\begin{cases}
Au_x + Bu_r - \frac{1}{2}v_E - \gamma_E(E)\omega(E)u - \gamma(E)v = C(E)u + q(x, r, E), \\
v(x, r, E) = (\omega(E)u)_{E|x, r, E}, \\
u(x, r, E_0) = \delta(x)\delta(r)u_0(E_0), \\
v(x, r, E_0) = -\delta(x)\delta(r)v_0(E_0), \quad u(x, r, 0) = 0, \\
v(x, r, 0) = 0.
\end{cases}
\]

Hence, using the notation \(\Gamma := (A, B), \nabla_x = (\partial_x, \partial_r),\) and \(D(E) = \gamma_E(E)\omega(E) + C(E),\) we may write the differential equations in (7.4) above as

\[
\begin{cases}
\Gamma \cdot \nabla x v - \frac{1}{2}v_E - \gamma(E)v = D(E)u + q, \\
v = (\omega(E)u)_E.
\end{cases}
\]

7.1.1. Weak formulation. We use partial integration in \(E\) and the notation

\[
(f, g) := (f, g)_E = \int_0^{E_0} f(x, r, E)g(x, r, E)\, dE,
\]

to write

\[
\begin{aligned}
(\Gamma \cdot \nabla x v, w) &= (Av_x + Bv_r, w) = (A(\omega(E)u)_{E|x} + B(\omega(E)u)_{E|r}, w) \\
&= -(A(\omega(E)u)_{x|} + B(\omega(E)u)_{r|}, w) = (Av_{x|} + Bv_{r|} + B(\omega(E)u(E_0))_{r|}, w(E)) \\
&= -((\omega(E)u)_{E|x} + (Av_{x|} + Bv_{r|} + B(\omega(E)u(E_0))_{r|}, w(E)) \\
&= -\left(\frac{1}{2}w(E)v_E\right) + S(E)v + D(E)\omega(E)u + \omega(E)q, \quad w \in H^1,
\end{aligned}
\]

and

\[
(\omega(E)u)_E, \chi_E) = (v, \chi_E), \quad \forall \chi \in H^1_0.
\]

7.1.2. Energy estimates. We consider finite element subspaces \(S_h \subset H^1_0(\Omega),\) and \(W_h \subset H^1(\Omega)\) with the following approximation properties: For \(1 \leq p \leq \infty\) and \(\ell > 0, s > 0\) integers, there is a constant \(C\) independent of \(h\) such that, see [5]

\[
\inf_{\chi \in S_h} \{||g - \chi||_{L^p(I_E)} + h||g - \chi||_{W^{1,p}(I_E)} \leq C h^{\ell+1}||g||_{W^{\ell+1,p}(I_E)}, \quad \forall g \in H^1_0 \cap W^{\ell+1,p}(I_E),
\]

and

\[
\inf_{\rho \in W_h} \{||\rho - \zeta||_{L^p(I_E)} + h||\rho - \zeta||_{W^{1,p}(I_E)} \leq C h^{s+1}||\rho||_{W^{s+1,p}(I_E)}, \quad \forall \rho \in W^{s+1,p}(I_E).
\]
Motivated by the weak (variational) formulation (7.6) and (7.7), we define a pair of semi-discrete finite element approximations \( \{ \tilde{\mathbf{u}}_h, \tilde{\mathbf{v}}_h \} : I_x \times I_r \rightarrow S_h \times W_h \) for \( \{ \mathbf{u}, \mathbf{v} \} \), respectively as solution of

\[
(7.10) \quad (\mathbf{f} \cdot \nabla_x \tilde{\mathbf{v}}_h, \mathbf{w}) = -\left( \frac{1}{2} (\omega(E)\tilde{\mathbf{v}}_h, E) + S(E)\tilde{\mathbf{v}}_h + D(E)\omega(E)\tilde{\mathbf{u}}_h + \omega(E)\tilde{\mathbf{q}}_h, \mathbf{w}_E \right) \\
+ (\omega(E)\tilde{\mathbf{u}}_h(E_0), x) + B\omega(E)\tilde{\mathbf{u}}_h(E_0)\mathbf{w}(E_0), \quad \forall \mathbf{w} \in W_h,
\]

and

\[
(7.11) \quad \left( (\omega(E)\tilde{\mathbf{u}})_h, \chi_E \right) = (\tilde{\mathbf{v}}_h, \chi_E), \quad \forall \chi \in S_h.
\]

where \( \tilde{\mathbf{u}}_h(\cdot, E_0) \in S_h \) is such that

\[
(7.12) \quad \| \mathbf{u}(E_0) - \tilde{\mathbf{u}}_h(E_0) \| \leq C(\mathbf{u}(E_0)) h^s.
\]

We assume that \( \omega(E) \) is sufficiently regular, so that the coefficient matrix corresponding to the left hand side in (7.11) is invertible. Then (7.10)-(7.11) yields a system of differential algebraic equations (DAEs) of "index one". For the subsequent error analysis, we now define the elliptic projection operators \( Q_h : H^1_0 \rightarrow S_h \) for \( \mathbf{u} \), (see [3]), by

\[
(7.13) \quad (\omega(E)(\mathbf{u}_E - Q_h \mathbf{u}_E), \chi_E) = 0, \quad \chi \in S_h, \quad (x, r) \in I_x \times I_r,
\]

and \( P_h : H^1 \rightarrow W_h \) for \( \mathbf{v} \) by

\[
(7.14) \quad A(\mathbf{v} - P_h \mathbf{v}, \rho) = 0, \quad \forall \rho \in W_h,
\]

where

\[
A(\rho, \zeta) = \frac{1}{2} \omega(E)\rho, \zeta ) + (S(E)\rho, \zeta ), \quad (D(E)\omega(E)\rho, \zeta ) + \Lambda((\rho, \zeta )
\]

\[
= \frac{1}{2} \omega(E)\rho, \zeta ) + (S(E) + D(E)\omega(E))\rho, \zeta ) + \Lambda((\rho, \zeta )).
\]

Here \( \Lambda \) is chosen appropriately so that \( A \) is \( H^1 \)-coercive, i.e. there is a parameter \( \alpha_0 > 0 \) such that

\[
(7.16) \quad A(\mathbf{v}, \mathbf{v}) \geq \alpha_0 \| \mathbf{v} \|^2.
\]

**Remark 7.1.** Note that in this sections all norms are with respect to the energy variable \( E \).

We let now \( \mathbf{u}_h = Q_h \mathbf{u}, \mathbf{v}_h = P_h \mathbf{v}, \eta = \mathbf{u} - \mathbf{u}_h \) and \( \xi = \mathbf{v} - \mathbf{v}_h \), then the \( L_2 \)-error estimates for \( \eta \) and \( \xi \) are derived using an extended version of a result by M. Wheeler [16].

**Lemma 7.1.** Let \( \{ \mathbf{u}, \mathbf{v} \} \) be a pair of solutions of (7.5). Further, let \( \{ \mathbf{u}_h, \mathbf{v}_h \} \) satisfy (7.10)-(7.11). Then, there is a constant \( C \) independent of \( h \) such that for \( j = 0, 1 \)

\[
(7.17) \quad \| \eta \|_j + \| \nabla_x \eta \|_j \leq C h^{\ell+1-j} \left( \| \mathbf{u} \|_{\ell+1} + \| \nabla_x \mathbf{u} \|_{\ell+1} \right), \quad \ell = 0, 1, \ldots,
\]

and

\[
(7.18) \quad \| \xi \|_j + \| \nabla_x \xi \|_j \leq C h^{s+1-j} \left( \| \mathbf{v} \|_{s+1} + \| \nabla_x \mathbf{v} \|_{s+1} \right), \quad s = 0, 1, \ldots
\]

Further for \( j = 0, 1 \) and \( 1 \leq p \leq \infty \), we have that

\[
(7.19) \quad \| \eta \|_{W^{\ell,p}(I_E)} \leq C h^{\ell+1-j} \| \mathbf{u} \|_{W^{\ell+1,p}(I_E)}, \quad \ell = 0, 1, \ldots,
\]

\[
(7.20) \quad \| \xi \|_{W^{s,p}(I_E)} \leq C h^{s+1-j} \| \mathbf{v} \|_{W^{s+1,p}(I_E)}, \quad s = 0, 1, \ldots
\]
To derive error estimates for the semi-discrete (discretization in $E$) approximation, we split the error as

\[ u - \tilde{u}_h = (u - u_h) - (\tilde{u}_h - u_h) := \eta - \varepsilon \]
\[ v - \tilde{v}_h = (v - v_h) - (\tilde{v}_h - v_h) := \xi - \nu. \]

Since the estimates for $\eta$ and $\xi$ are known from the Lemma 6.1, it is enough to estimate $\varepsilon$ and $\nu$. Taking difference between (7.6) and (7.10), and (7.7) and (7.11) and using the elliptic projections $Q_h$ and $P_h$ satisfying (7.13) and (7.14), we write the equations for $\varepsilon$ and $\nu$ as follows:

\[
(\Gamma \cdot \nabla_{x^r}(v - \tilde{v}_h), \zeta) = -\frac{1}{2}(\omega(E)(v - \tilde{v}_h)_E, \zeta_E) - (S(E)(v - \tilde{v}_h), \zeta_E)
- \left(D(E)\omega(E)(u - \tilde{u}_h)\xi_E\right) - (\omega(E)(q - \tilde{q}_h), \xi_E), \quad \zeta \in W_h,
\]

(7.21)

and

\[
(\omega(E)(u - \tilde{u}_h)_E, \chi_E) - (v - \tilde{v}_h), \chi_E) = 0.
\]

(7.22)

Note that

\[
\left(\omega(E)(u - \tilde{u}_h)_E, \chi_E\right) = (\omega(E)\eta_E, \chi_E) - (\omega(E)\varepsilon_E, \chi_E),
\]

where using the definition of $Q_h$ we have

\[
(\omega(E)(u - u_h, E) = (\omega(E)(u_E - Q_h u_E) = 0.
\]

(7.23)

Thus inserting (7.23) in (7.22) we get

\[
-(\omega(E)\varepsilon_E, \chi_E) = (\xi, \chi_E) - (\nu, \chi_E).
\]

(7.24)

Further (7.21) can be written as

\[
(\Gamma \cdot \nabla_{x^r} \nu, \zeta) = (\Gamma \cdot \nabla_{x^r} \xi, \zeta) + \frac{1}{2}(\omega(E)\xi_E, \zeta_E) - \frac{1}{2}(\omega(E)\nu_E, \zeta_E) + (S(E)\xi, \zeta_E) - ((S(E)\nu, \zeta_E)
+ (D(E)\omega(E)\eta, \zeta_E) - (D(E)\omega(E)\varepsilon, \zeta_E) + \left(\omega(E)(q - \tilde{q}_h), \xi_E\right).
\]

(7.25)

On the other hand we have that

\[
\mathcal{A}(\nu, \zeta) = \frac{1}{2}(\omega(E)\nu_E, \zeta_E) + ((S(E)\nu, \zeta_E) + (D(E)\omega(E)\nu, \zeta_E) + \Lambda(\nu, \zeta).
\]

(7.26)

Adding (7.25) and (7.26) we have that

\[
(\Gamma \cdot \nabla_{x^r} \nu, \zeta) + \mathcal{A}(\nu, \zeta) = (\Gamma \cdot \nabla_{x^r} \xi, \zeta) + \frac{1}{2}(\omega(E)\xi_E, \zeta_E) + (S(E)\xi, \zeta_E)
+ (D(E)\omega(E)(\eta - \varepsilon), \zeta_E) + (D(E)\omega(E)\nu_E, \zeta_E)
+ \left(\omega(E)(q - \tilde{q}_h), \xi_E\right) + \Lambda(\nu, \zeta).
\]

(7.27)
Now we let $\zeta = \nu$, use the coercivity assumption and write

$$
\begin{align}
& (\Gamma \cdot \nabla_x \nu, \nu) + \alpha_0 \|\nu\|^2 + \frac{1}{4} (\Gamma \cdot \nabla_x) \|\nu\|^2 \\
& + \| \omega(E) \|^2 \xi E \|^2 + \frac{1}{16} \| \omega(E) \| E \|^2 + 4 \| S(E) \|^2 \xi E \|^2 + \frac{1}{16} \| S(E) \|^2 \xi E \|^2 \\
& + 4 \| D(E) \| E \|^2 \eta \|^2 + \frac{1}{16} \| D(E) \|^2 \omega(E) \|^2 \\
& + 4 \| D(E) \|^2 \omega(E) \|^2 + \frac{1}{16} \| D(E) \|^2 \omega(E) \|^2 \\
& + \frac{1}{2} \| D(E) \|^2 \omega(E) \|^2 + \frac{1}{2} \| D(E) \|^2 \omega(E) \|^2 + \| A \|^2 \| \nu \|^2 \\
& + |(\omega(E)(\mathbf{q} - \bar{\mathbf{q}}_h), \nu_E)|.
\end{align}
$$

(7.28)

The last term in (7.28) is estimated as follows

$$
|\omega(E)(\mathbf{q} - \bar{\mathbf{q}}_h), \nu_E)| \leq 4 \| \omega(E) \|^2 (\mathbf{q} - \bar{\mathbf{q}}_h) \|^2 + \frac{1}{16} \| \omega(E) \|^2 \xi E \|^2.
$$

Hence, by a kick-back argument we hide all $\nu$-terms in the right, inside the left hand side. Except the $\varepsilon$-term, for all remaining $\xi$ and $\eta$ terms on the right hand side, we have theoretical error bounds. Thus it remains to estimate the $\varepsilon$-term. To this end we let $\chi = \varepsilon$ in (7.24), then

$$
\| \omega(E) \|^2 \xi E \|^2 \leq \| \omega(E) \|^2 \xi E \|^2 + \| \omega(E) \|^2 \xi E \|^2,
$$

so that

$$
\| \omega(E) \|^2 \xi E \|^2 \leq \| \omega(E) \|^2 \xi E \|^2 + \| \omega(E) \|^2 \xi E \|^2.
$$

(7.30)

Now for the contribution from the $\varepsilon$-term in (7.28), first we use Poincare inequality to write

$$
\| D(E) \|^2 \omega(E) \|^2 \leq \tilde{C} \| D(E) \|^2 \omega(E) \|^2 \leq \tilde{C} \| D(E) \|^2 (\| \omega(E) \|^2 \xi E \|^2 + \| \omega(E) \|^2 \xi E \|^2).
$$

An alternative estimate, for the $\varepsilon$-term, is obtained by letting $\chi_E = D(E)\varepsilon_E$ in (7.24). Then

$$
\begin{align}
\| D(E) \|^2 \omega(E) \|^2 & = (\xi, D(E)\varepsilon_E) - (\nu, D(E)\varepsilon_E) \\
& = (\omega(E)^{-1/2} D(E)^{1/2} \xi, \omega(E)^{1/2} D(E)^{1/2} \varepsilon_E) \\
& - (\omega(E)^{-1/2} D(E)^{1/2} \nu, \omega(E)^{1/2} D(E)^{1/2} \varepsilon_E) \\
& \leq \| \omega(E)^{-1/2} D(E)^{1/2} \xi \|^2 + \| \omega(E)^{-1/2} D(E)^{1/2} \nu \|^2 \\
& + \frac{1}{2} \| D(E) \|^2 \omega(E) \|^2.
\end{align}
$$

(7.31)

Once again, using Poincare inequality we get

$$
\begin{align}
\| D(E) \|^2 \omega(E) \|^2 & \leq \frac{\tilde{C}}{\min \omega(E)^2} (\| \omega(E)^{-1/2} D(E)^{1/2} \xi \|^2 + \| \omega(E)^{-1/2} D(E)^{1/2} \nu \|^2).
\end{align}
$$

(7.32)
Inserting (7.29) and (7.32) in (7.28) and rearranging the terms yields
\begin{equation}
(\Gamma \cdot \nabla x \nu, \nu) + \alpha_0 ||\nu||_2^2 \leq (\Gamma \cdot \nabla x \nu) ||\xi||_2^2 + \frac{1}{4}(\Gamma \cdot \nabla x \nu)||\nu||^2 + ||\omega(E)^{1/2}\xi_E||^2 \nonumber
\end{equation}
\begin{equation}
+ \frac{1}{8}||\omega(E)^{1/2}\nu_E||^2 + 4||S(E)^{1/2}\xi_E||^2 + \frac{1}{16}||S(E)^{1/2}\nu_E||^2 
onumber
\end{equation}
\begin{equation}
+ 4||D(E)^{1/2}\omega(E)^{1/2}\eta||^2 + \frac{5}{8}||D(E)^{1/2}\omega(E)^{1/2}\nu_E||^2 
onumber
\end{equation}
\begin{equation}
+ 4||D(E)^{1/2}\omega(E)^{1/2}\varepsilon||^2 + \frac{1}{2}||D(E)^{1/2}\omega(E)^{1/2}\nu||^2 
onumber
\end{equation}
\begin{equation}
+ \frac{C}{\min \omega(E)} \left( ||\omega(E)^{1/2}D(E)^{1/2}\xi||^2 + ||\omega(E)^{1/2}D(E)^{1/2}\nu||^2 \right) 
onumber
\end{equation}
\begin{equation}
+ 4||\omega(E)^{1/2}(q - \tilde{q}_h)||^2 + ||\Lambda^{1/2}\nu||^2. 
onumber
\end{equation}

By an elementary calculus one can show that the Poincare constant in here is \(\tilde{C} \sim |I_E| = E_0\). Now assuming that \(\min \omega(E_0) \geq 2\sqrt{E_0}\), and defining the triple norm as
\begin{equation}
||\nu||_1 = \left[ ||\omega(E)^{1/2}\nu_E||^2 + ||S(E)^{1/2}\nu_E||^2 + ||D(E)^{1/2}\omega(E)^{1/2}\nu_E||^2 \right]
\end{equation}
\begin{equation}
+ ||\omega(E)^{1/2}D(E)^{1/2}\varepsilon||^2 + ||\Lambda^{1/2}\nu||^2 \right]^{1/2},
\end{equation}
we get using a kick-back argument and with \(\alpha_0 \sim 1\) that
\begin{equation}
||(\Gamma \cdot \nabla x \nu)||^2 + \alpha_0' ||\nu||_1^2 \leq 4||(\Gamma \cdot \nabla x \nu)||^2 + 4||\omega(E)^{1/2}\xi_E||^2 + 16||S(E)^{1/2}\xi_E||^2 \nonumber
\end{equation}
\begin{equation}
+ 4||\omega(E)^{1/2}D(E)^{1/2}\xi||^2 + 16||D(E)^{1/2}\omega(E)^{1/2}\eta||^2 
onumber
\end{equation}
\begin{equation}
+ 16||\omega(E)^{1/2}(q - \tilde{q}_h)||^2,
\end{equation}
for some \(0 < \alpha_0' < \alpha_0 \sim 1\). Note that the norms of the projection errors, \(\eta\) and \(\xi\), on the right hand side in (7.35) are equivalent to their \(H^1\)-norms (assuming that all the energy dependent coefficients are absolutely bounded: \(\omega(E) \in L_\infty(I_E)\), \(S(E) \in L_\infty(I_E)\) and \(\omega(E)D(E) \in L_\infty(I_E)\)). Assuming also that the error in \(q - \tilde{q}_h\) is of the same order as in Lemma 6.1, we can apply Lemma 6.1 and the above estimates to obtain
\begin{equation}
||(\Gamma \cdot \nabla x \nu)||^2 + \alpha_0' ||\nu||_1^2 \leq C h^{2\min(\ell,s)} \left( ||u||^2_{L_\infty(H^{\ell+1})} + ||v||^2_{L_\infty(H^{\ell+1})} + ||\nabla x \cdot \nu||^2_{L_\infty(H^{\ell+1})} \right),
\end{equation}
which yields, e.g. the estimate
\begin{equation}
||(u - \tilde{u}_h)(x,r)|| + ||(v - \tilde{v}_h)(x,r)|| \nonumber
\end{equation}
\begin{equation}
\leq C h^{\min(\ell+1, s+1)} \left( ||u||_{L_\infty(H^{\ell+1})} + ||v||_{L_\infty(H^{\ell+1})} + ||\nabla x \cdot \nu||_{L_\infty(H^{\ell+1})} \right). 
\end{equation}
Hence, using a standard procedure and the above estimates we may derive the following a priori error estimates:

**Theorem 7.2.** Assume that \(\tilde{v}_h(0) = P_{EV_0}\) so that \(\nu(0) = 0\). Then there exists a constant \(C\) independent of \(h\) such that
\begin{equation}
||(v - \tilde{v}_h)(x,r)||_1 \leq C(E_0) h^{\min(\ell+1,s)} \left( ||u||_{L_\infty(H^{\ell+1})} + ||v||_{L_\infty(H^{\ell+1})} + ||\nabla x \cdot \nu||_{L_\infty(H^{\ell+1})} \right).
\end{equation}
Theorem 7.3. a) Under the assumption of the above theorem, the errors \( u - \tilde{u}_h \) and \( v - \tilde{v}_h \) can be estimated as

\[
\| (u - \tilde{u}_h)(x, r) \| + \| (v - \tilde{v}_h)(x, r) \| + h \| (v - \tilde{v}_h)(x, r) \|_1 \leq C(E_0) h^{\min(\ell+1, s+1)} \times
\]

\[
\left( \| u \|_{L_\infty^\infty (W^{\ell+1}, p)} + \| v \|_{L_\infty^\infty (W^{s+1}, p)} + \| \nabla_{xr} \cdot v \|_{L_2^2 (W^{s+1}, p)} \right).
\]

(7.39)

b) For \( 1 < p \leq \infty \) we have that

\[
\| (u - \tilde{u}_h)(x, r) \|_{L^p} + \| (v - \tilde{v}_h)(x, r) \|_{L^p} \leq C(E_0) h^{\min(\ell+1, s+1)} \times
\]

\[
\left( \| u \|_{L_\infty^\infty (W^{\ell+1}, p)} + \| v \|_{L_\infty^\infty (W^{s+1}, p)} + \| \nabla_{xr} \cdot v \|_{L_2^2 (W^{s+1}, p)} \right).
\]

(7.40)

These estimates are of optimal order due to the maximal available regularity in the degenerate type convection diffusion equation, see [10] and [13].

References


[8] J. Kempe and A. Brahme, Solution of the Boltzmann equation for primary light ions and the transport of their fragments, PhD Thesis J. Kempe, Medical Radiation Physics, Department of Oncology-Pathology, Stockholm University & Karolinska Institute, (2008).


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