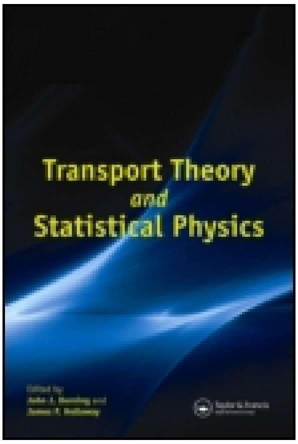

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Spherical Harmonics and a Semidiscrete Finite Element Approximation for the Transport Equation

Mohammad Asadzadeh [a] & Tobias Gebäck [a]
[a] Department of Mathematics, Chalmers University of Technology and University of Gothenburg, Göteborg, Sweden

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Spherical Harmonics and a Semidiscrete Finite Element Approximation for the Transport Equation

Mohammad Asadzadeh and Tobias Gebäck

Department of Mathematics, Chalmers University of Technology and University of Gothenburg, Göteborg, Sweden

This work is the first part in a series of two articles, 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 also considers the study of finite element discretizations in radial and spatial domains as well is the subject of a forthcoming article.

Keywords spherical harmonics; transport equation; finite element method; charged particle beams

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. A classical idea has been using

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Address correspondence to Mohammad Asadzadeh, Department of Mathematics, Chalmers University of Technology and University of Gothenburg, SE-412 96, Göteborg, Sweden. E-mail: mohammad@chalmers.se

asymptotic expansions to replace the scattering integral in the transport equation by a diffusion term, as, for example, in Pomraning's approach (1992). These approaches have been of a heuristic nature. We employ spherical harmonic expansions and derive a more general, nonasymptotic 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 modeling particle beams for radiation therapy applications are considering forward-peaked and/or broad beams. In this regard, for example, Prinja and Pomraning (1992) considered asymptotic scaling for forward-peaked transport, Börgers and Larsen (1996) derived the Fermi pencil beam equation, Asadzadeh and colleagues (2010b) studied Galerkin methods for broad beam transport, Asadzadeh and associates (2010a) extended the bipartition model for high energy electrons by Luo and Brahme (1992) to high energy ions and inhomogeneous media, and finally Kempe and Brahme (2010) studied the 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.

In a previous study (Asadzadeh et al., 2010a) 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 (2007).

An outline of this article is as follows. In Section 2 we start with a transport equation model under 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 CSDA. We also define the angle ψ such that

$$\begin{cases} y = r\cos\psi \\ z = r\sin\psi. \end{cases}$$

The equation is

$$\Omega \cdot \nabla f - \frac{1}{2}\frac{\partial^2 \omega(E) f}{\partial E^2} - \frac{\partial S(E) f}{\partial E} = C_f(x, r, E) + Q(x, r, \Omega, E), \tag{2.1}$$

where $\omega(E)$ is the energy loss straggling, $S(E)$ is the stopping power, (see Luo and Brahme, 1992 and the references therein), and $Q(x, r, \Omega, E)$ is a source term, either for incident primary electrons or for secondary electrons created in collisions between primary electrons and matter. Furthermore,

$$C_f(x, r, \Omega, E) = \int_{4\pi} \sigma_s(E, \Omega \cdot \Omega')\big(f(x, r, \Omega', E) - f(x, r, \Omega, E)\big)\, d\Omega' \tag{2.2}$$

is the collision factor, depending on the elastic scattering cross-section σ_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 θ is the angle from the x-axis,

$$\begin{aligned} f(x, r, \Omega, E) &= \sum_{n=0}^{\infty}\sum_{m=0}^{n} \frac{(n-m)!}{(n+m)!}\frac{2n+1}{4\pi}\alpha_m a_{n,m}(x, r, E)\cos(m\varphi)P_n^m(\cos\theta) \\ &\equiv \sum_{n=0}^{\infty}\sum_{m=0}^{n} \tilde{a}_{n,m}(x, r, E)Y_n^m(\Omega), \end{aligned} \tag{2.3}$$

with

$$\alpha_m = \begin{cases} 1 & m = 0, \\ 2 & m \geq 1, \end{cases}$$

where we have assumed that f is symmetric in φ so that the $\sin(m\varphi)$ terms vanish (although the analysis that follows 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 functions

$$P_n^m(\mu) = (1-\mu^2)^{m/2}\frac{d^m P_n(\mu)}{d\mu^m}, \tag{2.4}$$

$$P_n(\mu) = P_n^0(\mu) = 2^{-n}\sum_{k=0}^{[\frac{n}{2}]}(-1)^k\binom{n}{k}\binom{2n-2k}{n}\mu^{n-2k}. \tag{2.5}$$

Note that $P_n^m(\mu) \equiv 0$ 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 ψ), then

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

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

$$\cos\theta\, Y_n^m(\theta, \nu) \quad \text{and} \quad \sin\theta \cos\nu\, Y_n^m(\theta, \nu).$$

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

$$\begin{aligned} &\int_0^\pi \int_0^{2\pi} \left(\cos\theta \frac{\partial f}{\partial x} + \sin\theta \cos\nu \frac{\partial f}{\partial r} \right) P_j^k(\cos\theta) \cos(k\nu)\, d\nu \sin\theta\, d\theta \\ &= \sum_{n=0}^{\infty} \sum_{m=0}^{n} \frac{(n-m)!}{(n+m)!} \frac{2n+1}{4\pi} \alpha_m \\ &\quad \times \int_0^\pi \int_0^{2\pi} \left(\cos\theta \frac{\partial a_{n,m}}{\partial x} + \sin\theta \cos\nu \frac{\partial a_{n,m}}{\partial r} \right) P_j^k(\cos\theta) \cos(k\nu) P_n^m(\cos\theta) \\ &\quad \cos(m\nu)\, d\nu \sin\theta\, d\theta \\ &= \sum_{n \geq k-1} \left(A_{n,j}^k \frac{\partial a_{n,k}}{\partial x} + B_{n,j}^{+,k} \frac{\partial a_{n,k+1}}{\partial r} + B_{n,j}^{-,k} \frac{\partial a_{n,k-1}}{\partial r} \right), \end{aligned} \tag{3.1}$$

where

$$A_{n,j}^k = \frac{(n-k)!}{(n+k)!} \frac{2n+1}{2} \int_0^\pi \cos\theta P_j^k(\cos\theta) P_n^k(\cos\theta) \sin\theta\, d\theta, \tag{3.2}$$

$$B_{n,j}^{\pm,k} = \frac{(n-(k\pm1))!}{(n+(k\pm1))!} \frac{2n+1}{4} \int_0^\pi \cos\theta P_j^k(\cos\theta) P_n^{k\pm1}(\cos\theta) \sin\theta\, d\theta, \tag{3.3}$$

since

$$\int_0^{2\pi} \begin{pmatrix} 1 \\ \cos\nu \end{pmatrix} \cos(k\nu) \cos(m\nu) d\nu = \begin{cases} 2\pi \alpha_m^{-1} \delta_{mk} \\ \pi \alpha_m^{-1} (\delta_{m,k+1} + \delta_{m,k-1}), \end{cases}$$

where δ_{mk} is the Kronecker delta.

3.1 The Coefficients $A^k_{n,j}$

To evaluate the integral in (3.2), we set $\mu = \cos\theta$ and note that (see Holland, 1990)

$$\mu P_n^m(\mu) = \frac{n-m+1}{2n+1} P_{n+1}^m(\mu) + \frac{n+m}{2n+1} P_{n-1}^m(\mu), \tag{3.4}$$

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

$$\begin{aligned}\sum_{n\geq k} A^k_{n,j}\frac{\partial a_{n,k}}{\partial x} &= \sum_{n\geq k}\frac{(n-k)!}{(n+k)!}\frac{2n+1}{2}\frac{\partial a_{n,k}}{\partial x}\int_0^\pi \cos\theta P_j^k(\cos\theta)P_n^k(\cos\theta)\sin\theta\, d\theta \\ &= \sum_{n\geq k}\frac{(j+k)!}{(j-k)!}\frac{2}{2j+1}\frac{(n-k)!}{(n+k)!}\frac{2n+1}{2}\left(\frac{n-k+1}{2n+1}\frac{\partial a_{n,k}}{\partial x}\delta_{n+1,j} + \frac{n+k}{2n+1}\frac{\partial a_{n,k}}{\partial x}\delta_{n-1,j}\right) \\ &= \frac{j+k}{2j+1}\frac{\partial a_{j-1,k}}{\partial x} + \frac{j-k+1}{2j+1}\frac{\partial a_{j+1,k}}{\partial x},\end{aligned} \tag{3.5}$$

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

3.2 The Coefficients $B^{\pm,k}_{n,j}$

Similarly, we wish to evaluate the sums

$$\begin{aligned}\sum_{n\geq k-1} B^{\pm,k}_{n,j}\frac{\partial a_{n,k\pm1}}{\partial r} &= \sum_{n\geq k\pm1}\frac{(n-(k\pm1))!}{(n+(k\pm1))!}\frac{2n+1}{4}\frac{\partial a_{n,k\pm1}}{\partial r} \\ &\quad\times\int_0^\pi \sin\theta P_j^k(\cos\theta)P_n^{k\pm1}(\cos\theta)\sin\theta\, d\theta,\end{aligned} \tag{3.6}$$

which turns out to be a bit more difficult. We may transform $\sin\theta P_n^m(\cos\theta)$, with $m = k\pm1$ into a linear combination of "pure" Legendre polynomials $P_{n'}^{m'}$ by repeatedly using the relation (see Holland, 1990)

$$\begin{aligned}\sin\theta P_n^m(\cos\theta) &= 2(m-1)\cos\theta P_n^{m-1}(\cos\theta) - (n-m+2) \\ &\quad\times(n+m-1)\sin\theta P_n^{m-2}(\cos\theta), \qquad m\geq 2\end{aligned} \tag{3.7}$$

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

$$\sin\theta P_n^1(\cos\theta) = nP_{n-1}(\cos\theta) - n\cos\theta P_n(\cos\theta) \tag{3.8}$$

$$\sin\theta P_n(\cos\theta) = \frac{1}{2n+1}\left(P_{n+1}^1(\cos\theta) - P_{n-1}^1(\cos\theta)\right). \tag{3.9}$$

The final expressions are

$$\sin\theta P_n^m(\mu) = \begin{cases} \dfrac{1}{2n+1}\left(P_{n+1}^1(\mu) - P_{n-1}^1(\mu)\right) & \text{if } m = 0 \\ \displaystyle\sum_{l=2}^{m/2} q_{n,m}(2l-1)R_n^{2l-1}(\mu) + \frac{q_{n,m}(1)}{2n+1} & \text{if } m \text{ even,} \\ \quad \times\big((n+1)(n+2)P_{n-1}^1(\mu) & \quad m > 0 \\ \quad - n(n-1)P_{n+1}^1(\mu)\big) & \\ \displaystyle\sum_{l=1}^{(m-1)/2} q_{n,m}(2l)R_n^{2l}(\mu) & \text{if } m \text{ odd} \\ \quad + q_{n,m}(0)\dfrac{n(n+1)}{2n+1}(P_{n-1}(\mu) - P_{n+1}(\mu)) & \end{cases} \tag{3.10}$$

with

$$R_n^m(\mu) = \frac{2m}{2n+1}\left((n-m+1)P_{n+1}^m(\mu) + (n+m)P_{n-1}^m(\mu)\right) \tag{3.11}$$

$$q_{n,m}(l) = (-1)^{\frac{m-l-1}{2}} \frac{(n-l-1)!!}{(n-m)!!}\frac{(n+m-1)!!}{(n+l)!!} \qquad \text{if } m-l \text{ odd, m} \geq l+1 \tag{3.12}$$

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 in (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_j^p in the sum (3.10) will have p even (odd)). The integrals may be evaluated using the definition (2.5) directly as

$$\begin{aligned} I_{j,q}^{k,p} &= \int_0^{\pi} (\sin\theta)^{k+p+1}\left(\frac{d^k}{d\mu^k}P_j(\mu)\frac{d^p}{d\mu^p}P_q(\mu)\right)\Bigg|_{\mu=\cos\theta} d\theta \\ &= 2^{-(j+q)}\sum_{\kappa=0}^{[\frac{j-k}{2}]}\sum_{\lambda=0}^{[\frac{q-p}{2}]}(-1)^{\kappa+\lambda}\frac{(2j-2\kappa)!}{\kappa!(j-\kappa)!(j-k-2\kappa)!}\frac{(2q-2\lambda)!}{\lambda!(q-\lambda)!(q-p-2\lambda)!} \\ &\quad\times\int_0^{\pi}(\sin\theta)^{k+p+1}(\cos\theta)^{j+q-(p+k)-2(\kappa+\lambda)}\,d\theta. \end{aligned} \tag{3.13}$$

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 π. Otherwise, that is if $k+p$ is even and

$j+q$ is even, we use the formula involving the Γ 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 Γ function for the integers; see, e.g., Folland, 1992, and Szegö, 1957),

$$I_{j,q}^{k,p} = 2^{-(j+q-(k+p)/2)}\left(\frac{k+p}{2}\right)! \sum_{\kappa=0}^{[\frac{j-k}{2}]} \sum_{\lambda=0}^{[\frac{q-p}{2}]} (-1)^{\kappa+\lambda} \frac{(2j-2\kappa)!}{\kappa!(j-\kappa)!(j-k-2\kappa)!}$$
$$\times \frac{(2q-2\lambda)!}{\lambda!(q-\lambda)!(q-p-2\lambda)!} \cdot \frac{(j+q-(k+p)-2(\kappa+\lambda)-1)!!}{(j+q-2(\kappa+\lambda)+1)!!}. \qquad (3.14)$$

We note that both double factorials contain only odd numbers.

Thus, we conclude

$$B_{n,j}^{\pm,k} = \begin{cases} 0 & \text{if } n+j \text{even} \\ \frac{1}{4}\left(I_{j,n+1}^{1,1}(\mu) - I_{j,n-1}^{1,1}(\mu)\right) & \text{if } n+j\text{odd,} \\ & \quad -\text{case, } k=1 \\ \frac{1}{2}\sum_{l=2}^{(k\pm1)/2} \tilde{q}_{n,k\pm1}(2l-1)J_{j,n}^{k,2l-1} + \frac{\tilde{q}_{n,k\pm1}(1)}{4} & \text{if } n+j\text{odd,} \\ \quad \times \left((n+1)(n+2)I_{j,n-1}^{k,1} - n(n-1)I_{j,n+1}^{k,1}\right) & \quad k \text{ odd,} \\ & \quad -\text{case: } k>1 \\ \frac{1}{2}\sum_{l=1}^{(k\pm1-1)/2} \tilde{q}_{n,k\pm1}(2l)J_{j,n}^{k,2l} & \text{if } n+j \text{ odd,} \\ \quad +\tilde{q}_{n,k\pm1}(0)\frac{n(n+1)}{4}\left(I_{j,n-1}^{k,0} - I_{j,n+1}^{k,0}\right) & \quad k\,\text{even} \end{cases} \qquad (3.15)$$

where

$$J_{j,n}^{k,m} = m\left((n-m+1)I_{j,n+1}^{k,m} + (n+m)I_{j,n-1}^{k,m}\right) \qquad (3.16)$$

$$\tilde{q}_{n,m}(l) = \frac{(n-m)!}{(n+m)!}q_{n,m}(l) = (-1)^{\frac{m-l-1}{2}}\frac{(n-m-1)!!}{(n+m)!!}\frac{(n-l-1)!!}{(n+l)!!}. \qquad (3.17)$$

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 $m=k\pm1$ and $n+j$ odd, in addition to the contribution from (3.5) when $m=k$ and $n=j\pm1$.

4. EXPANDING THE COLLISION INTEGRAL

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

$$\begin{aligned} C_f(x, r, \Omega, E) &= \int_{4\pi} \sigma_s(E, \Omega \cdot \Omega') \big(f(x, r, \Omega', E) - f(x, r, \Omega, E) \big) \, d\Omega' \\ &= \sum_{n=0}^{\infty} \sum_{m=0}^{n} C_f^{n,m}(x, r, E) Y_n^m(\Omega), \end{aligned} \tag{4.1}$$

where

$$C_f^{n,m}(x, r, E) = \frac{(n-m)!}{(n+m)!} \frac{2n+1}{2\pi} \int_{4\pi} C_f(x, r, \Omega, E) Y_n^m(\Omega) \, d\Omega. \tag{4.2}$$

By expanding f in its spherical harmonics expansion with coefficients $a_{n,m}$, we may get a simple expression for the coefficients $C_f^{n,m}$. The second term in (4.1) is easy enough to evaluate, and the first term may be evaluated by expanding σ_s in Legendre polynomials in terms of $\Omega \cdot \Omega'$ and then using the addition formula for Legendre polynomials (see Holland, 1990). Due to orthogonality of spherical harmonics, the final result simplifies to

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

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 Luo (1985),

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

where f_p is the fluence of primary electrons, σ_c is the collision cross-section, and

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

specifies the direction of motion of the secondary electron with kinetic energy E' and direction Ω' given a primary electron with kinetic energy E and direction Ω, through $\Omega \cdot \Omega' = \phi(E', E)$. 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

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

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 δ-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

$$\sum_{n \geq k} \left(A^k_{n,j} \frac{\partial a_{n,k}}{\partial x} + B^k_{n,j} \frac{\partial a_{n,k}}{\partial r} \right) - \frac{1}{2} \frac{\partial^2 \omega(E) a_{j,k}}{\partial E^2} - \frac{\partial S(E) a_{j,k}}{\partial E}$$
$$= C_f^{j,k}(x, r, E) + Q^{j,k}(x, r, E). \tag{6.1}$$

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

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

where A and B are matrices containing the coefficients $A^k_{n,j}$ and $B^{\pm,k}_{n,j}$, 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.

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 article we shall study spatial discretization in (x, r).

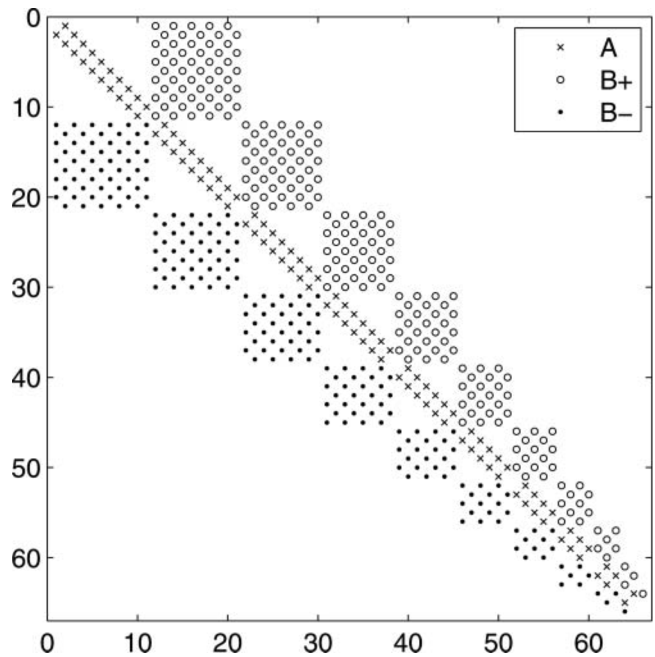

Figure 1: The non-zero elements of the matrices A and B for N = 10.

7.1 Notation

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 Equation (6.2) as a first order system viz,

$$\begin{cases} A\dfrac{\partial \mathbf{u}}{\partial x}+B\dfrac{\partial \mathbf{u}}{\partial r}-\dfrac{1}{2}\dfrac{\partial^2(\omega(E)\mathbf{u})}{\partial E^2}-\dfrac{\partial(S(E)\mathbf{u})}{\partial E}=C(E)\mathbf{u}+\mathbf{q}(x,r,E),\\ \mathbf{v}=\dfrac{\partial(\omega(E)\mathbf{u})}{\partial E}. \end{cases} \tag{7.1}$$

We use a change of variable as $\tilde{E}=E_0-E$ and supply the boundary condition as the energy from its peak $\mathbf{u}(0)$ at $\tilde{E}=0$ in the energy interval $\tilde{E}\in[0,E_0]$ corresponding to $E_0\overset{E}{\leftrightarrow}0$, and $(x,r)=(0,0)$. Then, evidently $\frac{\partial \mathbf{G}}{\partial E}=-\frac{\partial \mathbf{G}}{\partial \tilde{E}}$ and $\frac{\partial^2 \mathbf{G}}{\partial E^2}=\frac{\partial^2 \mathbf{G}}{\partial \tilde{E}^2}$. Further, to use the second relation in (7.1) we write

$$S(E)\mathbf{u}=\frac{S(E)}{\omega(E)}\omega(E)\mathbf{u}\equiv\gamma(E)\omega(E)\mathbf{u}. \tag{7.2}$$

Thus,

$$\frac{\partial(S(E)\mathbf{u})}{\partial E} = \frac{\partial\gamma(E)}{\partial E}\omega(E)\mathbf{u} + \gamma(E)\frac{\partial(\omega(E)\mathbf{u})}{\partial E}. \tag{7.3}$$

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

$$\begin{cases} A\mathbf{u}_x + B\mathbf{u}_r - \frac{1}{2}\mathbf{v}_E - \gamma_E(E)\omega(E)\mathbf{u} - \gamma(E)\mathbf{v} = C(E)\mathbf{u} + \mathbf{q}(x, r, E), \\ \mathbf{v}(x, r, E) = (\omega(E)\mathbf{u})_E(x, r, E), \\ \mathbf{u}(x, r, E_0) = \delta(x)\delta(r)\mathbf{u}_0(E_0), \qquad \mathbf{u}(x, r, 0) = 0, \\ \mathbf{v}(x, r, E_0) = -\delta(x)\delta(r)\mathbf{v}_0(E_0), \qquad \mathbf{u}(x, r, 0) = 0. \end{cases} \tag{7.4}$$

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

$$\begin{cases} \Gamma \cdot \nabla_{xr}\mathbf{u} - \frac{1}{2}\mathbf{v}_E - \gamma(E)\mathbf{v} = D(E)\mathbf{u} + \mathbf{q}, \\ \mathbf{v} = (\omega(E)\mathbf{u})_E. \end{cases} \tag{7.5}$$

7.1.1 *Weak formulation*

We use partial integration in E and the notation

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

to write

$$\begin{aligned} (\Gamma \cdot \nabla_{xr}\mathbf{v}, \mathbf{w}) &= (A\mathbf{v}_x + B\mathbf{v}_r, \mathbf{w}) = (A(\omega(E)\mathbf{u})_{Ex} + B(\omega(E)\mathbf{u})_{Er}, \mathbf{w}) \\ &= -(A(\omega(E)\mathbf{u})_x + B(\omega(E)\mathbf{u})_r, \mathbf{w}_E) + (A\omega(E)\mathbf{u_0}(E_0)_x \\ &\quad + B\omega(E)\mathbf{u}(E_0)_r)\mathbf{w}(E_0) \\ &= -(\Gamma\omega(E) \cdot \nabla_{xr}\mathbf{u}, \mathbf{w}_E) + (A\omega(E)\mathbf{u_0}(E_0)_x + B\omega(E)\mathbf{u}(E_0)_r)\mathbf{w}(E_0) \\ &= -\left(\frac{1}{2}(\omega(E)\mathbf{v}_E) + S(E)\mathbf{v} + D(E)\omega(E)\mathbf{u} + \omega(E)\mathbf{q}, , \mathbf{w}_E\right) \\ &= +(A\omega(E)\mathbf{u_0}(E_0)_x + B\omega(E)\mathbf{u}(E_0)_r)\mathbf{w}(E_0), \qquad \forall \mathbf{w} \in \mathcal{H}^1, \end{aligned} \tag{7.6}$$

and

$$((\omega(E)\mathbf{u})_E, \chi_E) = (v, \chi_E), \qquad \forall \chi \in \mathcal{H}_0^1. \tag{7.7}$$

7.1.2 *Energy estimates*

We consider finite element subspaces $S_h \subset \mathcal{H}_0^1(\Omega)$, and $W_h \subset \mathcal{H}^1(\Omega)$ with the following approximation properties: For $1 \le p \le \infty$ and $\ell > 0$, $s > 0$ integers, there is a constant C independent of h such that (see Ciarlet, 1978)

$$\inf_{\chi\in S_h}\{||g-\chi||_{L_p(I_E)}+h||g-\chi||_{W^{1,p}(I_E)}\}\le Ch^{\ell+1}||g||_{W^{\ell+1,p}(I_E)},$$
$$\forall g\in\mathcal{H}_0^1\cap W^{\ell+1,p}(I_E), \qquad (7.8)$$

and

$$\inf_{\zeta\in W_h}\{||\rho-\zeta||_{L_p(I_E)}+h||\rho-\zeta||_{W^{1,p}(I_E)}\}\le Ch^{s+1}||\rho||_{W^{s+1,p}(I_E)},$$
$$\forall\rho\in W^{s+1,p}(I_E). \qquad (7.9)$$

Motivated by the weak (variational) formulation (7.6) and (7.7), we define a pair of semidiscrete finite element approximations $\{\tilde{\mathbf{u}}_h, \tilde{\mathbf{v}}_h\} : I_x\times I_r\to S_h\times W_h$ for $\{\mathbf{u},\mathbf{v}\}$, respectively as solution of

$$(\Gamma\cdot\nabla_{xr}\tilde{\mathbf{v}}_h,\mathbf{w})=-\left(\frac{1}{2}(\omega(E)\tilde{\mathbf{v}}_{h,E})+S(E)\tilde{\mathbf{v}}_h+D(E)\omega(E)\tilde{\mathbf{u}}_h+\omega(E)\tilde{\mathbf{q}}_h,\mathbf{w}_E\right)$$
$$+(A\omega(E)\tilde{\mathbf{u}}_h(E_0)_x+B\omega(E)\tilde{\mathbf{u}}_h(E_0)_r)\mathbf{w}(E_0), \qquad \forall\mathbf{w}\in W_h, \quad (7.10)$$

and

$$((\omega(E)\tilde{\mathbf{u}})_{h,E},\chi_E)=(\tilde{\mathbf{v}}_h,\chi_E), \qquad \forall\chi\in S_h. \qquad (7.11)$$

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

$$||\mathbf{u}(E_0)-\tilde{\mathbf{u}}_h(E_0)||\le C(\mathbf{u}(E_0)h^s. \qquad (7.12)$$

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 $Q_h:\mathcal{H}_0^1\to S_h$ for $\mathbf{u}$ (see Brenner and Scott, 2008), by

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

and $P_h:\mathcal{H}^1\to W_h$ for $\mathbf{v}$ by

$$\mathcal{A}(\mathbf{v}-P_h\mathbf{v},\rho)=0, \qquad \forall\rho\in W_h, \qquad (7.14)$$

where

$$\mathcal{A}(\rho,\zeta)=\frac{1}{2}(\omega(E)\rho_E,\zeta_E)+(S(E)\rho,\zeta_E)+(D(E)\omega(E)\rho,\zeta_E)+\Lambda((\rho,\zeta)$$
$$=\frac{1}{2}(\omega(E)\rho_E,\zeta_E)+((S(E)+D(E)\omega(E))\rho,\zeta_E)+\Lambda((\rho,\zeta). \qquad (7.15)$$

Here Λ is chosen appropriately so that $\mathcal{A}$ is $\mathcal{H}^1$-coercive, i.e., there is a parameter $\alpha_0 > 0$ such that

$$\mathcal{A}(\mathbf{v}, \mathbf{v}) \geq \alpha_0 |||\mathbf{v}|||_1^2. \tag{7.16}$$

Remark 7.1 *Note that in this section 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 η and ξ are derived using an extended version of a result by Wheeler (1973).

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 $j = 0, 1$*

$$\|\eta\|_j + \|\nabla_{xv}\eta\|_j \leq Ch^{\ell+1-j}(\|\mathbf{u}\|_{\ell+1} + \|\nabla_{xv}\mathbf{u}\|_{\ell+1}), \qquad \ell = 0, 1, \ldots, \tag{7.17}$$

and

$$\|\xi\|_j + \|\nabla_{xv}\xi\|_j \leq Ch^{s+1-j}(\|\mathbf{v}\|_{s+1} + \|\nabla_{xv}\mathbf{v}\|_{s+1}), \qquad s = 0, 1, \ldots \tag{7.18}$$

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

$$\|\eta\|_{W^{j,p}(I_E)} \leq Ch^{\ell+1-j}\|\mathbf{u}\|_{W^{\ell+1,p}(I_E)}, \qquad \ell = 0, 1, \ldots, \tag{7.19}$$

$$\|\xi\|_{W^{j,p}(I_E)} \leq Ch^{s+1-j}\|\mathbf{v}\|_{W^{s+1,p}(I_E)}, \qquad s = 0, 1, \ldots. \tag{7.20}$$

To derive error estimates for the semidiscrete (discretization in E) approximation, we split the error as

$$\mathbf{u} - \tilde{\mathbf{u}}_h = (\mathbf{u} - \mathbf{u}_h) - (\tilde{\mathbf{u}}_h - \mathbf{u}_h) := \eta - \varepsilon$$

$$\mathbf{v} - \tilde{\mathbf{v}}_h = (\mathbf{v} - \mathbf{v}_h) - (\tilde{\mathbf{v}}_h - \mathbf{v}_h) := \xi - \nu.$$

Since the estimates for η and ξ are known from the Lemma 6.1, it is enough to estimate ε and ν. Taking the 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 ε and ν as follows:

$$\begin{aligned}
&(\Gamma \cdot \nabla_{xr}(\mathbf{v} - \tilde{\mathbf{v}}_h), \zeta) \\
&\quad = -\frac{1}{2}(\omega(E)(\mathbf{v} - \tilde{\mathbf{v}}_h)_E, \zeta_E) - (S(E)(\mathbf{v} - \tilde{\mathbf{v}}_h), \zeta_E) \\
&\qquad - (D(E)\omega(E)(\mathbf{u} - \tilde{\mathbf{u}}_h)\zeta_E) - (\omega(E)(\mathbf{q} - \tilde{\mathbf{q}}_h)\zeta_E), \quad \zeta \in W_h,
\end{aligned} \tag{7.21}$$

and

$$(\omega(E)(\mathbf{u}-\tilde{\mathbf{u}}_h)_E,\, \chi_E) - (\mathbf{v}-\tilde{\mathbf{v}}_h),\, \chi_E) = 0. \tag{7.22}$$

Note that

$$(\omega(E)(\mathbf{u}-\tilde{\mathbf{u}}_h)_E,\, \chi_E) = (\omega(E)\eta_E,\, \chi_E) - (\omega(E)\varepsilon_E,\, \chi_E),$$

where using the definition of Q_h we have

$$(\omega(E)(\mathbf{u}_E - \mathbf{u}_{h,E}) = (\omega(E)(\mathbf{u}_E - Q_h\mathbf{u}_E) = 0. \tag{7.23}$$

Thus inserting (7.23) in (7.22) we get

$$-(\omega(E)\varepsilon_E,\, \chi_E) = (\xi,\, \chi_E) - (\nu,\, \chi_E). \tag{7.24}$$

Further (7.21) can be written as

$$\begin{aligned}(\Gamma\cdot\nabla_{xr}\nu,\, \zeta) = {} & (\Gamma\cdot\nabla_{xr}\xi,\, \zeta) + \frac{1}{2}(\omega(E)\xi_E,\, \zeta_E) - \frac{1}{2}(\omega(E)\nu_E,\, \zeta_E) + (S(E)\xi,\, \zeta_E)\\ & -((S(E)\nu,\, \zeta_E) + (D(E)\omega(E)\eta,\, \zeta_E) - (D(E)\omega(E)\varepsilon,\, \zeta_E)\\ & + (\omega(E)(\mathbf{q}-\tilde{\mathbf{q}}_h),\, \zeta_E).\end{aligned} \tag{7.25}$$

On the other hand we have that

$$\mathcal{A}(\nu,\zeta) = \frac{1}{2}(\omega(E)\nu_E,\, \zeta_E) + ((S(E)\nu,\, \zeta_E) + (D(E)\omega(E)\nu,\, \zeta_E) + \Lambda(\nu,\zeta). \tag{7.26}$$

Adding (7.25) and (7.26) we have that

$$\begin{aligned}(\Gamma\cdot\nabla_{xr}\nu,\, \zeta) + \mathcal{A}(\nu,\zeta) = {} & (\Gamma\cdot\nabla_{xr}\xi,\, \zeta) + \frac{1}{2}(\omega(E)\xi_E,\, \zeta_E) + (S(E)\xi,\, \zeta_E)\\ & + (D(E)\omega(E)(\eta-\varepsilon),\, \zeta_E) + (D(E)\omega(E)\nu_E,\, \zeta_E)\\ & + (\omega(E)(\mathbf{q}-\tilde{\mathbf{q}}_h),\, \zeta_E) + \Lambda(\nu,\zeta).\end{aligned} \tag{7.27}$$

Now we let $\zeta = \nu$ use the coercivity assumption and write

$$\begin{aligned}(\Gamma\cdot\nabla_{xr}\nu,\, \nu) + \alpha_0|||\nu|||_1^2 \le {} & (\Gamma\cdot\nabla_{xr}\nu,\, \nu) + \mathcal{A}(\nu,\nu) \le (\Gamma\cdot\nabla_{xr})\|\xi\|^2 + \frac{1}{4}(\Gamma\cdot\nabla_{xr})\|\nu\|^2\\ & + \|\omega(E)^{1/2}\xi_E\|^2 + \frac{1}{16}\|\omega(E)^{1/2}\nu_E\|^2 + 4\|S(E)^{1/2}\xi_E\|^2 + \frac{1}{16}\|S(E)^{1/2}\nu_E\|^2\\ & + 4\|D(E)^{1/2}\omega(E)^{1/2}\eta\|^2 + \frac{1}{16}\|D(E)^{1/2}\omega(E)^{1/2}\nu_E\|^2\\ & + 4\|D(E)^{1/2}\omega(E)^{1/2}\varepsilon\|^2 + \frac{1}{16}\|D(E)^{1/2}\omega(E)^{1/2}\nu_E\|^2\\ & + \frac{1}{2}\|D(E)^{1/2}\omega(E)^{1/2}\nu\|^2 + \frac{1}{2}\|D(E)^{1/2}\omega(E)^{1/2}\nu_E\|^2 + \|\Lambda^{1/2}\nu\|^2\\ & + |(\omega(E)(\mathbf{q}-\tilde{\mathbf{q}}_h),\, \nu_E)|.\end{aligned} \tag{7.28}$$

The last term in (7.28) is estimated as follows:

$$|(\omega(E)(\mathbf{q}-\tilde{\mathbf{q}}_h), \nu_E)| \le 4\|\omega(E)^{1/2}(\mathbf{q}-\tilde{\mathbf{q}}_h)\|^2 + \frac{1}{16}\|\omega(E)^{1/2}\nu_E\|^2. \qquad (7.29)$$

Next, we employ a kick-back argument, i.e., we hide all ν-terms in the right, inside the left-hand side. Except the ε-term, for all remaining ξ and η terms on the right-hand side, we have theoretical error bounds. Thus it remains to estimate the ε-term. To this end we let $\chi = \varepsilon$ in (7.24), then

$$\|\omega(E)^{1/2}\varepsilon_E\|^2 \le \|\omega(E)^{-1/2}\xi\|\|\omega(E)^{1/2}\varepsilon_E\| + \|\omega(E)^{-1/2}\nu\|\|\omega(E)^{1/2}\varepsilon_E\|,$$

so that

$$\|\omega(E)^{1/2}\varepsilon_E\| \le \|\omega(E)^{-1/2}\xi\| + \|\omega(E)^{-1/2}\nu\|. \qquad (7.30)$$

Now for the contribution from the ε-term in (7.28), first we use Poincare inequality to write $\|D(E)^{1/2}\omega(E)^{1/2}\varepsilon\|^2 \le \tilde{C}\|D(E)^{1/2}\omega(E)^{1/2}\varepsilon_E\|^2 \le \tilde{C}\|D(E)\|_\infty(\|\omega(E)^{-1/2}\xi\| + \|\omega(E)^{-1/2}\nu\|)$. An alternative estimate for the ε-term is obtained by letting $\chi_E = D(E)\varepsilon_E$ in (7.24). Then

$$\begin{aligned}\|D(E)^{1/2}\omega(E)^{1/2}\varepsilon_E\|^2 &= (\xi, D(E)\varepsilon_E) - (\nu, D(E)\varepsilon_E)\\ &= (\omega(E)^{-1/2}D(E)^{1/2}\xi, \omega(E)^{1/2}D(E)^{1/2}\varepsilon_E)\\ &- (\omega(E)^{-1/2}D(E)^{1/2}\nu, \omega(E)^{1/2}D(E)^{1/2}\varepsilon_E)\\ &\le \|\omega(E)^{-1/2}D(E)^{1/2}\xi\|^2 + \|\omega(E)^{-1/2}D(E)^{1/2}\nu\|^2\\ &+ \frac{1}{2}\|D(E)^{1/2}\omega(E)^{1/2}\varepsilon_E\|^2. \qquad (7.31)\end{aligned}$$

Once again, using Poincare inequality we get

$$\begin{aligned}\|D(E)^{1/2}\omega(E)^{1/2}\varepsilon\|^2 \le \frac{\tilde{C}}{|\min\omega(E)|^2}(&\|\omega(E)^{1/2}D(E)^{1/2}\xi\|^2\\ &+ \|\omega(E)^{1/2}D(E)^{1/2}\nu\|^2). \qquad (7.32)\end{aligned}$$

Inserting (7.29) and (7.32) in (7.28) and rearranging the terms yields

$$\begin{aligned}&(\Gamma\cdot\nabla_{xr}\nu, \nu) + \alpha_0|||\nu|||_1^2\\ &\le (\Gamma\cdot\nabla_{xr})\|\xi\|^2 + \frac{1}{4}(\Gamma\cdot\nabla_{xr})\|\nu\|^2 + \|\omega(E)^{1/2}\xi_E\|^2\\ &+ \frac{1}{8}\|\omega(E)^{1/2}\nu_E\|^2 + 4\|S(E)^{1/2}\xi_E\|^2 + \frac{1}{16}\|S(E)^{1/2}\nu_E\|^2\\ &+ 4\|D(E)^{1/2}\omega(E)^{1/2}\eta\|^2 + \frac{5}{8}\|D(E)^{1/2}\omega(E)^{1/2}\nu_E\|^2\\ &+ 4\|D(E)^{1/2}\omega(E)^{1/2}\varepsilon\|^2 + \frac{1}{2}\|D(E)^{1/2}\omega(E)^{1/2}\nu\|^2\end{aligned}$$

$$+\frac{\tilde{C}}{|\min\omega(E)|^2}(\|\omega(E)^{1/2}D(E)^{1/2}\xi\|^2+\|\omega(E)^{1/2}D(E)^{1/2}\nu\|^2)$$
$$+4\|\omega(E)^{1/2}(\mathbf{q}-\tilde{\mathbf{q}}_h)\|^2+\|\Lambda^{1/2}\nu\|^2. \tag{7.33}$$

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

$$|||\nu|||_1=[\|\omega(E)^{1/2}\nu_E\|^2+\|S(E)^{1/2}\nu_E\|^2+\|D(E)^{1/2}\omega(E)^{1/2}\nu_E\|^2$$
$$+\|\omega(E)^{1/2}D(E)^{1/2}\nu\|^2+\|\Lambda^{1/2}\nu\|^2]^{1/2}, \tag{7.34}$$

we get using a kick-back argument and with $\alpha_0\sim 1$ that

$$\|(\Gamma\cdot\nabla_{xr})\nu\|^2+\alpha_0'|||\nu|||_1^2\leq 4\|(\Gamma\cdot\nabla_{xr})\xi\|^2+4\|\omega(E)^{1/2}\xi_E\|^2+16\|S(E)^{1/2}\xi_E\|^2$$
$$+4\|\omega(E)^{1/2}D(E)^{1/2}\xi\|^2+16\|D(E)^{1/2}\omega(E)^{1/2}\eta\|^2$$
$$+16\|\omega(E)^{1/2}(\mathbf{q}-\tilde{\mathbf{q}}_h)\|^2, \tag{7.35}$$

for some $0<\alpha_0'<\alpha_0\sim 1$. Note that the norms of the projection errors, η and ξ, 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 $\mathbf{q}-\tilde{\mathbf{q}}_h$ is of the same order as in Lemma 6.1, we can apply Lemma 6.1 and the previous estimates to obtain

$$\|(\Gamma\cdot\nabla_{xr})\nu\|^2+\alpha_0'|||\nu|||_1^2$$
$$\leq Ch^{2\min(\ell,s)}\big(\|\mathbf{u}\|^2_{L^\infty_{xr}(H^{\ell+1})}+\|\mathbf{v}\|^2_{L^\infty_{xr}(H^{s+1})}+\|\nabla_{xr}\cdot\mathbf{v}\|^2_{L^2_{xr}(H^{s+1})}\big), \tag{7.36}$$

which yields, e.g., the estimate

$$\|(\mathbf{u}-\tilde{\mathbf{u}}_h)(x,r)\|+\|(\mathbf{v}-\tilde{\mathbf{v}}_h)(x,r)\|$$
$$\leq Ch^{\min(\ell+1,s+1)}\big(\|\mathbf{u}\|_{L^\infty_{xr}(H^{\ell+1})}+\|\mathbf{v}\|_{L^\infty_{xr}(H^{s+1})}+\|\nabla_{xr}\cdot\mathbf{v}\|_{L^2_{xr}(H^{s+1})}\big). \tag{7.37}$$

Hence, using a standard procedure and the previous estimates we may derive the following *a priori error estimates*.

Theorem 7.2 *Assume that* $\tilde{\mathbf{v}}_h(0)=P_E\mathbf{v}_0$ *so that* $\nu(0)=0$. *Then there exists a constant* C *independent of* h *such that*

$$\|(\mathbf{v}-\tilde{\mathbf{v}}_h)(x,r)\|_1\leq C(E_0)h^{\min(\ell+1,s)}\big(\|\mathbf{u}\|_{L^\infty_{xr}(H^{\ell+1})}+\|\mathbf{v}\|_{L^\infty_{xr}(H^{s})}+\|\nabla_{xr}\cdot\mathbf{v}\|_{L^2_{xr}(H^{s+1})}\big). \tag{7.38}$$

Theorem 7.3 (a) *Under the assumption of the previous theorem, the errors* $\mathbf{u} - \tilde{\mathbf{u}}_h$ *and* $\mathbf{v} - \tilde{\mathbf{v}}_h$ *can be estimated as*

$$\|(\mathbf{u} - \tilde{\mathbf{u}}_h)(x,r)\| + \|(\mathbf{v} - \tilde{\mathbf{v}}_h)(x,r)\| + h\|(\mathbf{v} - \tilde{\mathbf{v}}_h)(x,r)\|_1 \leq C(E_0)h^{\min(\ell+1,s+1)} \times \left(\|\mathbf{u}\|_{L^\infty_{xr}(H^{\ell+1})} + \|\mathbf{v}\|_{L^\infty_{xr}(H^{s+1})} + \|\nabla_{xr} \cdot \mathbf{v}\|_{L^2_{xr}(H^{s+1})}\right). \tag{7.39}$$

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

$$\|(\mathbf{u} - \tilde{\mathbf{u}}_h)(x,r)\|_{L^p} + \|(\mathbf{v} - \tilde{\mathbf{v}}_h)(x,r)\|_{L^p} + \leq C(E_0)h^{\min(\ell+1,s+1)} \times \left(\|\mathbf{u}\|_{L^\infty_{xr}(W^{\ell+1,p})} + \|\mathbf{v}\|_{L^\infty_{xr}(W^{s+1,p})} + \|\nabla_{xr} \cdot \mathbf{v}\|_{L^2_{xr}(W^{s+1,p})}\right). \tag{7.40}$$

These estimates are of optimal order due to the maximal available regularity in the degenerate type convection diffusion equation (see Lions , 1961 and Pani, 1998).

8. CONCLUSIONS

We have considered solving transport equation for, symmetrically distributed, charged radiation particles, using the continuous slowing down assumption. The underlying equation is of the form of a degenerate type (diffusive only in energy variable) convection-diffusion equation with a collision integral corresponding to the elastic scattering. Both stopping power and energy loss straggling (coefficients in first- and second-order derivatives in energy variable, respectively) were modeled in the equation. We performed spherical harmonic expansions for the convection term, collision integral, and source term for secondary collisions and obtained a system of partial differential equations for the coefficient matrices. We have performed a semidiscrete finite element approximation of the energy variable and derived optimal convergence rates up to the maximal available regularity of the exact solution. In summary this approach was for a general form of energy-dependent transport equation, rather than assuming forward peaked scattering. The fully discrete (discretization on the radial variable and penetration direction) approximation as well as numerical implementations is the subject of future work.

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