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ION TRANSPORT IN INHOMOGENEOUS MEDIA II. GALERKIN METHODS FOR PRIMARY IONS

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ABSTRACT. This is Part II of our investigation of ion transport problem. The study concerns the energy deposition of high-energy (e.g., $\approx 50-1000$ MeV) proton and carbon ions and light ions (high-energy electrons of ≈ 50 MeV), in inhomogeneous media. The original effort was to develop a flexible model incorporated with the analytic theory for electrons: the bipartition model. In this model the transport equation is split into a, coupled, system of convection diffusion equations controlled by a bipartition condition. This paper concerns convergence analysis for both semi-discrete and fully discrete Galerkin approximations of a such obtained equation for a broad beam model. In this setting we also study the characteristic Galerkin and streamline diffusion methods. The analytic broad beam model of the light ion absorbed dose were compared with the results of the modified Monte Carlo (MC) code SHIELD-HIT+ and those of Galerkin streamline diffusion approach.

1. INTRODUCTION

In the present paper we, primarily, assume a broad beam of *forward-directed* ions normally incident at the boundary of a semi infinite medium entering the domain in a direction labeled as the positive direction of the x-axis. As a result of collisions (because of the forward-directness assumption), only, very small portion of the ions is scattered to *large angles*. These are, except at very low energies, very few ions with a directional change beyond a certain minimal angle θ_m, determined by the *bipartition condition below*, which have a *diffusion-like* transport behavior and an, almost, isotropic angular distribution. The remaining significant portion of the ion particles, deflecting slightly ($< \theta_m$) from the original direction, are convective ions and refereed to as *forward-directed* ions. To separate the large-angle scattered and forward-directed ions properly, the partition condition is introduced. The current model is based on a split, of the scattering integral (kernel), through adding and subtracting the diffusion ion source to the diffusion and straightforward equations, respectively. A similar approach is given through the split of the scattering cross-section into the hard and soft parts, see [16].

The first part of this investigation was devoted to the study of an ion transport model describing the actual process of energetic ions in absorbing media under continuously slowing down assumption, see [19], and retain of the energy straggling (a term with a second order derivative in the energy variable). In Part I, the bipartition model was applied to solving three type of problems for ion transport in

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inhomogeneous media: (i) normally incident ion transport in a slab; (ii) obliquely incident ion transport in a semi-infinite medium; (iii) energy deposition of ions in a multilayer medium.

In the present paper we consider the case of, forward directed, ions injected into a medium with large atomic weight. The underlying partial differential equation is therefore the Boltzmann equation within the Fokker-Planck realm. More specifically, we shall study the finite element approximation for a broad beam model. For the asymptotic expansion procedure and some relevant studies of resulting Fermi and Fokker-Planck pencil beam equations, see, e.g. [24], [15]-[16] and [3]-[7].

Neutral (photon, i.e. x-ray) and charged (electron and ion) particle beams are extensively used in radiation therapy both for early cancer detection and dose computation algorithms see, e.g. [8], [9], [18]-[20] and [23].

An outline of this paper is as follows: In Section 2 we give a brief description of the ion transport model under continuously slowing down assumption. In Section 3 we introduce the standard Galerkin procedure. In Section 4 we consider semi-discrete problem: Galerkin finite element approximation applied for a convection-diffusion problem of a broad beam model, where the penetration variable is treated like time variable, in the multilayer setting. We study stability and convergence of the semi-discrete problem. Section 5 is devoted to the fully discrete problem. In Section 6 we formulate the characteristic Galerkin and streamline diffusion methods for the broad beam model and give the corresponding error estimates. In our concluding Section 7 we discuss some simulation results for the bipartition and Galerkin approaches and compare them with results from Monte Carlo simulations.

2. Ion transport models under CSDA

The ion transport describing the actual process of energetic ions in absorbing media is formulated as follows: Let $f(\mathbf{x}, \mathbf{v}, E)$ denote the ion distribution function, (also called the *ion fluence differential* in angle and energy), then $f(\mathbf{x}, \mathbf{v}, E)d\mathbf{v}dE$ represents the ion fluence at point $\mathbf{x} \in \mathbb{R}^3$, with direction between $\mathbf{v}$ and $\mathbf{v}+d\mathbf{v}$ and energy between E and $E + dE$ ($\mathbf{v} \in \mathbb{R}^3$, $E \in \mathbb{R}^+$). Due to the statistical balance principle we may write the following ion transport equation derived from the linear transport equation by Lewis and Miller in [17]

$$\begin{aligned}\mathbf{v}\cdot\nabla_{\mathbf{x}} f - \frac{\partial(\rho f)}{\partial E} = \frac{1}{2}\frac{\partial^2(\Omega f)}{\partial E^2} + \kappa_N \int_{4\pi} d\mathbf{v}'\{[f(\mathbf{x},\mathbf{v}',E) - f(\mathbf{x},\mathbf{v},E)] \\ \times\, \sigma_n(E', E(1-\mathbf{v}\cdot\mathbf{v}')\} + S(\mathbf{x},\mathbf{v},E),\end{aligned} \tag{2.1}$$

where ρ denotes the stopping power and Ω is the energy loss straggling factor, κ_N is a constant depending on N the number of atoms and σ_n is the elastic cross section. We consider an ion beam of energy E_0 normally incident on the hypersurface of a semi-infinite medium. We let the outward normal to the semi-infinite region on the left to be along the positive x-axis inside the medium (we use the standard vector notation $\mathbf{x} = (x, y, z)$). In the bipartition strategy, the scattering integral is divided into two parts, of which one is the comparatively isotropic diffusion ion source S_d, including almost all of the "large-angle" scattered ions, the other is the remaining part that spreads mainly in the forward, small-angle, direction. The latter, convective part, is normally of negative value, indicating that the number of ions that leave the forward small-angle direction due to elastic scattering is larger than that of ions that enter the small-angle directions caused by elastic scattering.

For our physical model we have considered a scattering kernel with strong algebraic fall-off behavior from its peaks at zero angle and zero energy. To this end we have assumed an inverse power function approximation for the elastic cross-section, viz

$$\sigma_n(E, \mathbf{v}\cdot\mathbf{v}') \approx CE^{-2k}(1-\mathbf{v}\cdot\mathbf{v}')^{-1-k}, \tag{2.2}$$

where C is a constant, k is a positive integer, which corresponds to the Jacobian of the algebraic fall-offs. See [2], [20] and [24] for details. We also use the notation

$$Q := \frac{1}{2\pi}\delta(x)\delta(E-E_0)\delta(1-\mu),$$

where μ is the cosine of the angle between the direction of the ions and the x-axis,and denote the scattering integral by

$$C_f := CE^{-2k}\int_{4\pi} d\mathbf{v}'[f_s(\mathbf{x},\mu',E) - f_s(x,\mu,E)] \times (1-\mathbf{v}\cdot\mathbf{v}')^{-k-1}. \tag{2.3}$$

C_f represents the net increase in the number of particles per unit solid angle $\mathbf{v}$, passing through a unit distance, caused by elastic scattering. Now we split f as:

$$f(x,\mu,E) = f_s(x,\mu,E) + f_d(x,\mu,E), \tag{2.4}$$

where f_s is the forward-directed ion distribution satisfying

$$-\frac{\partial(\rho f_s)}{\partial E} + \mu\frac{\partial f_s}{\partial x} - \frac{1}{2}\frac{\partial^2(\Omega f_s)}{\partial E^2} = -S_d + Q + C_f, \tag{2.5}$$

and f_d is the distribution of the diffusion ion particles satisfying

$$-\frac{\partial(\rho f_d)}{\partial E} + \mu\frac{\partial f_d}{\partial x} - \frac{1}{2}\frac{\partial^2(\Omega f_d)}{\partial E^2} = S_d + C_f. \tag{2.6}$$

From the equation (2.1) and the property that the small-angle elastic scattering of ions is dominating, the main characteristics of C_f and S_d can be featured as shown in Fig 1., below.

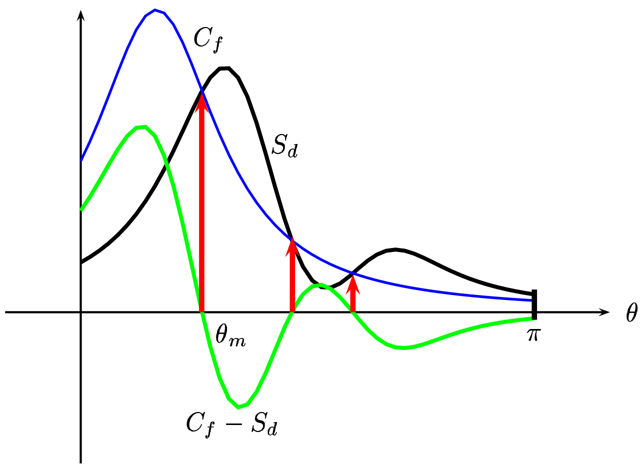

Figure 1: The extract of diffusion source S_d from the collision term C_f.

Physically, the collision term represents a scattering source. Thus, using the bipartition model we deduct the large-angle scattering source from the collision term in the straight-forward ion transport equation (2.1) by means of subtracting $S_d(x, \mu, E)$. Consequently, in (2.5) the scattering process generating large-angle ions is removed from the forward-directed ion transport equation (2.1). *The partition condition* is given by

$$S_d(x, \mu_i, E) = C_{f_s}(x, \mu_i, E), \qquad i = 0, 1, \ldots, m, \tag{2.7}$$

indicating that all the large-angle scattered ions in the straight-forward ion group are regarded as the secondary diffusion ion source S_d. *Then, to define the bipartition condition, we require that the intensity of this diffusion ion source, at the $m+1$ large angle directions, to be exactly equal to the values of collision integral at the same directions.*

3. Standard Galerkin for ion transport in isotropic media

We focus on broad beam model for ion transport and relay on Fokker-Planck development of the beam model (as an alternative to the bipartition model by Luo et al [18]-[20]). We use Pomraning's approach based on asymptotic expansions in isotropic media [24] (extended to anisotropic media by Asadzadeh in [6]), and split the equation into a *pencil beam model* and a *broad beam model*. As for the pencil beam model there is an extensive amount of literature for the Fermi equation [12] see, e.g. [3]-[7], [15], [24]. Here, we consider a broad beam model, which is compatible with the bipartition model studied in Part I, and study its Galerkin finite element approximations. To this end we start with the final form of the steady state Fokker-Planck equation

$$\begin{aligned}\mathbf{v}\cdot\nabla_x f + \sigma_a(E) f(\mathbf{x}, E, \mathbf{v}) &= T(E)\Big[\frac{\partial}{\partial\mu}(1-\mu^2)\frac{\partial}{\partial\mu} + \frac{1}{1-\mu^2}\frac{\partial^2}{\partial\varphi^2}\Big] f(\mathbf{x}, E, \mathbf{v}) \\ &+ \frac{\partial}{\partial E}\Big[S(E) f(\mathbf{x}, E, \mathbf{v})\Big] + \frac{\partial^2}{\partial E^2}\Big[R(E) f(\mathbf{x}, E, \mathbf{v})\Big] \\ &+ Q(\mathbf{x}, E, \mathbf{v}) + \mathcal{O}\Big(\frac{\delta^2 + \varepsilon\delta + \varepsilon^3}{\Delta}\Big),\end{aligned} \tag{3.1}$$

where δ, ε and Δ (mean free path) are certain smallness parameters (see [24]) and

$$\begin{aligned} S(E) &= 2\pi \int_0^\infty dE' \int_{-1}^1 d\mu (E - E')\sigma_s(E, E', \mu) = \mathcal{O}\Big(\frac{\varepsilon}{\Delta}\Big), \\ T(E) &= \pi \int_0^\infty dE' \int_{-1}^1 d\mu (1-\mu)\sigma_s(E, E', \mu) = \mathcal{O}\Big(\frac{\delta}{\Delta}\Big), \\ R(E) &= 2\pi \int_0^\infty dE' \int_{-1}^1 d\mu (E - E')^2\sigma_s(E, E', \mu) = \mathcal{O}\Big(\frac{\varepsilon^2}{\Delta}\Big), \end{aligned} \tag{3.2}$$

where σ_a and σ_s are absorption and scattering cross-sections, respectively. For comparison purpose we choose a coordinates system as is customary in the medical physics literature, where the orientation corresponds to a counter clock-wise rotation of the standard mathematical coordinates by $\pi/2$, and write

$$v = (\mu, \eta, \xi) = (\cos\theta, \sin\theta\cos\varphi, \sin\theta\sin\varphi).$$

In this setting, for a pencil beam model we may assume that the penetration direction of the beam is along the y-axis and the problem is independent of the energy

E, the spatial variable x and $\mu = \cos\theta \approx 0$. Thus, the Fokker-Planck equation is reduced to the pencil beam problem

$$\cos\varphi \frac{\partial}{\partial y} f_p(y,z,\varphi) + \sin\varphi \frac{\partial}{\partial z} f_p(y,z,\varphi) = T(E) \frac{\partial^2}{\partial \varphi^2} f_p(y,z,\varphi). \tag{3.3}$$

As for the case of broad beam model we have chosen the x-axis as the penetration direction and, due to symmetry, the beam is independent of y, z and φ variables, however it depends on x, μ and the energy variable E. Hence, the corresponding equation is

$$\begin{aligned} \mu \frac{\partial}{\partial x} f_b(x,\mu,E) + \sigma_a(E) f_b(x,\mu,E) &= T(E) \Big[\frac{\partial}{\partial \mu} (1-\mu^2) \frac{\partial}{\partial \mu} f_b(\mathbf{x},\mu,E) \Big] \\ &+ \frac{\partial}{\partial E} \Big[S(E) f_b(\mathbf{x},\mu,E) \Big] + \frac{\partial^2}{\partial E^2} \Big[R(E) f_b(\mathbf{x},\mu,E) \Big] + Q, \end{aligned} \tag{3.4}$$

where, because of the energy dependence we retain both absorption and source terms only in the broad beam model.

To proceed we consider the equation (3.4) for forward-directed broad beams ($\mu > 0$) in a bounded domain $D := \{(x,\mu,E) : 0 < x < L,\ 0 < \mu < 1,\ 0 < E < E_0\}$, associated with some physically relevant boundary conditions. Recall that by (3.2) we have $S(E) = \mathcal{O}\big(\frac{\varepsilon}{\Delta}\big)$, $T(E) = \mathcal{O}\big(\frac{\delta}{\Delta}\big)$ and $R(E) = \mathcal{O}\big(\frac{\varepsilon^2}{\Delta}\big)$, with $\varepsilon \approx \delta \approx \Delta$. Suppressing, the subscript b the broad beam equation is now

$$\sigma_a(E) f + \mu \frac{\partial f}{\partial x} - \frac{\partial f}{\partial E} = \frac{\partial}{\partial \mu} \Big[(1-\mu^2) \frac{\partial}{\partial \mu} f \Big] + \varepsilon \frac{\partial^2 f}{\partial E^2} + Q. \tag{3.5}$$

The equation (3.5) is degenerate convection-diffusion equation with convection in x and E and diffusion in μ and E variables. If we disregard the forward directed property, then $\mu \in [-1,1]$ yields a so called *Forward-backward problem* which is studied in connection with the Kolmogorov equations, see [26].

Since the collisions often appear as sudden changes in the energy and direction of the particles on each collision site. Therefore the discontinuous Galerkin method, in all three variables x, μ and E, is the more adequate finite approach for the numerical study of this problem. However, in the original bipartition model, the discontinuities caused by small changes are not considered to be severe. In such cases the jumps in energy and direction of the beam can be approximated by continuous functions resulting to approximate beam configurations with the same in- and outward profiles as the original ones. We reformulate the problem (3.5) by interpreting the source term Q as an inflow boundary condition on

$$\Gamma_\beta^{-(+)} := \{x_\perp \in \Gamma := \partial I_\perp : \mathbf{n}(x_\perp) \cdot \beta < 0 (> 0)\}, \tag{3.6}$$

where $x_\perp = (\mu, E)$, $I_\perp = I_\mu \times I_E$, $I_\mu = [0,1]$, $I_E = [0, E_0]$, $\beta = (0,-1)$ and $\mathbf{n}(x_\perp)$ is the outward unit normal to the boundary Γ at $x_\perp \in \Gamma$. Hence the final form of our broad beam problem will be a boundary value problem where for $x = 0$ (3.5) is associated with an inflow boundary condition viz

$$\begin{cases} \sigma_a(E) f + \mu \frac{\partial f}{\partial x} - \frac{\partial f}{\partial E} = \frac{\partial}{\partial \mu} \Big[(1-\mu^2) \frac{\partial}{\partial \mu} f \Big] + \varepsilon \frac{\partial^2 f}{\partial E^2}, & (x,\mu,E) \in I_x \times I_\perp, \\ f(0,\mu,E_0) = \delta(1-\mu)\tilde{\delta}(E-E_0), & \text{on } \Gamma_\beta^-, \\ f(x,\mu,E) = 0, & \text{on } \Gamma_\beta^+ \cup \Gamma_\beta^0. \end{cases} \tag{3.7}$$

Remark 3.1. Here $\tilde{\delta}(E-E_0)$ is a smooth approximation for the $\delta(E-E_0)$ function. In what follows, due to the nature of Dirac δ function we will be forced to such smooth replacements, otherwise the energy estimates (involving L_2 norms) will deteriorate.

4. The Semi-discrete Problem

We introduce a finite dimensional function space $V_{h,\beta} \subset H^1_\beta(I_\perp)$ with,

$$H^1_\beta(I_\perp) = \Big\{ f \in H^1(I_\perp): \;\; f = 0 \;\text{ on } \Gamma^0, \;\; v = \delta(1-\mu)\tilde{\delta}(E-E_0) \;\text{ on } \Gamma^-_\beta \Big\}, \tag{4.1}$$

such that, $\forall f \in H^1_\beta(I_\perp) \cap H^r(I_\perp)$,

$$\inf_{\chi \in V_{h,\beta}} \|f - \chi\|_j \le C h^{\alpha - j} \|f\|_\alpha, \quad j = 0, 1 \;\text{ and }\; 1 \le \alpha \le r, \tag{4.2}$$

where for positive integer s, $\|\cdot\|_s$ denotes the L_2-based Sobolev norm of functions with all their partial derivatives of order $\le s$ in L_2. An example of such $V_{h,\beta}$ is the set of sufficiently smooth piecewise polynomials $P(x_\perp)$ of degree $\le r$, satisfying the boundary condition given in (3.6).

To proceed we introduce a bilinear form, $A : H^1_\beta(I_\perp) \times H^1_\beta(I_\perp)$, defined by

$$A(f,\chi)_\perp := (\sigma_a(E)\, f, \chi)_\perp + (\mu f_x, \chi)_\perp - (f_E, \chi)_\perp, \quad \forall f, \chi \in H^1_\beta(I_\perp). \tag{4.3}$$

Then the continuous variational problem is: find a solution f to (3.7) such that

$$\begin{cases} A(f,\chi)_\perp + ((1-\mu^2) f_\mu, \chi_\mu)_\perp + (\varepsilon f_E, \chi_E)_\perp = 0, \quad \forall \chi \in H^1_\beta(I_\perp), \\ f(0, x_\perp) = \tilde{g}(x_\perp) := \tilde{\delta}(x_\perp), \end{cases} \tag{4.4}$$

where $\tilde{g}(x_\perp) := \tilde{\delta}(x_\perp) \approx \delta(1-\mu)\delta(E-E_0)$ is a smooth approximation for the product of the above two Dirac δ functions. Let now $\tilde{f} \in V_{h,\beta}$ be an auxiliary interpolant of the solution u of (3.5) defined by

$$A(f - \tilde{f}, \chi) = 0, \quad \forall \chi \in V_{h,\beta}. \tag{4.5}$$

Our objective is to solve the following discrete variational problem: find $f_h \in V_{h,\beta}$, such that

$$\begin{cases} A(f_h,\chi)_\perp + ((1-\mu^2) f_{h,\mu}, \chi_\mu)_\perp + (\varepsilon f_{h,E}, \chi_E)_\perp = 0, \quad \forall \chi \in V_{h,\beta}, \\ f_h(0, x_\perp) = \tilde{\delta}_h(x_\perp). \end{cases} \tag{4.6}$$

where $\tilde{\delta}_h$ is assumed to be a finite element approximation of $\tilde{\delta}$ which coincides with the interpolant $\tilde{f}(0,x_\perp)$ of $f(0,x_\perp)$. Here, $(f,g)_\perp = \int_{I_\perp} f(x_\perp) g(x_\perp)\, dx_\perp$ and $\|f\|_{L_2(I_\perp)} = (f,f)_\perp^{1/2}$. To distinguish, we use the following inner products notations: $(\cdot,\cdot)_\perp$ and $(\cdot,\cdot)_\Omega$, where $\Omega = [0,L] \times I_\perp := I_x \times I_\perp$, for integrations over $I_\perp$ and $I_x \times I_\perp$, respectively. Finally, we assume that the mesh size h is related to ε according to:

$$h^2 \le \varepsilon \le h.$$

4.1. **Stability.** In this part we prove a stability lemma in both inner products, $(\cdot,\cdot)_\perp$ and $(\cdot,\cdot)_\Omega$, to guarantee the control of both continuous and discrete solutions by the data. For simplicity we introduce the triple norm,

$$|||w|||^2_{\tilde\beta} = \frac{1}{2}\int_{\Gamma^+_{\tilde\beta}} w^2(\mathbf{n}\cdot\tilde\beta)\, d\Gamma + \|\sqrt{\sigma(E)}w\|^2_{L_2(\Omega)} + \|\sqrt{1-\mu^2}w_\mu\|^2_{L_2(\Omega)} + \|\sqrt{\varepsilon}w_E\|^2_{L_2(\Omega)},$$

where $\tilde\beta = (\mu,\beta)$ and $\Gamma^+_{\tilde\beta} := \Gamma\setminus\Gamma^-_{\tilde\beta} = [0,L]\times\Gamma^+_{\beta}\cup\{\{L\}\times I_\perp\}$. Or, alternatively,

$$|||w|||^2_{\tilde\beta} = \frac{1}{2}\int_{\Gamma^+_{\tilde\beta}} w^2(\mathbf{n}\cdot\tilde\beta)\, d\Gamma + \|w\|^2_{L_2(\Omega,\,\sigma_a(E))} + \|w_\mu\|^2_{L_2(\Omega,\,1-\mu^2)} + \|w_E\|^2_{L_2(\Omega,\,\varepsilon)},$$

where $\|\cdot\|_{L_2(D,\,\omega)} := \Big(\int_D \omega|\cdot|^2\Big)^{1/2}$, is the ω-weighted L_2-norm over D.

Lemma 4.1. *For f satisfying* (3.7) *we have that,*

$$\sup_{x\in I_x}\|\sqrt{\mu}f(x,\cdot)\|^2_{L_2(I_\perp)} \le \int_{\Gamma^-_\beta} f^2\,|\mathbf{n}\cdot\beta|\; d\Gamma, \tag{4.7}$$

$$|||f|||^2_{\tilde\beta} = \frac{1}{2}\int_{\Gamma^-_{\tilde\beta}} f^2\,\Big|\mathbf{n}\cdot\tilde\beta\Big|\; d\Gamma. \tag{4.8}$$

Proof. We let $\chi = f$, in the first equation, in the first equation in (4.4). Using (4.3) and partial integration, in the f_E term we, compute

$$\begin{aligned}&\Big\|\sqrt{\sigma_a(E)}f\Big\|^2_{L_2(I_\perp)} + \frac{1}{2}\frac{d}{dx}\|\sqrt{\mu}f\|^2_{L_2(I_\perp)} - \frac{1}{2}\int_0^1 f^2(x,\mu,E_0)\,d\mu\\ &+\frac{1}{2}\int_0^1 f^2(x,\mu,0)\,d\mu + \Big\|\sqrt{1-\mu^2}f_\mu\Big\|^2_{L_2(I_\perp)} + \Big\|\varepsilon^{1/2}f_E\Big\|^2_{L_2(I_\perp)} = 0.\end{aligned} \tag{4.9}$$

Integrating over $x\in(0,\bar x)$, $\bar x\le L$ we get

$$\begin{aligned}&\|f\|^2_{L_2(\bar\Omega,\sigma_a(E))} + \frac{1}{2}\int_{I_\perp}\mu f^2(\bar x,\mu,E)\,dx_\perp - \frac{1}{2}\int_{I_\perp}\mu f^2(0,\mu,E)\,dx_\perp\\ &\quad -\frac{1}{2}\int_0^{\bar x}\int_0^1 f^2(x,\mu,E_0)\,d\mu\,dx + \frac{1}{2}\int_0^{\bar x}\int_0^1 f^2(x,\mu,0)\,d\mu\,dx\\ &\quad +\|f_\mu\|^2_{L_2(\bar\Omega,1-\mu^2)} + \|f_E\|^2_{L_2(\bar\Omega,\varepsilon)} = 0,\end{aligned} \tag{4.10}$$

where $\bar\Omega := (0,\bar x)\times I_\perp$. Consequently $\forall \bar x\le L$, we have that

$$\int_{I_\perp}\mu f^2(\bar x,\mu,E)\,dx_\perp \le \int_{I_\perp}\mu f^2(0,\mu,E)\,dx_\perp + \int_0^{\bar x}\int_0^1 f^2(x,\mu,E_0)\,d\mu\,dx,$$

which gives the first assertion of the lemma. Note that the two integrals with positive sign in (4.10) add up to $\frac12\int_{\Gamma^+_{\tilde\beta}} f^2(\mathbf{n}\cdot\tilde\beta)\;d\Gamma$, whereas those with negative sign add up to $-\frac12\int_{\Gamma^-_{\tilde\beta}} f^2|\mathbf{n}\cdot\tilde\beta|\;d\Gamma$. Transferring the negative integrals to the right hand side we obtain the second assertion of the lemma and the proof is complete. □

From the proof of above lemma we can deduce a control of a quantity involving a norm of the form

$$\|[w]\|^2_{L_2(\bar\Omega)} := \|f\|^2_{L_2(\bar\Omega,\sigma_a(E))} + \|f_\mu\|^2_{L_2(\bar\Omega,1-\mu^2)} + \|f_E\|^2_{L_2(\bar\Omega,\varepsilon)} + \sup_{x\in I_x}\|\sqrt{\mu}f(x,\cdot)\|^2_{L_2(I_\perp)}.$$

Corollary 4.2. *There, is constant C such that*

$$\|[w]\|^2_{L_2(\bar{\Omega})} + \int_{I_\perp} \mu f^2(\bar{x}, \mu, E)\, dx_\perp \le C \int_{\Gamma^-_\beta} f^2\, |\mathbf{n}\cdot\beta|\ d\Gamma. \tag{4.11}$$

The interesting feature in the relation (4.11) is that, roughly speaking, it controls a quantity corresponding to the contribution of the $|||\cdot|||$-norm at each collision site $\bar{x} \in (0, L)$.

By the same argument as in the above Lemma we obtain the semidiscrete version of the stability estimate for SG problem:

Corollary 4.3. *The solution f_h of problem* (4.6) *satisfies the stability relations,*

$$\sup_{x\in I_x} \|\sqrt{\mu} f_h(x,\cdot)\|^2_{L_2(I_\perp)} \le \int_{\Gamma^-_\beta} f_h^2\, |\mathbf{n}\cdot\beta|\ d\Gamma, \tag{4.12}$$

$$|||f_h|||^2_{\tilde{\beta}} = \frac{1}{2}\int_{\Gamma^-_{\tilde{\beta}}} f_h^2 \left|\mathbf{n}\cdot\tilde{\beta}\right|\ d\Gamma. \tag{4.13}$$

For convenience, in the sequel we shall use the following boundary integral notation:

$$(p,q)_{\alpha^{+(-)}} = \int_{\Gamma^{+(-)}_\alpha} pq(\mathbf{n}\cdot\alpha)d\Gamma, \quad |p|^2_{\alpha^{+(-)}} = \int_{\Gamma^{+(-)}_\alpha} p^2|\mathbf{n}\cdot\alpha|d\Gamma, \tag{4.14}$$

where $\alpha = \beta$ or $\alpha = \tilde{\beta}$ (then $\mathbf{n} := \tilde{\mathbf{n}}$), will be obvious from the content.

4.2. **Convergence.** In this part we state and prove convergence rates, both in the L_2-norm and in the triple norm, for the SG-method for the semidiscrete problem with weakly imposed boundary conditions. Our main results are Lemma 4.4 and Theorem 4.6 below. For the hyperbolic problems with an absorption term of $\mathcal{O}(1)$, and $f \in H^r(\Omega)$, the optimal convergence rate for the standard Galerkin in the L_2 norm is $\mathcal{O}(h^{r-1})$. Our equation, although degenerate, is not purely hyperbolic: the diffusive terms in (μ, E) on the right hand side corresponds to add of artificial viscosity, of order $\mathcal{O}(\varepsilon)$, $\varepsilon \sim (1-\mu)$, in the (μ, E) variables. This improves the triple norm estimate by $\mathcal{O}(\sqrt{\varepsilon}) \sim \mathcal{O}(\sqrt{h})$. However, turning to the L_2 norm estimate because of the lack of full convection (no first order derivatives in μ) we shall need some further corrections, that may cause for a somewhat weaker convergence rate.

Lemma 4.4 (error estimate in the triple norm). *Assume that f and f_h satisfy* (4.4) *and* (4.6)*, respectively. Let $f \in H^r(\Omega)$, $r \ge 2$ (motivated by the estimates in the next theorem), then there is a constant C such that,*

$$|||f_h - f|||_{\tilde{\beta}} \le C h^{r-1/2}\, \|f\|_r\, . \tag{4.15}$$

Proof. Subtracting first equations in (4.4) and (4.6) we get, using (4.3), and

$$G(f,\chi)_\perp := ((1-\mu^2)f_\mu, \chi_\mu)_\perp + (\varepsilon f_E, \chi_E)_\perp$$

that

$$A(f_h - \tilde{f}, \chi)_\perp + G(f_h - \tilde{f}, \chi)_\perp = A(f - \tilde{f}, \chi)_\perp + G(f - \tilde{f}, \chi)_\perp = G(f - \tilde{f}, \chi)_\perp,$$

or equivalently, we get

$$\begin{aligned}
&(\sigma_a(E)(f_h-\tilde f),\chi)_\perp+(\mu(f_h-\tilde f)_x,\chi)_\perp-((f_h-\tilde f)_E,\chi)_\perp\\
&\qquad((1-\mu^2)(f_h-\tilde f)_\mu,\chi_\mu)_\perp+(\varepsilon(f_h-\tilde f)_E,\chi_E)_\perp\\
&\quad=(\sigma_a(E)(f,\chi))_\perp(\mu f_x,\chi)_\perp-(f_E,\chi)_\perp\\
&\qquad((1-\mu^2)(f_\mu,\chi_\mu)_\perp+(\varepsilon f_E,\chi_E)_\perp\\
&\qquad+((1-\mu^2)(f-\tilde f))_\mu,\chi_\mu)_\perp+(\varepsilon(f-\tilde f)_E,\chi_E)_\perp\\
&\quad=0-((1-\mu^2)(f-\tilde f)_\mu,\chi_\mu)_\perp+(\varepsilon(f-\tilde f)_E,\chi_E)_\perp.
\end{aligned}$$

Let now $\chi=f_h-\tilde f$, then using the same argument as in the stability estimate we may write,

$$\begin{aligned}
&\left\|f_h-\tilde f\right\|^2_{L_2(I_\perp,\sigma_a(E))}+\frac12\frac{d}{dx}\left\|f_h-\tilde f\right\|^2_{L_2(I_\perp,\mu)}\\
&-\frac12\int_{\Gamma^-_\beta}|\mathbf n\cdot\beta|(f_h-\tilde f)^2(x,\mu,E_0)\,d\Gamma+\frac12\int_{\Gamma^+_\beta}(\mathbf n\cdot\beta)(f_h-\tilde f)^2(x,\mu,0)\,d\Gamma\\
&+\left\|(f_h-\tilde f)_\mu\right\|^2_{L_2(I_\perp,1-\mu^2)}+\left\|(f_h-\tilde f)_E\right\|^2_{L_2(I_\perp,\varepsilon)}\\
&\le\frac12\left\|(f_h-\tilde f)_\mu\right\|^2_{L_2(I_\perp,1-\mu^2)}+\frac12\left\|(f-\tilde f)_\mu\right\|^2_{L_2(I_\perp,1-\mu^2)}\\
&+\frac12\left\|(f_h-\tilde f)_E\right\|^2_{L_2(I_\perp,\varepsilon)}+\frac12\left\|(f-\tilde f)_E\right\|^2_{L_2(I_\perp,\varepsilon)}.
\end{aligned}$$

or equivalently,

$$\begin{aligned}
&\left\|f_h-\tilde f\right\|^2_{L_2(I_\perp,2\sigma_a(E))}+\frac{d}{dx}\left\|f_h-\tilde f\right\|^2_{L_2(I_\perp,\mu)}-\left|f_h-\tilde f\right|^2_{\Gamma^-_\beta}+\left|f_h-\tilde f\right|^2_{\Gamma^+_\beta}\\
&+\left\|(f_h-\tilde f)_\mu\right\|^2_{L_2(I_\perp,1-\mu^2)}+\left\|(f_h-\tilde f)_E\right\|^2_{L_2(I_\perp,\varepsilon)}\\
&\le\left\|(f-\tilde f)_\mu\right\|^2_{L_2(I_\perp,1-\mu^2)}+\left\|(f-\tilde f)_E\right\|^2_{L_2(I_\perp,\varepsilon)}.
\end{aligned}$$

Now integrating over $x\in[0,L]$, implies that

$$\begin{aligned}
&\left\|f_h-\tilde f\right\|^2_{L_2(\Omega,2\sigma_a(E))}+\left\|(f_h-\tilde f)(L,\cdot)\right\|^2_{L_2(I_\perp,\mu)}-\left\|(f_h-\tilde f)(0,\cdot)\right\|^2_{L_2(I_\perp,\mu)}\\
&-\left|f_h-\tilde f\right|^2_{\Gamma^-_{\tilde\beta}\setminus\Gamma_0}+\left|f_h-\tilde f\right|^2_{\Gamma^+_{\tilde\beta}\setminus\Gamma_L}+\left\|(f_h-\tilde f)_\mu\right\|^2_{L_2(\Omega,1-\mu^2)}+\left\|(f_h-\tilde f)_E\right\|^2_{L_2(\Omega,\varepsilon)}\\
&\le\left\|(f-\tilde f)_\mu\right\|^2_{L_2(\Omega,1-\mu^2)}+\left\|(f-\tilde f)_E\right\|^2_{L_2(\Omega,\varepsilon)}.
\end{aligned}$$

where $\Gamma_p=\{\{p\}\times I_\perp\}$, $p=0$ or $p=L$. Thus recalling $f_h(0,\cdot)=\tilde f(0,\cdot)=g_h(\cdot)$, and the definition of the $|||\cdot|||_{\tilde\beta}$ norm we have

$$|||f_h-\tilde f|||^2_{\tilde\beta}\le\left\|\sqrt{1-\mu^2}(f-\tilde f)_\mu\right\|^2_{L_2(\Omega)}+\left\|\varepsilon^{1/2}(f-\tilde f)_E\right\|^2_{L_2(\Omega)}. \tag{4.16}$$

Now the desired result follows from the following interpolation estimate: □

Proposition 4.5. *Let $h^2 \le \sigma_a(E) \sim \varepsilon(x,\mu) \sim (1-\mu^2) \le h$, then there is a constant $\tilde{C}$ such that,*

$$|||f-\tilde{f}|||_{\tilde{\beta}} \le \tilde{C} h^{r-1/2} \|f\|_r . \tag{4.17}$$

Proof. The proof is based on classical interpolation error estimates, see [10]: Let $f \in H^r(\Omega)$, then there exists an interpolant $\tilde{f} \in V_{h,\beta}$, of f and interpolation constants C_1 and C_2 such that

$$\|f-\tilde{f}\|_s \le \quad C_1 h^{r-s}\|f\|_r, \qquad s=0,1 \tag{4.18}$$

$$|f-\tilde{f}|_{\tilde{\beta}} \le \quad C_2 h^{r-1/2}\|f\|_r, \tag{4.19}$$

where

$$|w|_{\tilde{\beta}} = \left(\int_{\Gamma^+_{\tilde{\beta}}} w^2(\tilde{\mathbf{n}}\cdot\tilde{\beta})\, d\Gamma\right)^{1/2}. \tag{4.20}$$

Now recalling the definition of $|||\cdot|||_{\tilde{\beta}}$ we have,

$$\begin{aligned}
|||f-\tilde{f}|||^2_{\tilde{\beta}} &= \frac{1}{2}|f-\tilde{f}|^2_{\tilde{\beta}} + \left\|\sqrt{\sigma_a(E)}(f-\tilde{f})\right\|^2_{L_2(\Omega)} \\
&+ \left\|\sqrt{1-\mu^2}(f-\tilde{f})_\mu\right\|^2_{L_2(\Omega)} + \left\|\sqrt{\varepsilon}(f-\tilde{f})_E\right\|^2_{L_2(\Omega)} \\
&\le \frac{1}{2}|f-\tilde{f}|^2_{\tilde{\beta}} + \|\sigma_a(E)^{1/2}\|^2_{L_\infty(\Omega)} \left\|f-\tilde{f}\right\|_{L_2(\Omega)} \\
&+ \|(1-\mu^2)^{1/2}\|^2_{L_\infty(\Omega)} \left\|(f-\tilde{f})_\mu\right\|^2_{L_2(\Omega)} + \|\varepsilon^{1/2}\|^2_{L_\infty(\Omega)} \left\|(f-\tilde{f})_E\right\|^2_{L_2(\Omega)} \\
&\le \frac{1}{2}|f-\tilde{f}|^2_{\tilde{\beta}} + \left(\sup_{I_E}\sigma_a + 2\sup_{I_x\times I_\mu}\varepsilon\right)\|f-\tilde{f}\|^2_{H^1(\Omega)} \\
&\le \frac{1}{2}C_2^2 h^{2r-1}\|u\|^2_r + C_1^2\tilde{\varepsilon}h^{2r-2}\|u\|^2_r \le Ch^{2r-1}\|u\|^2_r,
\end{aligned}$$

where in the last step we used $\tilde{\varepsilon} := \sup_{I_E}\sigma_a + 2\sup\varepsilon \le 3h$ and $C = \max(3C_1^2, C_2^2/2)$. Letting now $\tilde{C} = C^{1/2}$ the proof is complete. □

From this result we now obtain the desired estimate in the L_2 norm:

Theorem 4.6. *For $f \in H^r(\Omega)$, satisfying (4.4) and with f_h being the solution of (4.6), there is a constant $C = C(\Omega, g)$ such that*

$$\|f-f_h\|_{L_2(\Omega)} \le Ch^{r-3/2}\|f\|_r. \tag{4.21}$$

Proof. Recalling the definition of the triple norm we have that

$$\left\|\sqrt{\sigma_a(E)}(f-f_h)\right\|_{L_2(\Omega)} \le |||f-\tilde{f}|||_{\tilde{\beta}} \le Ch^{r-1/2}\|f\|_r. \tag{4.22}$$

Thus, since $\sigma_a(E) \ge h^2$, we obtain (4.21). □

Observe that in $C = C(\Omega, g)$, the Ω dependence is because of the E depending $\sigma_a(E)$ and the fact that $\varepsilon = \varepsilon(x,\mu)$, while the g dependence comes from the assumed identity $u_h(0) := \tilde{u}(0) = g$.

5. The Fully Discrete Problem

In this section, we derive the algorithms corresponding to the SG for $I_\perp$ combined with discontinuous Galerkin (DG), backward-Euler (BE) and Crank-Nicholson (CN) methods for the penetration interval I_x. So far our approximation techniques were designed for discretizations in the transversal variable $x_\perp = (\mu, E)$. We could include the penetration variable x, in this procedure as an additional space variable, as it is, see the analysis in [7], where full discretizations are made in all three variables using both the usual streamline diffusion and the discontinuous Galerkin methods. This however, due to the lack of a diffusion term in x, would yield a degenerate type PDE requiring more involved technicalities. Such studies are inevitable for the pencil beam problems where, in spite of interpreting x as a time variable, the degeneracy nature remains in the differential operators over $x_\perp$ domain. See, e.g. [5]-[7]. Therefore, here in order to efficiently determine the beam intensity at different transversal cross sections, discretization procedures for the penetration variable x is treated separately and as a time variable, as in the similar time dependent convection-diffusion problems. Thus, in extending our semidiscrete algorithms to a higher dimensional case containing also discretizations in x, we consider the time discretization schemes for I_x, such as DG, BE and CN.

To continue, we introduce the bilinear forms:

$$a(f,\chi) := (\sigma_a(E)f,\chi)_\perp + ((1-\mu^2)f_\mu,\chi_\mu)_\perp + (\varepsilon f_E,\chi_E)_\perp + \frac{1}{2}\int_{\Gamma_\beta^+}(\mathbf{n}\cdot\beta)f\chi\,d\Gamma, \tag{5.1}$$

and

$$b(f,\chi) := \delta(\mu f,\chi)_\perp + \frac{1}{2}\int_{\Gamma_\beta^-}(\mathbf{n}\cdot\beta)g\chi\,d\Gamma, \tag{5.2}$$

and rewrite the problem (4.4) as finding a solution $f \in H_\beta^1(I_\perp)$ such that,

$$b(f_x,\chi) + a(f,\chi) = 0, \quad \forall \chi \in H_\beta^1(I_\perp). \tag{5.3}$$

We subsequently use the finite dimensional subspace $V_{h,\beta} \subset H_\beta^1(I_\perp)$ and represent the discrete solution f_h by a separation of variables viz:

$$f_h(x,y,z) = \sum_{j=1}^{M} \xi_j(x)\phi_j(\mu,E), \tag{5.4}$$

where $M \sim 1/h$. Now we let $v = \phi_i$ for $i = 1,\dots,M$, and insert (5.4) into the semidiscrete counterpart of (5.3) to obtain,

$$\sum_{j=1}^{M} \xi_j^{'}(x) b(\phi_i,\phi_j) + \sum_{j=1}^{M} \xi_j(x) a(\phi_i,\phi_j) = 0, \qquad i = 1,\dots,M. \tag{5.5}$$

In the matrix form (5.5) may be represented by $B\xi^{'}(x) + \mathcal{A}\xi(x) = 0$, where $B = (b_{ij})$ with $b_{ij} = b(\phi_i,\phi_j)$ and $\mathcal{A} = (a_{ij})$ with $a_{ij} = a(\phi_i,\phi_j)$. More specifically the matrix $\mathcal{A}$ is given by

$$\mathcal{A} := M_{\sigma_a(E)} + S^\mu_{1-\mu^2} + S^E_\varepsilon, \tag{5.6}$$

where $M_{\sigma_a(E)}$ is the $\sigma_a(E)$-weighted mass matrix, $S^\mu_{1-\mu^2}$ is the $(1-\mu^2)$-weighted stiffness matrix in μ and S^E_ε is the ε-weighted stiffness matrix in E. One can show that the matrix B is positive definite and therefore invertible. Hence we can reformulate (5.5) as,

$$\xi'(x) + \bar{\mathcal{A}}\xi(x) = 0, \tag{5.7}$$

where $\bar{\mathcal{A}} = B^{-1}\mathcal{A}$. However inverting B is among other things expensive. Therefore we instead consider a Choleski decomposition of $B = \Lambda^T\Lambda$, which leads to

$$\eta'(x) + \tilde{\mathcal{A}}\eta(x) = 0, \qquad \eta(0) = \eta_0, \tag{5.8}$$

where now $\tilde{\mathcal{A}} = (\Lambda^{-1})^T\mathcal{A}\Lambda^{-1}$ and $\eta = \Lambda\xi$. The (stiff) solution of (5.8) is:

$$\eta(x) = \eta_0 \exp(-\tilde{\mathcal{A}}x). \tag{5.9}$$

The matrix equations presented in this section can now be easily implemented for usual finite element test functions. Now a fully discrete scheme is obtained by also discretizing (5.7) in the x variable. Below we combine both SG and semi-streamline diffusion (SSD) schemes [4], for discretization in $x_\perp$, with the most common time discretization techniques applied to our x variable. To achieve the most general schemes for the x discretization we extract them from Pade approximations of the form, $F^{n+1} = E_{\mu\nu}F^n$ for $n \geq 0$, where $E_{\mu\nu} = r_{\mu\nu}(\tilde{G})$. Here, $r_{\mu\nu}(x) = \frac{\eta_{\mu\nu}(x)}{d_{\mu\nu}(x)}$ with,

$$\eta_{\mu\nu}(x) = \sum_{j=0}^{\nu} \frac{(\mu+\nu-j)!\nu!}{(\mu+\nu)!j!(\nu-j)!}(-x)^j, \tag{5.10}$$

$$d_{\mu\nu}(x) = \sum_{j=0}^{\mu} \frac{(\mu+\nu-j)!\mu!}{(\mu+\nu)!j!(\mu-j)!}x^j. \tag{5.11}$$

For instance $r_{01}(x) = 1 - x$ corresponds to forward Euler, $r_{10}(x) = 1/(1+x)$ to backward Euler and r_{11} to Crank-Nicholson scheme:

$$\left(\frac{F_h^n - F_h^{n-1}}{k_n}\right) + \bar{A}F_h^n = 0, \quad \text{backward Euler}, \tag{5.12}$$

$$\left(\frac{F_h^n - F_h^{n-1}}{k_n}\right) + \bar{A}\left(\frac{F_h^n + F_h^{n-1}}{2}\right) = 0, \quad \text{Crank Nicholson}. \tag{5.13}$$

Other such choices will easily provide comparisons for alternative methods.

6. Streamline diffusion method

Due to the fact that $\tilde{\varepsilon}/|\beta| = \max(1-\mu^2, \varepsilon)$ is very small; both broad beam as well as Fermi and Fokker-Planck equations are convection dominated convection-diffusion equations. To obtain approximate solutions for these types of equations, we may use a certain type of the Galerkin method: the streamline diffusion finite element method. Because of a lack of stability of the standard Galerkin finite element method (SGM) , the Galerkin approximation contain oscillations not present in the true solution in convection dominated problems. So we need to improve the stability properties of the SGM without sacrificing accuracy. We consider two ways of enhancing the stability of SGM. (a) introduction of weighted least squares terms; (b) introduction of artificial viscosity based on the residual. We refer to the Galerkin finite element method with these modifications as the streamline diffusion method (Sd). Both modifications enhance stability without a strong effect on the accuracy. We begin by describing the Sd-method for an abstract linear problem

$$\mathcal{L}f = g, \tag{6.1}$$

for which SGM reads: find $F \in V_h$ such that

$$(\mathcal{L}F, \varphi) = (g, \varphi), \qquad \forall \varphi \in V_h, \tag{6.2}$$

where $\mathcal{L}$ is a linear operator on a vector space V and V_h is a finite dimensional subspace of V. In our problem, $\mathcal{L}$ is a convection-diffusion absorption operator:

$$\mathcal{L}w := \sigma_a w + \partial_x w + \beta \cdot \nabla_\perp w. \tag{6.3}$$

The least squares method for (6.1) is to find $F \in V_h$ that minimizes the residual over V_h in an appropriate norm, that is

$$||\mathcal{L}F - g||^2 = min_{\varphi \in V_h} ||\mathcal{L}\varphi - g||^2. \tag{6.4}$$

where $||\cdot||$ denotes, e.g. the usual L_2 norm.

This is a convex minimization problem and the solution F is characterized by

$$(\mathcal{L}F, \mathcal{L}\varphi) = (g, \mathcal{L}\varphi), \qquad \forall \varphi \in V_h. \tag{6.5}$$

We now formulate a Galerkin/least squares finite element method for (6.2) by taking a weighted combination of (6.4) and (6.5): compute $F \in V_h$ such that

$$(\mathcal{L}F, \varphi) + (\delta \mathcal{L}F, \mathcal{L}\varphi) = (g, \varphi) + (\delta g, \mathcal{L}\varphi), \qquad \forall \varphi \in V_h, \tag{6.6}$$

where δ is a parameter to be chosen. We may rewrite the relation (6.6) as

$$(\mathcal{L}F, \varphi + \delta \mathcal{L}\varphi) = (f, \varphi + \delta \mathcal{L}\varphi), \qquad \forall \varphi \in V_h. \tag{6.7}$$

Adding the artificial viscosity modification yields the Sd-method in abstract form: find $F \in V_h$ such that

$$(\mathcal{L}F, \varphi + \delta \mathcal{L}\varphi) + (\varepsilon \nabla F, \nabla \varphi) = (f, \varphi + \delta \mathcal{L}\varphi), \qquad \forall \varphi \in V_h, \tag{6.8}$$

where ε is the artificial viscosity defined in terms of the residual $R(F) = \mathcal{L}F - g$.

Now we return to our broad beam equation (3.7) and perform the differentiation with respect to μ to obtain

$$\sigma_a(E) f + \mu f_x + 2\mu f_\mu - f_E = (1-\mu^2) f_{\mu\mu} + \varepsilon f_{EE} + Q, \quad (x, \mu, E) \in I_x \times I_\perp, \tag{6.9}$$

which is of degenerate form, where the convection is on the direction of $\beta_c := (\mu, 2\mu, -1)$ while the diffusion is in $x_\perp$. Now, since the beam is forward directed hence $\mu \neq 0$ ($\mu = \cos\theta \approx 1$), therefore we may divide by μ to obtain

$$f_x + \tilde{\sigma} f + \tilde{\beta} \cdot \nabla_\perp f - \tilde{\varepsilon} \Delta_\perp f = Q, \tag{6.10}$$

where $\tilde{\sigma} = \tilde{\sigma}(\mu, E) := \sigma_a(E)/\mu$, $\tilde{\beta} := (2, -1/\mu)$ and, assuming $\varepsilon \approx 1 - \mu^2$, $\tilde{\varepsilon} = \varepsilon/\mu$. The equation (6.10) has a *user friendly form* in the sense that: interpreting $x > 0$ as a time variable both convection and diffusion are then in $x_\perp = (\mu, E)$ and hence we have a, non-degenerate, "time dependent", convection dominated ($\tilde{\varepsilon} << |\tilde{\beta}|$), convection-diffusion equation. A study of this type of time dependent convection-diffusion problems is outlined in [11]. A desirable closing for equation (6.10) would be stating the problem in unbounded domain associated with a compact support as a boundary data, viz

$$\begin{cases} f_x + \tilde{\sigma} f + \tilde{\beta} \cdot \nabla_\perp f - \tilde{\varepsilon} \Delta_\perp f = Q, & \text{in } \mathbb{R}^2 \times (0, \infty), \\ f(x, x_\perp) \to 0, & \text{for } x > 0 \text{ as } |x_\perp| \to \infty, \\ f(0, \cdot) = f_0, & \text{in } \mathbb{R}^2. \end{cases} \tag{6.11}$$

As a matter of fact, this is the most natural initial-boundary value problem for a forward directed charged particle beam, simply because there are no particles with infinite energy range as $|x_\perp|^2 = \mu^2 + E^2 \to \infty$. However, in the radio therapy applications, the physical medium is bounded and therefore we state an initial-boundary value problem in a bounded domain:

$$\text{(6.12)} \qquad \begin{cases} f_x + \tilde{\sigma} f + \tilde{\beta} \cdot \nabla_\perp f - \tilde{\varepsilon} \Delta_\perp f = Q, & \text{in } I \times I_\perp, \\ f(x, x_\perp) = g_-, & \text{on } (I \times \partial I_\perp)_-, \\ f(x, x_\perp) = g_+, \text{ or } \tilde{\varepsilon} \partial_n f = g_+ & \text{on } (I \times \partial I_\perp)_+, \\ f(0, \cdot) = f_0, & \text{in } I \times I_\perp, \end{cases}$$

where we recall that $I \times I_\perp := (0, L) \times (-1, 1) \times (0, E_0)$ and

$$\text{(6.13)} \qquad (I \times \partial I_\perp)_{-(+)} := \{(x, x_\perp) \in I \times \partial I_\perp : \tilde{\beta}(x, x_\perp) \cdot \mathbf{n}(x_\perp) < 0 (\geq 0)\}.$$

On each collision site the particle changes (decrease) its "speed"($|\mu|$) and energy. We assume $x_i, i = 1, \dots N$ to be the collision sites and let a partitioning of I into subintervals $I_n = (x_{n-1}, x_n)$, $n = 1, 2, \dots, N$. We use the space "time" slabs $S_n = I_n \times I_\perp$. We divide each slab into prisms $I_n \times K$, where $\mathcal{T}_n = \{K\}$ is a triangulation of $I_\perp$ with mesh function h_n. Now streamline diffusion method is a finite element method based on using approximations consisting of continuous piecewise linear functions in $x_\perp$ and discontinuous polynomials of degree r in x: This is denoted, in short, by $cG(1)dG(r)$ method. We define the trial space W_k^r to be the set of functions $w(x, x_\perp)$ defined on $I_x \times I_\perp$ such that the restriction $w|_{S_n}$ is continuous and piecewise linear in $x_\perp$ and a polynomial of degree r in x. Thus, on each slab S_n, we seek the approximate solution for the equation (6.12), in the streamline diffusion space $w|_{S_n} \in W_{kn}^r$:

$$\text{(6.14)} \qquad W_{kn}^r := \{w : w(x, x_\perp) = \sum_{j=0}^{r} x^j w_j(x_\perp), \; w_j \in V_n, \; (x, x_\perp) \in S_n\},$$

where $V_n = V_{h_n}$ is the space of continuous piecewise linear functions vanishing on $\partial I_\perp$. We denote by $\hbar$ and h the mesh parameters in I_x and $I_\perp$, respectively and use the usual notation

$$\text{(6.15)} \qquad [w_n] = w_n^+ - w_n^-, \qquad w_n^{+(-)} = \lim_{s \to 0^{+(-)}} w(x_n + s).$$

In this setting, the method reads as: Compute $F \in W_k^r$ such that for $n = 1, 2, \dots, N$ and for $w \in W_{kn}^r$,

$$\text{(6.16)} \qquad \begin{aligned} \int_{I_n} \Big(\mathcal{B}(F), w + \delta \mathcal{B}(w)\Big)\, dx + \int_{I_n} (\hat{\varepsilon} \nabla_\perp F, \nabla_\perp w)\, dx + \Big([F_{n-1}], v_{n-1}^+\Big) \\ = \int_{I_n} \Big(Q, w + \delta \mathcal{B}(w)\Big)\, dx, \end{aligned}$$

where

$$\text{(6.17)} \qquad \mathcal{B}(g) = \tilde{\sigma} g + g_x + \tilde{\beta} \cdot \nabla_\perp w,$$

$$\text{(6.18)} \qquad \delta = \frac{1}{2}\Big(\hbar_n^{-2} + h_n^{-2} |\beta|^2\Big)^{-1/2},$$

$$\text{(6.19)} \qquad \hat{\varepsilon} = \max\{\tilde{\varepsilon}, \alpha_1 h^2 \mathcal{R}(F), \alpha_2 h^{3/2}\},$$

$$\text{(6.20)} \qquad \mathcal{R}(F) = |\mathcal{B}(F) - Q| + |[F_{n-1}]| / \hbar_n, \qquad \text{on } S_n,$$

for positive constants α_i, $i = 1, 2$.

The error estimate procedure is simplified using the transformation between Euler and Lagrange coordinates (see [11]) by letting $(x, x_\perp) = (\bar{x}, \bar{x}_\perp + \bar{x}\tilde{\beta})$. Then we have for $\bar{f}(\bar{x}, \bar{x}_\perp) = f(x, x_\perp)$, by the chain rule, that

$$\frac{\partial \bar{f}}{\partial \bar{x}} = \frac{\partial}{\partial \bar{x}} f(\bar{x}, \bar{x}_\perp + \bar{x}\tilde{\beta}) = \frac{\partial f}{\partial x} + \tilde{\beta}\nabla_\perp f. \tag{6.21}$$

Below we summarize a priori and a posteriori error estimates for the $cG(1)dG(0)$ scheme, described in (6.16), derived for the local Lagrangian coordinates $(\bar{x}, \bar{x}_\perp)$.

Theorem 6.1. *If $\nu\hbar_n\tilde{\varepsilon} \geq h_n^2$, for sufficiently small ν and $\hat{\varepsilon} = \tilde{\varepsilon}$, then for each $M, 1 \leq M \leq N$,*

$$\|\bar{f}(x_M, \cdot) - \bar{F}_M\| \leq L_M C_i \max_{1\leq n\leq M}\Big(\hbar\Big\|\frac{\partial \bar{f}}{\partial \bar{x}}\Big\|_{I_n} + \|h_n^2 D^2 \bar{u}\|_{I_n}\Big),$$

and

$$\|\bar{f}(x_M, \cdot) - \bar{F}_M\| \leq L_M C_i \max_{1\leq n\leq M}\Big(\|\hbar\mathcal{R}_{0\hbar}(\bar{F})\|_{I_n} + \Big\|\frac{h_n^2}{\varepsilon\hbar_n}[\bar{F}_{n-1}]\Big\|^\star + \|h_n^2\mathcal{R}(\bar{F})\|_{I_n}\Big),$$

where

$$L_M = \Big(\max((\log(x_M/\hbar_M))^{1/2}, \log(x_M/\hbar_M)\Big) + 2, \tag{6.22}$$

$$\mathcal{R}_{0\hbar}(\bar{F}) = |Q| + \big|[\bar{F}]\big|/\hbar, \tag{6.23}$$

$$\mathcal{R}(\bar{F}) = \frac{1}{\varepsilon}|Q| + \frac{\tilde{\varepsilon}}{2}\max_{S\subset\partial K} h_K^{-1}\,|[\partial_S F]|\,, \qquad on\ K \in \mathcal{T}_h, \tag{6.24}$$

where $[\partial_S w]$ denotes the jump across the side $S \subset \partial K$ in the normal derivative of the function $w \in V_h$ (see Fig.2. below). Finally, the star indicates that the corresponding term is present only if V_{n-1} is not a subset of V_n.

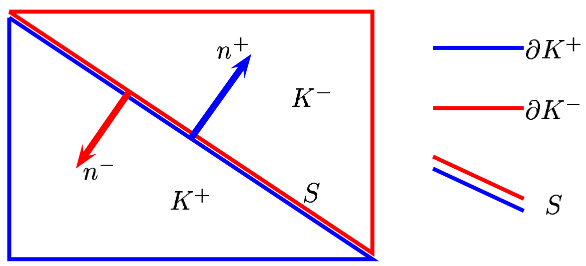

Figure 2: Two neighboring elements K^+ and K^-, their boundaries ∂K^+ and ∂K^-, and their interior side S.

The convergence rates in this theorem hold in the Euler coordinates $(x, x_\perp)$, provided that there exists an affine bijection $\mathcal{G}_n : S_n \to S_n$ defined by

$$(x, x_\perp) = \mathcal{G}_n(\bar{x}, \bar{x}_\perp) = (x_{\perp,n}(\bar{x}, \bar{x}_\perp), \bar{x}), \quad \text{for} \quad (\bar{x}, \bar{x}_\perp) \in S_n, \tag{6.25}$$

i.e., $\mathcal{G}_n : S_n \to S_n$ takes a non-oriented grid in $(\bar{x}, \bar{x}_\perp)$ to an oriented grid in $(x, x_\perp)$, as illustrated in Fig. 3. below. Let now

$$(x_{\perp,n}(\bar{x}, \bar{x}_\perp), \bar{x}) = \bar{x}_\perp + (\bar{x} - x_{n-1})\tilde{\beta}_n^h(x_\perp), \qquad \bar{x} \in I_n, \tag{6.26}$$

with $\tilde{\beta}_n^h \in V_n$ denoting the nodal interpolant of $\tilde{\beta}_n = \tilde{\beta}(x_{n-1}, \cdot)$. By the inverse mapping theorem, $\mathcal{G}_n : S_n \to S_n$ is invertible, if there is a sufficiently small constant c_0 such that

$$\max_{I_\perp} \left(\hbar_n \left| \bar{\nabla} \tilde{\beta}_n^h \right| \right) \le c_0, \tag{6.27}$$

where $\bar{\nabla}$ denotes the Jacobian with respect to $\bar{x}_\perp$:

$$\bar{\nabla} x_{\perp,n}(\bar{x}, \bar{x}_\perp) = \mathcal{I} + (\bar{x} - x_{n-1}) \bar{\nabla} \tilde{\beta}_n^h(\bar{x}_\perp), \tag{6.28}$$

where $\mathcal{I}$ is the identity operator. The proof of the above theorem is a lengthy

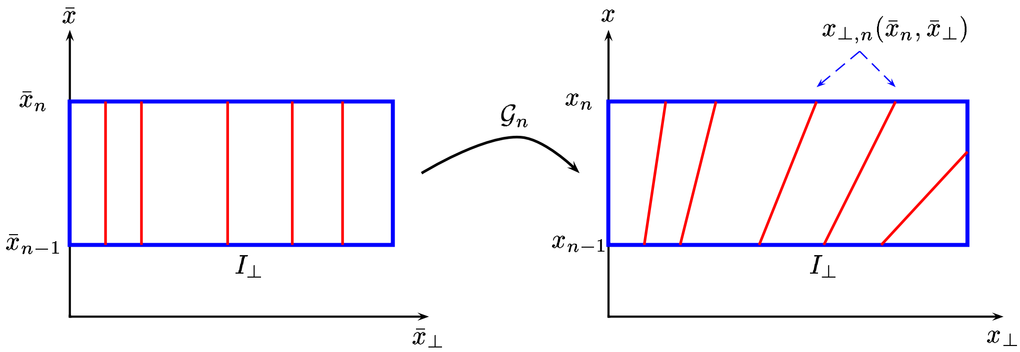

Figure 3: The map $\mathcal{G}_n$ between local Lagrangian and Euler coordinates

modification of the a priori and a posteriori error estimates for heat equation based on a dual problem approach derived in [11]. The reader can get an idea about how much involved are the actual error estimates in the Euler coordinates. We skip theses seemingly involved details and instead focus on some numerical results comparing the Sd, bipartition and Monte-Carlo methods.

So far, to keep the computational costs in a realistic level, our simulation results concern the energy ranges $\le 30 MeV$ (adequate for light ions and high-energy electron particles). These results are for broad beam configurations derived using bipartition model, see [28]. The final equation is identical to the broad beam equation, in here, resulting from a Fokker-Planck development based on asymptotic expansions. There are simulation results available for both bipartition model and MC method for high-energy ions (see Part I; [2] for energy ranges $\le 200 MeV$, and [13] for $\le 600 MeV$). We plan to perform Sd simulations in high energy cases and compare them with the bipartition and MC results. For the purpose of clinical applications, the accuracy of the simulations in a moderate energy range of, say, $\sim 50 - 100 MeV$ are more desirable than the simulations for very high energies.

7. Numerical simulations

We shall use the following Boundary conditions for the broad beam model: Given a function $g := g(\mu, E)$, we define the boundary conditions for the broad beam model as the following:

$$
(7.1)\qquad \begin{cases}
f(0,\mu,E) = g, & (\mu,E) \in [-1,1]\times[0,E_0] \qquad (BC1)\\
f(x_0,\mu,E) = 0, & (\mu,E) \in [-1,1]\times[0,E_0] \qquad (BC2)\\
\frac{\partial}{\partial\mu} f(x,1,E) = 0, & (x,E) \in (0,x_0)\times(0,E_0] \qquad (BC3)\\
f(x,-1,E) = 0, & (x,E) \in (0,x_0)\times(0,E_0] \qquad (BC4)\\
\frac{\partial}{\partial E} f(x,\mu,E_0) = 0, & (x,\mu) \in (0,x_0)\times(-1,1] \qquad (BC5)\\
f(x,\mu,0) = 0, & (x,\mu) \in (0,x_0)\times[-1,1] \qquad (BC6).
\end{cases}
$$

The function g is an smooth approximation of the original source function $Q = \frac{1}{2\pi}\delta(x)\delta(1-\mu)\delta(E_0 - E)$. We have considered the broad beam problem (6.10) associated with the boundary condition (7.1) and derived numerical algorithms for a Standard Galerkin the streamline diffusion finite element method (Sd), which coincides with a Characteristic Galerkin (CG)- and a Characteristic Streamline Diffusion (CSD)-method, studied for the Fermi equation in[4]. Here, we present only the results of the Sd method. For the sake of completeness we also comment the results of our observations testing other methods than the Sd: we have carried out implementations to illustrate the applicability of the algorithms using different types of initial data approximating the Dirac δ function. To begin with, semi-streamline diffusion (SSD) and characteristic streamline diffusion (CSD) methods are more stable and accurate than the standard Galerkin (SG) and characteristic Galerkin (CG) methods for all the canonical forms of the initial data (approximating a Dirac δ function beam source by a Maxwellian, cone, cylinder and a hyperbolic beam). As for the convergence: solutions with modified Dirac initial condition are suited in both CS and SSD. However, Maxwellian initial conditions produce accurate results in the CSD scheme, whereas the hyperbolic initial conditions produce more accurate results in the SSD scheme. The oscillatory behavior, while considering non smooth initial data, can be eliminated by modifying the L_2-projection. The formation of layers can be avoided taking small steps in the penetration variable. However, a better approach to deal with this phenomenon is through adaptive refinement.

7.1. **Results.** We use Sd-method to solve (6.10) with the boundary condition (7.1) and integrate $f(x,\mu,E)$ over μ and E to get the energy and angular distributions for different depths. We compare the results of dose delivery with the intensity of 10, 20, 30 MeV electron transport in water, with those of the bipartition model and Monte Carlo (MC) method . Here, we have neglected the contributions from the secondary particles. In Fig. 5, 8 and 11 we can see that our results are very close to MC, only the positions of the maximum values are different. The reason is that the stopping power that we have used is somewhat different from that of MC. We use the same stopping power with the bipartition model, so we could find that the positions of the maximum values are very close as seen in Fig. 4, 7 and 10. The bipartition model use CSDA and neglect the particles which have larger variations in energy and angle. In this way the energy distributions are very narrow and the maxima drop exponentially fast. Similar phenomena appears for the angular distributions in Fig. 6 and 9.

7.2. **Conclusion.** In this paper we start from a broad beam equation derived using a bipartition model for the linear (ion) transport equation for both low- and high-energy ions as well as high energy electrons in inhomogeneous media Our derivation is based on an split of the source term to diffusion and forward-directed particles combined with a Legendre series expansion approach.

This split may be used, as an alternative for asymptotic expansions, to derive P_1, Fokker-Planck and Fermi approximations of a pencil beam model associated with the bipartition model problem.

In this paper we have descritized the, Fokker-Planck type, broad beam equation by a variety of finite element approximations. We have derived stability and convergence estimates for a semi-discrete standard Galerkin method. We have also formulated both fully discrete and streamline diffusion Galerkin methods and give the sharp error bounds in local Lagrangian coordinates. Under certain assumption on the characteristics and by the inverse mapping theorem, these bounds are valid in a more concrete Euler coordinates as well.

In the implementation part, we use the streamline diffusion method to calculate the energy and angular distributions for the electron, and light ion, transport equation and compare the results with those obtained by bipartition model and Monte Carlo simulation. In our knowledge, this approach is not considered elsewhere. Our ambition is to solve 3D pencil beam and broad models and show the advantages of FEM in comparison with bipartition model and MC method, in particular in the cases of inhomogeneous data and media as well as irregular geometry. In a forthcoming paper we shall study the error analysis for FEM applied to these cases, extend our implementations to high energy ions and include secondary particles.

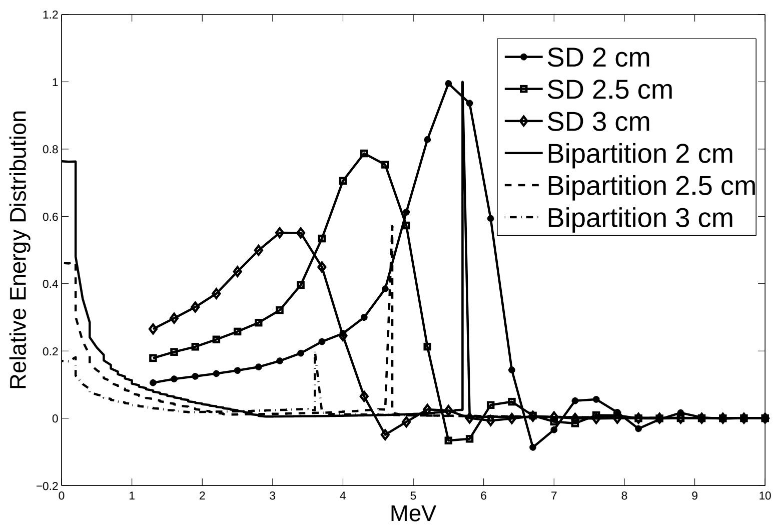

Figure 4: 10MeV Relative Energy Distribution

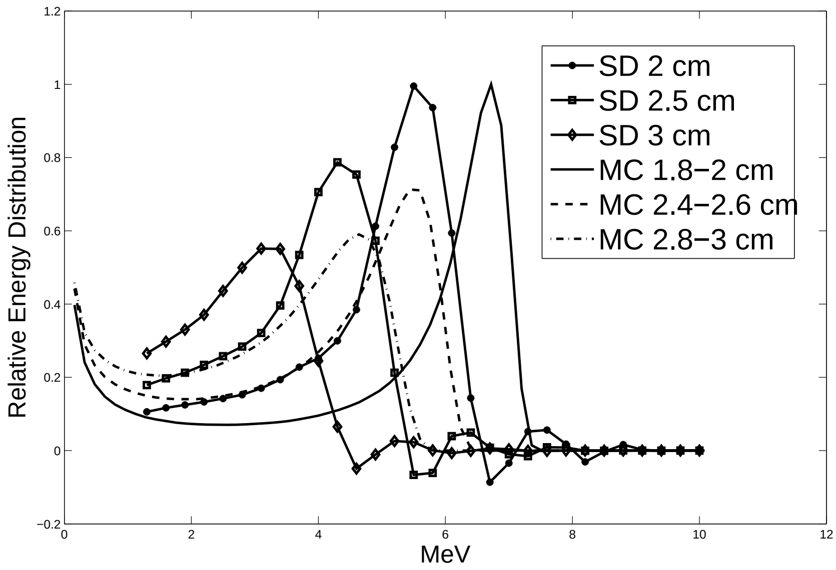

Figure 5: 10MeV Relative Energy Distribution

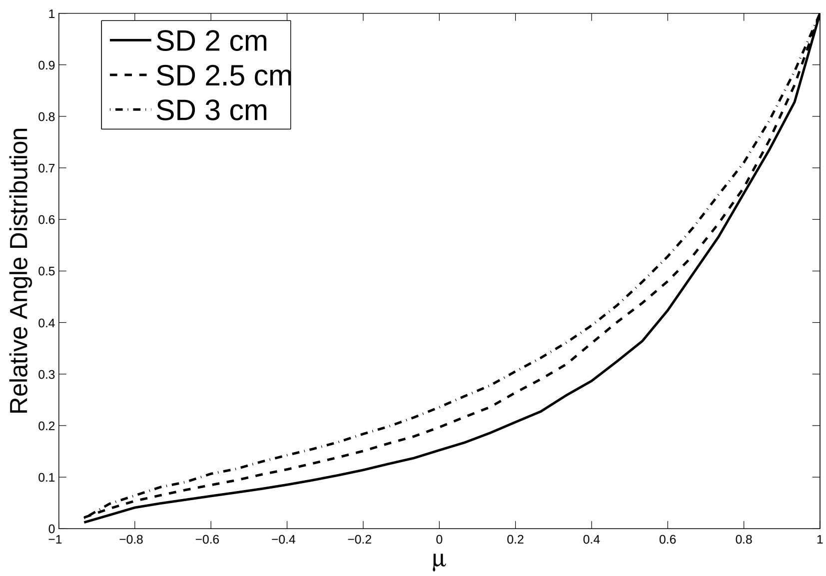

Figure 6: 10MeV Relative Angle Distribution

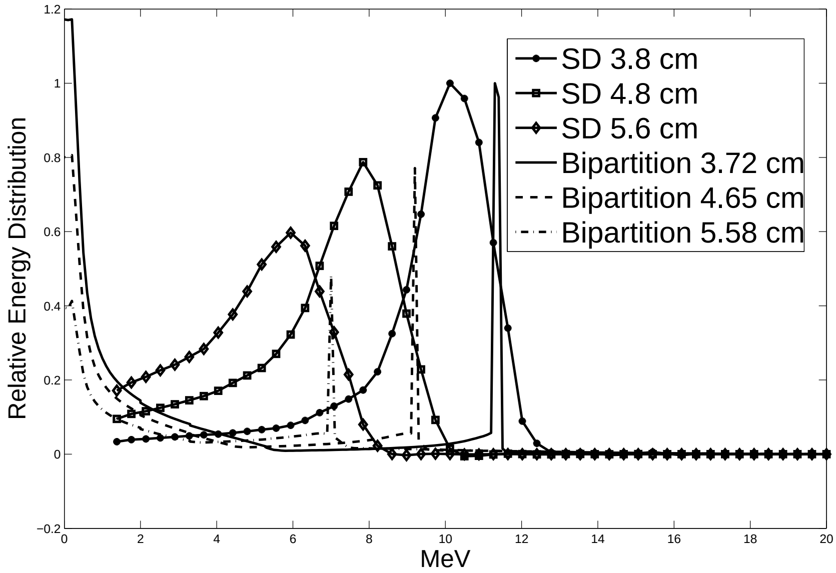

Figure 7: 20MeV Relative Energy Distribution

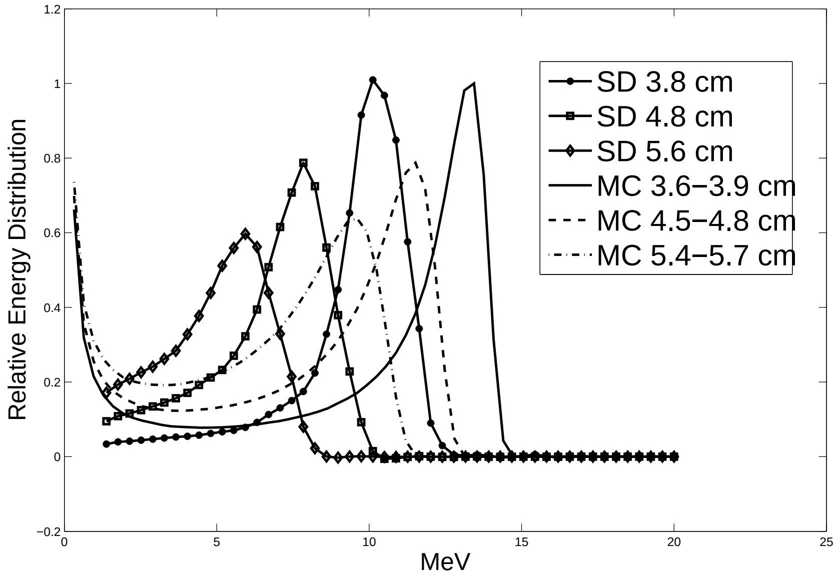

Figure 8: 20MeV Relative Energy Distribution

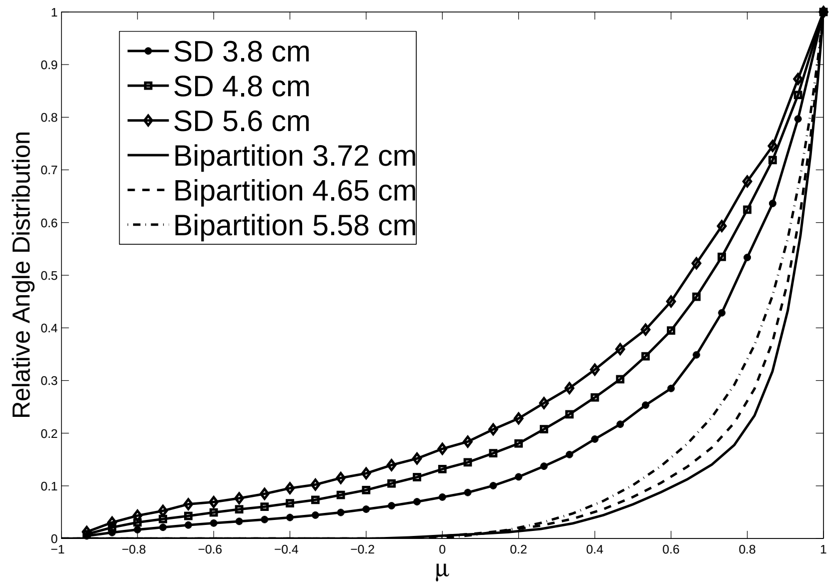

Figure 9: 20MeV Relative Angle Distribution

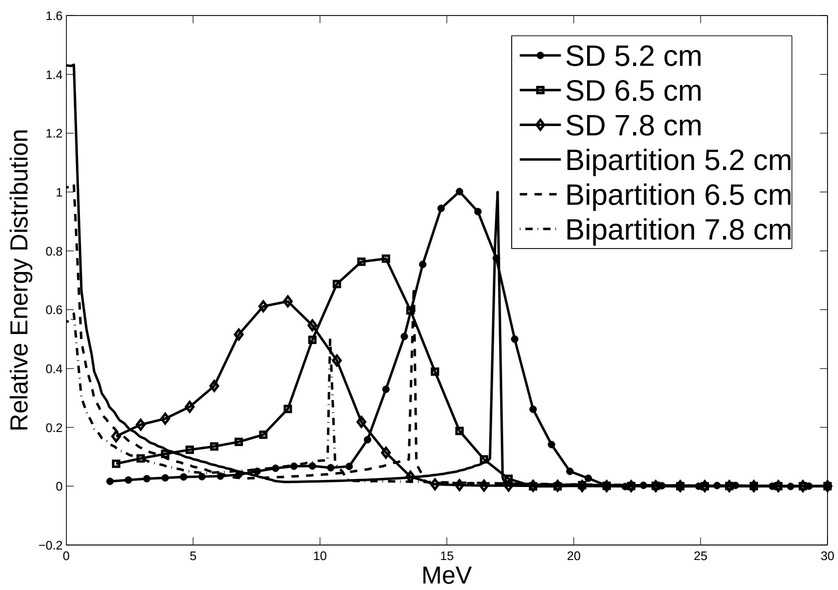

Figure 10: 30MeV Relative Energy Distribution

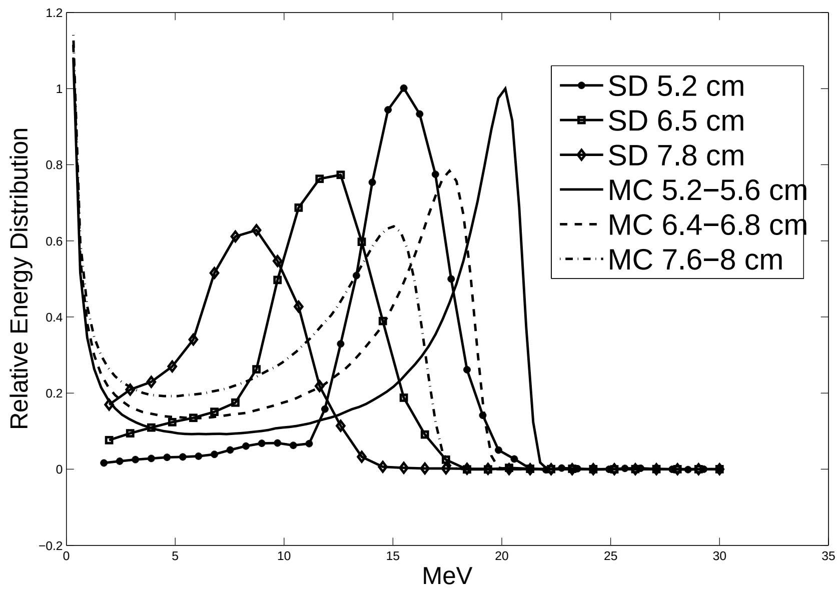

Figure 11: 30MeV Relative Energy Distribution

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