A novel upwind stabilized discontinuous finite element angular framework for deterministic dose calculations in magnetic fields

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Abstract
Angular discretization impacts nearly every aspect of a deterministic solution to the linear Boltzmann transport equation, especially in the presence of magnetic fields, as modeled by a streaming operator in angle. In this work a novel stabilization treatment of the magnetic field term is developed for an angular finite element discretization on the unit sphere, specifically involving piecewise partitioning of path integrals along curved element edges into uninterrupted segments of incoming and outgoing flux, with outgoing components updated iteratively. Correct order-of-accuracy for this angular framework is verified using the method of manufactured solutions for linear, quadratic, and cubic basis functions in angle. Higher order basis functions were found to reduce the error especially in strong magnetic fields and low density media. We combine an angular finite element mesh respecting octant boundaries on the unit sphere to spatial Cartesian voxel elements to guarantee an unambiguous transport sweep ordering in space. Accuracy for a dosimetrically challenging scenario involving bone and air in the presence of a 1.5 T parallel magnetic field is validated against the Monte Carlo package GEANT4. Accuracy and relative computational efficiency were investigated for various angular discretization parameters. 32 angular elements with quadratic basis functions yielded a reasonable compromise, with gamma passing rates of 99.96% (96.22%) for a 2%/2 mm (1%/1 mm) criterion. A rotational transformation of the spatial calculation geometry is performed to orient an arbitrary magnetic field vector to be along the z-axis, a requirement for a constant azimuthal angular sweep ordering. Working on the unit sphere, we apply the same rotational transformation to the angular domain to align its octants with the rotated Cartesian mesh. Simulating an oblique 1.5 T magnetic field against GEANT4 yielded gamma passing rates of 99.42% (95.45%) for a 2%/2 mm (1%/1 mm) criterion.

1. Introduction

Accurate radiotherapy dose calculations in the presence of a strong magnetic field has become increasingly relevant with the clinical adoption of hybrid magnetic resonance imaging (MRI) guided radiation delivery technologies which simultaneously image and irradiate the patient while immersed in a strong magnetic field. Dose-depositing electrons undergo continuous deflection by the Lorentz force in a manner dependent on the magnetic field strength and field orientation relative to the radiation beam. The ultimate impact of this deflection on the final dose distributions depends on the mean free path length of electrons in the surrounding medium.

Linac-MRI hybrid systems can be classified by their geometry. By integrating a linear accelerator in-line with a rotating biplanar superconducting MRI magnet (Fallone et al 2007, 2009, Fallone 2014) irradiation is parallel to the magnetic field at all gantry angles relative to the patient. Dosimetric consequences of this configuration are increased collimation, and a reduction in the penumbra due to electron confinement in helical trajectories along magnetic field lines (Litzenberg et al 2001, Kirkby et al 2010), with only a marginal increase in skin dose (Keyvanloo et al 2016). An alternative class of geometries rotates the radiation source around the axis of a fixed cylindrical magnet, such that the beam remains perpendicular to a stationary magnetic field (Raaymakers et al 2009, Mutic et al 2014). The dose profile is asymmetrically shifted by the Lorentz force (Raaymakers et al 2004), while the elec-
tron return effect (ERE) has been shown to increase exit-dose at interfaces between tissue and low density lung or air, while decreasing surface doses (Raaijmakers et al 2005).

Historically, all calculations of magnetic field effects on patient dose have relied on Monte Carlo techniques which represent a stochastic solution to the linear Boltzmann transport equation (LBTE), the governing equation for particle transport in heterogeneous media. Monte Carlo codes are generally considered the gold standard for accuracy when benchmarked with magnetic fields in radiotherapy (Raaymakers et al 2007, Reynolds et al 2013, Ghila et al 2017), but always result is some degree of statistical uncertainty.

Recent developments at the Cross Cancer Institute (St-Aubin et al 2015, 2016) and at Sandia Labs (Pautz et al 2014) have successfully incorporated the Lorentz force operator into a deterministic framework which directly solves the LBTE in terms of discretized variables in space, angle, and energy.

Angular discretization in particular plays a central role towards an accurate and efficient deterministic solution, as this fundamentally governs the ability to model directional anisotropy, both in representing the angular fluence solution, and in the coupling between transport directions as particles are scattered by the interaction cross section of each material. The inclusion of magnetic fields (St-Aubin et al 2015) adds further anisotropy through an angular streaming operator which also introduces stability requirements for the numerical solution in angle.

Discrete ordinates (DO) represents a classical angular technique where the LBTE is solved along discrete transport directions which are chosen from numerical quadrature sets (Lewis and Miller 1993). It has been successfully applied to radiotherapy (Vassiliev et al 2010, Failla et al 2010), however in the presence of magnetic fields, the solution stability was found to be conditional on many parameters including magnetic field strength, and the material interaction cross section (St-Aubin et al 2015, Zelyak et al 2018).

Finite element methods have been investigated in the angular domain to yield improved approximations and mitigation of ray-effects (Miller et al 1973, Briggs et al 1975, Martin and Duderstadt 1977, Martin et al 1981, Boman et al 2005, Merton et al 2008, Kophazi and Lathouwers 2015). There exists an important interdependence between discontinuous angular and spatial finite elements. In order to achieve stability of the solution for the first order LBTE using a Galerkin FEM approach, an upwind stabilization procedure (Lewis and Miller 1993, Wareing et al 2001) is required. In a standard upwinding procedure the surface terms for every spatial element face is separated into either an outgoing or incoming fluence contribution (i.e. fluence exits through the element surface, or enters through the element surface). Elements from which fluence flows into the element in question are considered upwind elements, and elements into which the fluence flows are considered down-wind elements. For angular finite elements that span a large range of angles, any given spatial finite element face in an unstructured mesh can contain both outgoing and incoming fluences, thus the standard upwinding procedure cannot be applied.

There exist several approaches to rectify this, the simplest being the refinement of the angular finite elements to a point where each angular finite element spans a small enough angular range to minimize the probability that any given spatial finite element face on an unstructured grid contains both incoming and outgoing contributions. With this mitigation strategy, a standard upwinding scheme can be employed as was the case in the previous work (St-Aubin et al 2016). However, a high angular mesh refinement level was necessary in this case which leads to a very high computational burden. Another technique is described by Kophazi and Lathouwers where each spatial finite element surface in the unstructured grid is separated into outgoing and incoming contributions through a Riemann decomposition (Kophazi and Lathouwers 2015). As mentioned in their work, performing the Reimann decomposition can be computationally burdensome, especially for a large number of spatial finite elements. In addition, a new iterative upwinding scheme is required which can lead to an increased number of iterations required for the solution to converge. These issues can be overcome by using a structured spatial mesh, such as the Cartesian hexahedral elements chosen in this work. Furthermore, if angular finite elements remain strictly contained within each octant of the unit sphere, then each spatial element surface of the structured mesh contains exclusively incoming or outgoing fluence contributions over the range of angles spanned by any given angular element. Consequently, a standard upwinding procedure can be adopted, with angular finite elements able to encompass a much larger range of angles as long as they do not cross octant boundaries.

In this work, higher order angular basis functions on the unit sphere are used to better model anisotropy within each element. When a magnetic field is introduced to the LBTE, curved element edges on the unit sphere can simultaneously contain both incoming and outgoing fluence contributions. We introduce a simple iterative technique to resolve cyclic dependencies in angle, thus preserving upwind stabilization and solution accuracy in the context of an angular sweeping method associated with the magnetic field operator. Finally, a rotational formalism is developed to simulate magnetic fields at oblique orientations while preserving alignment between spatial element faces and octant boundaries.

Following a standard approach for new formalisms (Salari and Knupp 2000, Oberkampf and Roy 2010), we first verify correctness of the implementation of our mathematical framework by order of convergence tests using the method of manufactured solution (MMS). As code verification by MMS is not designed to validate the accuracy of a given formalism, we performed validation studies comparing to Monte Carlo for several dosimetrically challenging radiotherapy cases in the presence of magnetic fields. Within this framework, the impact of angular mesh refinement levels and the use of higher order angular finite element basis functions are investigated.
2. Methods

2.1. The continuous slowing down linear Boltzmann transport equation with magnetic fields

A deterministic solution to the transport equation solves for the angular fluence of dose-depositing particles \( \psi(\vec{r}, E, \hat{\Omega}) \) which is a 6-dimensional function of space, energy, and angle. Specifically, in the presence of a magnetic field, the steady state continuous slowing down (CSD) LBTE for secondary electrons is (St-Aubin et al 2015),

\[
\hat{\Omega} \cdot \nabla \psi(\vec{r}, E, \hat{\Omega}) + \frac{d}{dE} \hat{\sigma}(\vec{B}, \hat{\Omega}) \cdot \nabla_{\Omega} \psi(\vec{r}, E, \hat{\Omega}) + \sigma(\vec{r}, E) \psi(\vec{r}, E, \hat{\Omega}) = \frac{d}{dE} \left( \beta_s(\vec{r}, E) \psi(\vec{r}, E, \hat{\Omega}) \right) = Q(\vec{r}, E, \hat{\Omega}) + S(\vec{r}, E, \hat{\Omega}).
\] (1a)

With vacuum boundary conditions,

\[
\psi = 0, \quad \hat{\Omega} \cdot \hat{n} < 0
\] (1b)

where \( \hat{n} \) is the outward normal of the domain boundary.

In equation (1), the following symbolic definitions apply:

- \( \psi(\vec{r}, E, \hat{\Omega}) \) = Angular fluence
- \( \Omega = (\sin \theta \cos \varphi, \sin \theta \sin \varphi, \cos \theta) \)
- \( \varphi \) = azimuthal angle in spherical coordinates
- \( \theta \) = polar angle in spherical coordinates
- \( \sigma(\vec{r}, E) \) = macroscopic total cross section
- \( \beta_s(\vec{r}, E) \) = restricted mass stopping power

\( \hat{\sigma}(\vec{B}, \hat{\Omega}) = \frac{1}{\sqrt{1 - \cos^2 \theta}} \left[ \left( \hat{\Omega} \times \left( \hat{\Omega} \times \vec{B} \right) \right) \hat{z} - \left( \hat{\Omega} \times \vec{B} \right) \hat{z} \right] \)

\( \vec{B} \) = magnetic field in Teslas
\( q \) = particle charge
\( \vec{p} \) = particle momentum.

\( \nabla_{\Omega} = \frac{1}{\sqrt{1 - \cos^2 \theta}} \left( \frac{\partial}{\partial \varphi} \hat{\varphi} + \frac{\partial}{\partial \theta} \hat{\theta} \right) \)

\( S(\vec{r}, E, \hat{\Omega}) \) = external source.

By expanding the macroscopic differential cross sections in Legendre polynomials and the angular fluence in spherical harmonics (Lewis and Miller 1993), the scattering integral \( Q \) in equation (1) can be expressed,

\[
Q(\vec{r}, E, \hat{\Omega}) = \int_{\Delta} dE \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \sigma_l(\vec{r}, E' \rightarrow E) \phi_{lm}(\vec{r}, E') Y_{lm}(\hat{\Omega})
\] (2)

where the following definitions apply,

- \( \sigma_l = \) Legendre polynomial moments of the macroscopic differential cross section
- \( \phi_{lm}(\vec{r}, E') = \int_{\Omega} Y_{lm}(\hat{\Omega}) \Psi(\vec{r}, \hat{\Omega}, E') \ d\hat{\Omega} = \) angular fluence moments
- \( Y_{lm}(\hat{\Omega}) = \) Spherical harmonics

and where \( \Delta \) is the cutoff energy for the CSD operator which accounts for soft collisions at energies lower than \( \Delta \). In this work, the CSD operator in equation (1) is discretized using a diamond difference approach (Morel 1985), whose form is similar to the scattering integral in equation (2). As such, the CSD operator will not be shown explicitly in further discussions. Practically, the Legendre expansion of the macroscopic differential cross sections in equation (2) is truncated at order \( L \). For radiotherapy calculations, a partial coupling technique is employed where photons create electrons, but electrons do not create photons (i.e. positrons are treated as electrons, and the energy from photons produced by electrons is deposited locally). Thus only downscatter is included in equation (2) (Vassiliev et al 2010).

2.2. Source iteration

Due to the complexity of integro-differential equations such as the CSD-LBTE with magnetic fields (equation (1)), numerical iterative schemes are often required. Source Iteration (Lewis and Miller 1993) is a stationary Richardson iteration technique which can be used to solve the LBTE. Equation (1) recast in the form of an unaccelerated Source Iteration becomes,

\[
\hat{\Omega} \cdot \nabla \psi^{(t+1)}(\vec{r}, E, \hat{\Omega}) + \frac{d}{dE} \hat{\sigma}(\vec{B}, \hat{\Omega}) \cdot \nabla_{\Omega} \psi^{(t+1)}(\vec{r}, E, \hat{\Omega}) + \sigma(\vec{r}, E) \psi^{(t+1)}(\vec{r}, E, \hat{\Omega}) = Q(\vec{r}, E, \hat{\Omega}) + S(\vec{r}, E, \hat{\Omega}).
\] (3)
\[
\phi_{lm}^{(t)}(\hat{r}, \hat{E}) = \int_{\Omega} Y_{lm}^*(\hat{\Omega}) \Psi^{(t)} (\hat{r}, \hat{E}, \hat{\Omega}) \, d\hat{\Omega}.
\] (4)

At each iteration, the angular fluence \(\phi^{(t+1)}\) is updated using the angular fluence moments from the previous iteration, \(\phi^{(t)}\). For conciseness we omit the iteration index \(t\) in further discussions.

2.3. Energy discretization

A Multigroup approach (Lewis and Miller 1993) is used to discretize the energy variable into groups denoted by their index \(g\). Within each group, energy dependence is considered to be piecewise constant. Equation (3) becomes

\[
\hat{\Omega} \cdot \nabla \psi_{g} (\hat{r}, \hat{\Omega}) + \kappa_{g} \psi_{g} (\hat{r}, \hat{\Omega}) \cdot \nabla_{\hat{\Omega}} \psi_{g} (\hat{r}, \hat{\Omega}) + \sigma_{g} (\hat{r}) \psi_{g} (\hat{r}, \hat{\Omega}) = \sum_{g'} \sum_{i=0}^{I} \sum_{m=-1}^{1} \sigma_{g' \rightarrow g} (\hat{r}) \phi_{g'}^{m} (\hat{r}) Y_{lm}(\hat{\Omega}) + S_{g} (\hat{r}, \hat{\Omega}).
\] (5)

Where the multigroup magnetic field parameter is calculated to be (St-Aubin et al 2015, 2016)

\[
\kappa_{g} = \frac{q c}{E_{g} - E_{g+1}} \ln \left( \frac{E_{g} + m_{c}c^{2} + \sqrt{(E_{g} + m_{c}c^{2})^{2} - (m_{c}c^{2})^{2}}}{E_{g+1} + m_{c}c^{2} + \sqrt{(E_{g+1} + m_{c}c^{2})^{2} - (m_{c}c^{2})^{2}}} \right)
\] (6)

with \(c\) being the speed of light and \(m_{c}\) denoting the rest mass of the particle.

In further discussions we omit the energy group index \(g\) without loss of generality, and consider the spatially uniform \(\hat{B}(\hat{r}) = \hat{B}_{0}\) of the MRI.

2.4. Finite element method

For each energy group, the problem domain in space and angle are partitioned into local subdomains (elements). The space and angle variables of equation (5) are approximated by independent basis functions over each element,

\[
\psi (\hat{r}, \hat{\Omega}) = \sum_{i=1}^{I} \sum_{p=1}^{P} \psi_{i,p} \lambda_{i}(\hat{r}) \gamma_{p}(\hat{\Omega})
\] (7)

where \(I\) and \(P\) represent the number of nodes, or degrees of freedom, for the spatial and angular elements respectively. In this study, \(\gamma_{p}(\hat{\Omega})\) are polynomial basis functions for angular elements conformal to the unit sphere, while \(\lambda_{i}(\hat{r})\) denote trilinear basis functions for the spatial elements chosen to be hexahedral voxels structured as a Cartesian grid. \(\psi_{i,p}\) denotes the coefficient indexed to the \(i\)th local node in space and \(p\)th local node in angle of this space-angle system.

2.5. Discontinuous finite element system of equations

The Galerkin method is applied by substituting equation (7) into equation (5), multiplying each term by weighting functions \(\lambda_{i}(\hat{r})\) and \(\gamma_{p}(\hat{\Omega})\), and integrating over phase-space to yield the weak-form system of equations. To establish a discontinuous finite element framework, the divergence theorem is applied to all first order derivatives, in this case the spatial and angular gradient terms (St-Aubin et al 2016).

\[
\sum_{i=1}^{I} \sum_{p=1}^{P} \sum_{k=1}^{K} \psi_{i,p,k} \int_{\Omega_{n}} d\Omega \gamma_{p} (\hat{\Omega}) \gamma_{q} (\hat{\Omega}) \hat{\Omega} \cdot \hat{n}_{k} \int_{S} dS \lambda_{i}(\hat{r}) \lambda_{j}(\hat{r})
\]

\[
- \int_{\Omega_{n}} \psi_{i} \int_{\Omega_{n}} d\Omega \gamma_{p}(\hat{\Omega}) \gamma_{q}(\hat{\Omega}) \hat{\Omega} \cdot \partial V \lambda_{i}(\hat{\Omega}) dV \lambda_{j}(\hat{r})
\]

\[
+ \kappa \sum_{i=1}^{I} \sum_{p=1}^{P} \sum_{k=1}^{K} \psi_{i,p,k} \int_{\Omega_{n}} d\Omega \gamma_{p}(\hat{\Omega}) \gamma_{q}(\hat{\Omega}) \hat{\Omega} \cdot \partial V \lambda_{i}(\hat{\Omega}) dV \lambda_{j}(\hat{r})
\]

\[
- \kappa \int_{\Omega_{n}} \psi_{i} \int_{\Omega_{n}} d\Omega \gamma_{p}(\hat{\Omega}) \gamma_{q}(\hat{\Omega}) \hat{\Omega} \cdot \partial V \lambda_{i}(\hat{\Omega}) dV \lambda_{j}(\hat{r})
\]

\[
+ \int_{\Omega_{n}} \psi_{i} \int_{\Omega_{n}} d\Omega \gamma_{p}(\hat{\Omega}) \gamma_{q}(\hat{\Omega}) \hat{\Omega} \cdot \partial V \lambda_{i}(\hat{\Omega}) dV \lambda_{j}(\hat{r})
\]

\[
= \int_{\Omega_{n}} \hat{\Omega} \int_{V} dVQ (\hat{r}, \hat{\Omega}) \gamma_{q}(\hat{\Omega}) \lambda_{j}(\hat{r})
\]

\[
+ \int_{\Omega_{n}} \hat{\Omega} \int_{V} dV S (\hat{r}, \hat{\Omega}) \gamma_{q}(\hat{\Omega}) \lambda_{j}(\hat{r})
\]

(8a)

with boundary conditions
along an element edge, and the unit radial vector \( \mathbf{\hat{r}} \) for face \( k \) of a spatial element and \( \mathbf{\hat{n}}_k (\hat{\Omega}) \) refers to the outward unit-normal vector along edge \( k' \) of an angular element, tangential to the surface of the unit sphere. This is formally defined in equation (8d) with respect to the differential path \( \mathbf{dl} \) along an element edge, and the unit radial vector \( \mathbf{\hat{r}} \). Consequently, the angular edge outward normal orientation varies with angle \( \hat{\Omega} \) due to the curvature on the sphere’s surface. In this discretization scheme, the material cross section \( \sigma \) (\( \mathbf{\hat{r}} \)) remains constant over each spatial element.

\[\psi_{l,p,k} = \begin{cases} \psi_{l,p}^{inc} \cdot \mathbf{\hat{n}}_k < 0 \text{ (down-wind)} \\ \psi_{l,p} \cdot \mathbf{\hat{n}}_k > 0 \text{ (upwind)} \end{cases} \tag{8b}\]

and

\[\psi_{l,p,k'} = \begin{cases} \psi_{l,p}^{inc} \cdot (\mathbf{\hat{B}}, \mathbf{\hat{\Omega}}) \cdot \mathbf{\hat{n}}_k (\hat{\Omega}) < 0 \text{ (down-wind)} \\ \psi_{l,p} \cdot (\mathbf{\hat{B}}, \mathbf{\hat{\Omega}}) \cdot \mathbf{\hat{n}}_k (\hat{\Omega}) > 0 \text{ (upwind)} \end{cases} \tag{8c}\]

where

\[\mathbf{\hat{n}}_k (\hat{\Omega}) = \frac{\mathbf{dl} \times \mathbf{\hat{r}}}{\mathbf{dl} \times \mathbf{\hat{r}}} \tag{8d}\]

In equation (8), \( \Omega_\alpha \) defines the angles subtended by the angular finite element \( \alpha \), \( \mathbf{\hat{n}}_k \) is the outward unit-normal vector for face \( k \) of a spatial element and \( \mathbf{\hat{n}}_k (\hat{\Omega}) \) refers to the outward unit-normal vector along edge \( k' \) of an angular element, tangential to the surface of the unit sphere. This is formally defined in equation (8d) with respect to the differential path \( \mathbf{dl} \) along an element edge, and the unit radial vector \( \mathbf{\hat{r}} \). Consequently, the angular edge outward normal orientation varies with angle \( \hat{\Omega} \) due to the curvature on the sphere’s surface. In this discretization scheme, the material cross section \( \sigma \) (\( \mathbf{\hat{r}} \)) remains constant over each spatial element.

### 2.6. Angular basis function definition and transformations

Angular basis functions are first defined with respect to canonical coordinates as \( \gamma (\varepsilon, \eta) \), each parameter spanning 0 to 1, as shown in figure 1(a). The three linear basis functions spanning the canonical triangle can thus be expressed as,

\[
\begin{align*}
\gamma_1 &= 1 - \varepsilon - \eta \\
\gamma_2 &= \varepsilon \\
\gamma_3 &= \eta.
\end{align*}
\tag{9}
\]

Higher order polynomial basis functions can be constructed in terms of this linear set (Jin 2014). In this work, linear, quadratic, and cubic orders having 3, 6, and 10 nodal degrees of freedom per angular element respectively are investigated.

Transformation from the canonical space, where the basis functions are defined, to the surface of the unit sphere is accomplished by a standard two stage projection technique (Hennink 2015, Hennink and Lathouwers 2018). First, each canonical element is mapped onto its corresponding triangle defined on the flat faces of the octahedron (figure 1(b)). A given element is uniquely defined by the coordinates of its corner vertices: \((X_1, Y_1, Z_1), (X_2, Y_2, Z_2), (X_3, Y_3, Z_3)\).

\[
\mathbf{\bar{t}} = \begin{bmatrix} x \\ y \\ z \end{bmatrix} = \begin{bmatrix} X_1 \\ Y_1 \\ Z_1 \end{bmatrix} + \begin{bmatrix} X_2 - X_1 \\ Y_2 - Y_1 \\ Z_2 - Z_1 \end{bmatrix} \cdot \begin{bmatrix} \varepsilon \\ \eta \end{bmatrix} + \begin{bmatrix} X_3 - X_1 \\ Y_3 - Y_1 \\ Z_3 - Z_1 \end{bmatrix} \cdot \begin{bmatrix} \varepsilon \\ \eta \end{bmatrix}. \tag{10}\]

Next, the elements on the octahedron are projected onto the curved surface of the unit-sphere (figure 1(c)) where the CSD-LBTE with magnetic fields is defined.

\[
\mathbf{\hat{\Omega}} = \begin{bmatrix} \Omega_x \\ \Omega_y \\ \Omega_z \end{bmatrix} = \frac{\mathbf{\bar{t}}}{|\mathbf{\bar{t}}|}. \tag{11}\]

The transformations of equations (10) and (11) (figure 1(c)) map the polynomial basis functions from canonical coordinates \( \gamma (\varepsilon, \eta) \) to the angular domain as \( \gamma (\hat{\Omega}) \).

Angular meshing begins on the faces of an octahedron with vertices at \( \pm 1 \) along the cardinal axes (figure 1(b)); the simplest case is a single angular element per octant (eight angular elements in total, figure 2(a)). Each face can undergo systematic refinement by recursively bisecting the edges of triangles generated on the octahedron, creating angular meshes with 32, 128, 512, 2048, and 8192 elements used in this work (first four refinements projected onto sphere shown in figure 2).
2.7. Interplay between space-angle discretization scheme and spatial sweep ordering

Upwind stabilization involves propagating a known angular fluence from an upwind element $\psi_{\text{inc}}^{i,p}$ across the down-wind faces of an element as specified by the boundary conditions in either equation (8b), or (8c). This process is performed for each solution direction and is known as a transport sweep. In space, the choice of hexahedral voxel elements aligned to the cardinal axes of a Cartesian grid yields the minimum possible set of 8 different sweep orderings. Each sweep ordering corresponds to the range of angles encompassed by an octant of the unit sphere. By ensuring all angular elements are fully contained in their respective octant, we can align octant boundaries of the angular mesh with the cardinal planes of the spatial Cartesian grid, such that each spatial voxel face $k$ (characterized by its normal vector $\hat{n}_k$) is unambiguously categorized as upwind $\hat{\Omega}_\alpha \cdot \hat{n}_k > 0$ or down-wind $\hat{\Omega}_\alpha \cdot \hat{n}_k > 0$ over the entire range of angles $\hat{\Omega}_\alpha$ encompassed by a given angular element $\alpha$ (i.e. the sign of $\hat{\Omega}_\alpha \cdot \hat{n}_k$ will not change for each face over the entire sweep octant). In the previous work (St-Aubin et al 2016) utilizing unstructured tetrahedral spatial meshes, spatial element faces are directed randomly and small angular elements were required to minimize the impact when the sign of $\hat{\Omega}_\alpha \cdot \hat{n}_k$ changed over the angular element $\alpha$. Thus a large number of angular elements were required to span the full unit-sphere leading to an overly complex calculation. However, by adopting a Cartesian grid and requiring angular elements to respect octant boundaries, an unambiguous spatial sweep ordering can be achieved for any mesh refinement level. Thus the mesh refinement is determined by the needed accuracy of the problem, and not the generation of the spatial sweep ordering.

2.8. Mechanism to preserve angular upwind stabilization

The sweep ordering of angular elements on the unit sphere is established by the boundary conditions of equation (8c). For upwind stabilization, as dictated by the boundary condition equation (8c), it is crucial that edges where $\tilde{\sigma} (\vec{B}, \vec{\Omega}) \cdot \hat{n}_k (\hat{\Omega}) < 0$ use incoming flux which has been solved in a down-wind angular sweep group. However, after projecting the canonical triangles in ($\varepsilon$, $\eta$) space onto the unit sphere, it was found that the sign of $\tilde{\sigma} (\vec{B}, \vec{\Omega}) \cdot \hat{n}_k (\hat{\Omega})$ can change even along a single edge of an angular element, causing it to contain both down-wind and upwind contributions. This phenomenon arises from either or a combination of two root causes, (1) the curved nature of the sphere allows the orientation of $\hat{n}_k$ to change over a given edge, and (2) the magnetic
For radiotherapy, we establish the patient coordinate frame $S = (x,y,z)$ as the Cartesian grid to which the spatial imaging voxels are aligned and whose cardinal planes divide the unit sphere into octants (figure 4(a)). These form the octant boundaries which angular mesh elements must respect in order to retain an unambiguous spatial sweep ordering.

Sweeping in the angular domain is characterized by the vector field $\vec{\tau}(\vec{B}, \hat{\Omega})$, shown in figure 3. In general, this flow can be quite complex, for which a well-defined angular sweep ordering is difficult to establish. It was shown that restricting the magnetic field to the z-axis ($B_y = B_z = 0$) results in a well-defined azimuthal flow (equation (13)), providing a simple sweep ordering (St-Aubin et al. 2016),

$$\vec{\tau}\left(\hat{\Omega}\right) = B_x \sin \theta \hat{\varphi}. \tag{13}$$

Consequently, for radiotherapy systems such as the Alberta Linac-MR (Fallone et al. 2009, Fallone 2014) which causes $\vec{B}_0$ to rotate with gantry angle $\chi$, a calculation coordinate frame $\mathcal{S}_\chi = (x,y,z)$ is established which orients the new $z_r$-axis parallel to the oblique magnetic field (e.g. $\chi = 37^\circ$ clockwise from the $z$-axis in the $y$-$z$ plane as shown in figure 4(b)). This recovers the simple azimuthal sweep ordering in $\mathcal{S}_\chi$, shown in figure 4(b), and expressed in equation (14).

$$\vec{\tau}\left(\hat{\Omega}_r\right) = B_x \sin \theta \hat{\varphi}. \tag{14}$$

As shown in figure 4(b), the transformation to $\mathcal{S}_\chi$ is simply achieved by rotating the angular elements on the unit sphere by the same angle $\chi$ counterclockwise about the $x$-axis. The same rotation applies to the spatial domain such that the relative orientation between voxel faces and angular elements are preserved, and spatial transport sweep orderings remain unaltered. However, in the rotated system, changes in the relative orientation between the sweep vector $\vec{\tau}$, and angular element edge normal $\hat{n}_E$ can occur. Thus the inflection points of $\vec{\tau}\left(\hat{\Omega}_r\right) \cdot \hat{n}_E$, and the resulting integrals (equation (8)) must be reevaluated and the sweep ordering on the unit-sphere needs to be
redefined for every magnetic field direction. As the number of angular elements is generally quite low, this is not a computationally intensive calculation.

2.10. Verification of mathematical framework

In scientific computing, code verification comprises a hierarchy of tests used to establish confidence that a proposed solution framework and its algorithmic implementation are correctly solving the underlying mathematical model. Most rigorous among these tests is the evaluation of the rate at which the code’s numerical solution converges to the exact analytic solution under systematic mesh refinement (Oberkampf and Roy 2010). Formally, this observed order-of-accuracy under mesh refinement (or $h$-refinement) can be compared with well-established theoretical values for the finite element method (Braess 2007).

A prerequisite to quantify error in the numerical solution is to have the analytic form of the exact solution. For complex systems such as the CSD-LBTE with magnetic fields, the method of manufactured solutions (MMS) is ideally suited as it starts by specifying the analytic solution, in this case chosen to be a spatially uniform, directionally anisotropic angular fluence of the form:

$$\psi_a (\hat{\Omega}) = P_{ms} \cdot \exp \left( \frac{\omega_x \Omega_x^2 + \omega_y \Omega_y^2 + \omega_z (\Omega_z - 0.9)^2}{4 \sigma^2} \right)$$

(15)

where $\hat{\Omega} = (\Omega_x, \Omega_y, \Omega_z)$ is the angular ordinate.
Although MMS does not require a physically realistic solution (Pautz 2001, Oberkampf and Roy 2010), the form of equation (15) and the choice of parameters \( \{ P_{\text{in}} = \pi \times 10^6 \text{ cm}^2, \omega_3 = 1, \omega_4 = 2, \omega_5 = 1, \vartheta = 1/4 \} \) was used to produce an angular fluence distribution resembling the electron fluence solution for the highest energy group (6 MeV) of the CSD-LBTE based on previous numerical radiotherapy calculations. Equation (15) is substituted into the monoenergetic CSD-LBTE with magnetic fields (equation (3)) to yield the corresponding source function:

\[
S_a(\Omega) = \sigma \psi_a(\Omega) + \kappa B_z \frac{\partial}{\partial \phi} \psi_a(\Omega) - \int d\Omega' \psi_a(\Omega') \sigma(\Omega \cdot \Omega') \psi_a(\Omega'') .
\]  

(16)

The macroscopic differential scattering cross section \( \sigma^s(\Omega \cdot \Omega') \) is approximated in the form of the Henyey-Greenstein model (Henyey and Greenstein 1941) as,

\[
\sigma^s(\Omega \cdot \Omega') = \frac{\sigma}{2 \left(1 - \zeta^2 \right)^{3/2}}
\]

with an anisotropy parameter of \( \zeta = 0.5 \). The scattering integral in equation (16) with the cross section of equation (17) is evaluated using a level symmetric \( S_{64} \) quadrature set comprising 8192-points, with \( \sigma^s(\Omega \cdot \Omega') \) expanded in Legendre polynomial moments \( \sigma_l \), where the maximum Legendre expansion order of \( L = 8 \) was chosen.

A numerical implementation of our mathematical framework is prototyped in Matlab (Mathworks Inc., Natick, MA). The angular finite element surface integrals in equation (8) are performed using an 88-point numerical quadrature with order 20 accuracy (Zhang et al 2009), found to be sufficient for regions up to an octant. The line integrals in equation (8) are performed using a 64-point Gaussian quadrature (order 127 accurate), the large number of points used to facilitate numerical determination of the inflection point between upwind and downwind regions. Unaccelerated source iteration (SI) was used to converge on the numerical solution for angular fluence, with the termination condition presented by Adams to avoid false convergence which can occur when the iteration count is very large (Adams and Larsen 2002),

\[
\frac{\| \phi_{lm}^{t-1} - \phi_{lm}^{t-2} \|}{1 - \| \phi_{lm}^{t-2} - \phi_{lm}^{t-1} \|} \leq 10^{-5} .
\]

(18)

The error between the code’s numerical solution \( \psi_n(\Omega) \) and the reference \( \psi_n(\Omega) \) is quantified using the \( L^2 \) norm over angle,

\[
\varepsilon = \| \psi_n - \psi_a \| = \sqrt{\int d\Omega (\psi_n(\Omega) - \psi_a(\Omega))^2} ,
\]

(19)

which is plotted as a function of elemental edge length of the octahedron \( h = \frac{\sqrt{2}}{2} \), with \( r = 1, 2, 3, \ldots \) being successive refinement levels. Observed order of convergence is obtained by evaluating the slope \( m \) of the converged plots,

\[
m = -\frac{\log_{10}\varepsilon}{\log_{10}(1/h)} .
\]

(20)

MMS was performed using linear, quadratic, and cubic basis functions in angle, for material cross sections with magnitudes of \( \sigma = 10^{-3}, 10^{0}, 10^{2} \text{ cm}^{-1} \), representative of air, water, and bone respectively. For example, the magnitude of the electron total cross section for air at 6 MeV is on the order of \( 10^{-3} \text{ cm}^{-1} \) while materials such as water and bone can have cross section magnitudes of \( 10^{2} \text{ cm}^{-1} \) at lower energies. For each of these cross section magnitudes, calculations were performed for a case with no magnetic fields, and for a magnetic field parameter of \( \kappa B_z = 10 \text{ cm}^{-1} \) which was chosen as an extreme case representative of a 20 T magnetic field.

2.11. Validation against Monte Carlo in heterogeneous phantom with magnetic fields

The deterministic framework’s accuracy is validated against the Monte Carlo package GEANT4 (Pia 2003, Allison et al 2006) over a range of angular discretization parameters for a dosimetrically challenging scenario containing high density bone (1.92 g cm\(^{-3}\)) immediately followed by low density air (1.02 \times 10^{-3} g cm\(^{-3}\)) in the presence of a strong 1.5 T magnetic field. This setup is actualized in the test geometry of a 10 \times 10 \times 10 cm\(^3\) heterogeneous phantom comprising slabs of water, bone, and air, irradiated by a polyenergetic 6 MV point source (St-Aubin et al 2015) at 100 cm SSD for a 2 \times 2 cm\(^2\) field size. For the standard test case, a constant 1.5 T magnetic field is oriented parallel to the beam (along z-axis). To benchmark accuracy at an oblique field orientation, the 1.5 T magnetic field was rotated 37° clockwise in the y-z plane. By choosing a non-cardinal angle, we test performance of this
framework in the most general case. Lastly, investigations were performed on a \( 30 \times 30 \times 30 \text{ cm}^3 \) phantom with a \( 10 \times 10 \text{ cm}^2 \) field size in the presence of a 1.5 T parallel as well as 3 T perpendicular magnetic fields.

The deterministic formalism in these calculations first solves the photon fluence from which the electron fluence and final dose was calculated. For simplicity, the photon finite element discretization was identical to the electron discretization. For the energy discretization, the Multigroup method used 32 photon and 40 electron energy groups. Material cross sections are generated using the CEPXS software (Lorence et al 1989) with a maximum Legendre expansion order of \( L = 5 \). These parameters were shown in our previous work (St-Aubin et al 2016) to be sufficiently fine to yield dose in close agreement with Monte Carlo and not be a limiting source of error.

Spatial discretization for the \( 10 \times 10 \times 10 \text{ cm}^2 \) test phantom used a Cartesian hexahedral grid with a minimum element size of \( 1.25 \times 1.25 \times 1.25 \text{ mm}^3 \) within the beam and penumbra, which grew by successive factors of 2 in edge dimension to \( 10 \times 10 \times 10 \text{ mm}^3 \) for the largest elements outside of the beam, for a total of 52 800 spatial elements. The larger \( 30 \times 30 \times 30 \text{ cm}^3 \) phantom used a minimum element size of \( 2.5 \times 2.5 \times 2.5 \text{ mm}^3 \) within the beam and penumbra, growing to a maximum of \( 10 \times 10 \times 10 \text{ mm}^3 \) outside the beam, for a total of 410 040 spatial elements. Notably, each discontinuous spatial finite element has 8 degrees of freedom, corresponding to dose at the corners, whereas the same sized voxel in Monte Carlo has 1 dose value ascribed to its centre.

The Monte Carlo calculations using GEANT4 replicated the same phantom geometry and test conditions used in the deterministic calculations, with low energy physics models in the radiotherapy regime derived from the Livermore evaluated photon and electron data libraries (EPDL and EEDL respectively), providing equivalent material cross sections as generated by CEPXS (Geant4 Collaboration 2011). For the \( 10 \times 10 \times 10 \text{ cm}^2 \) phantom, 5 billion histories were run with dose scored on a \( 1.25 \times 1.25 \times 1.25 \text{ mm}^3 \) voxel grid. For the \( 30 \times 30 \times 30 \text{ cm}^3 \) phantom, 20 billion histories were run with dose scored on a \( 2.5 \times 2.5 \times 2.5 \text{ mm}^3 \) voxel grid. The path length cutoff for production of secondary particles in GEANT4 is set to 10 \( \mu \text{m} \). Both the deterministic and Monte Carlo calculations are normalized to dose per particle fluence of primary photons (Gy cm\(^2\)).

Central axis depth dose and lateral profiles are compared for a variety of angular mesh refinement levels and angular basis function orders. For representative cases, a 3D gamma analysis (Low et al 1998) was performed using a 2%/2 mm as well as a 1%/1 mm global dose maximum Van Dyk gamma criterion (Van Dyk et al 1993, Templeton et al 2015), which evaluates dose differences relative to the global maximum of the corresponding Monte Carlo reference dose. Considering only voxels exceeding 10% of the global maximum dose limited their statistical uncertainty to less than 0.1%. Within a search radius of 3 mm, dose of the deterministic solution was evaluated on a 0.1 mm subgrid by interpolation along its trilinear spatial basis functions.

### 3. Results and discussion

#### 3.1. MMS order of convergence verification

Plotted in figure 5 is the \( L^2 \) norm of error in the numerical solution as a function of angular mesh refinement. Grouped by color are calculations performed with different polynomial orders of angular basis function. In the absence of magnetic fields, the numerical error was found to be the same for each cross section magnitude investigated, thus is presented as a solid baseline in each grouping of figure 5. As expected, for each mesh refinement level, higher order basis functions reduced the solution error. Theoretically, this is consistent with the assumption that increased degrees of freedom provided by a higher order polynomial approximation are better able to model angular anisotropy for a given mesh size.

In each case, adding magnetic fields (\( \kappa B_z = 10 \text{ cm}^{-1} \)) caused the error in the numerical solution to increase, the effect becoming progressively greater in materials with lower magnitude cross sections (i.e. \( \sigma = 10^{-3} \)). Physically, this corresponds to charged particles traversing longer path lengths under the influence of magnetic fields, especially in materials where the probability of interaction is small. Mathematically this is consistent with the magnetic field’s streaming operator (second term in equation (3)) playing a greater role relative to the terms involving material cross-section. Consequently, the solution appears to become increasingly sensitive to numerical error in calculating the angular derivative when subject to the increased anisotropy caused by magnetic fields. With linear basis functions, the margin of error for magnetic fields at low cross sections persists even under intensive mesh refinement. However, with quadratic and cubic basis functions, the error associated with magnetic fields at low cross sections converges to the same level observed for the larger cross sections upon mesh refinement. Practically, higher order basis functions can provide a means to better model increased angular anisotropy inherent to magnetic fields.

From the slopes in figure 5 (equation (20)), we extract the observed order of accuracy in the asymptotic limit of mesh refinement (table 1).

Order-of-accuracy is the most comprehensive and difficult verification criterion, encompassing all aspects of the code’s mathematical methods and programming implementation (Oberkampf and Roy 2010). Formal order of accuracy for Lagrange finite elements is expected to approach \( p + 1 \), where \( p \) is the polynomial order of the angular basis function (Braess 2007).
From table 1, it can be seen that even with strong magnetic fields in low density air, the observed order of accuracy was within 6% of the expected $p + 1$, establishing reasonable confidence in the correctness and implementation of our angular treatment of magnetic fields, specifically the splitting of finite element edge integrals to preserve angular upwind stabilization on the unit sphere.

### 3.2. Validation against Monte Carlo

To assess the practical implications of angular discretization parameters in challenging dosimetric scenarios, the accuracy of our code is validated against GEANT4 Monte Carlo calculations over a range of angular mesh refinements and basis function orders. One testing extremum made possible by discretization on the unit sphere is to simulate the minimum of eight angular elements (one element per octant), each characterizing a transport sweep ordering. Figure 6 compares the central axis depth dose against Monte Carlo for the small phantom in a 1.5 T magnetic field parallel to the beam. Figure 6(a) shows the effect of angular mesh refinement ($h$-refinement) while constrained to linear basis functions, and figure 6(b) shows the effect of higher order basis functions ($p$-refinement) while constrained to the minimum eight angular elements.

As expected, increasing the number of angular elements leads to improved agreement with Monte Carlo, especially in the air and distal regions (figure 6(a)), with peak percent difference dropping from 10% to 5% to 1.5% with successive $h$-refinement. Likewise, applying higher order basis functions over each angular element ($p$-refinement) is shown to improve agreement with Monte Carlo, such that even with 8 elements, cubic basis functions perform reasonably, where the depth dose deviates from Monte Carlo by a maximum of 4.3% in the air region (figure 6(b)).

It was observed each angular mesh refinement incurs approximately a 4.2-fold increase in computation time. This is expected given the intrinsic serial dependencies between discontinuous finite elements in angle when a magnetic field is present, requiring them to be solved in sequence. With each $h$-refinement, there is a 4-fold increase in the number of angular elements.

By contrast, each $p$-refinement was observed to increase computation time approximately 1.75-fold. While higher order angular basis functions require a larger matrix to model the increased degrees of freedom, these matrix operations are typically performed using highly efficient BLAS libraries. The spatial transport sweep is
Figure 6. Depth dose and percent difference against reference Monte Carlo in a $10 \times 10 \times 10 \text{ cm}^3$ phantom with 1.5 T parallel magnetic field for cases of (a) increasing the number of angular elements with linear basis functions, (b) increasing the order of angular basis functions for 8 angular elements.

Figure 7. Deterministic solution using 32 angular elements with quadratic basis functions compared to Monte Carlo. (a) Depth dose, and (b) cross-beam profiles taken halfway through the depth of each layer.

Figure 8. 2D coronal slice images for (a) Monte Carlo, (b) DFEM with 32 elements and quadratic basis functions, (c) gamma map at 2%/2 mm criterion for $2 \times 2 \text{ cm}^2$ beam in 1.5 T parallel field.

by far the most computationally intensive step. Fewer angular elements lead to proportionally fewer transport sweeps, regardless of hardware implementation platform.

Starting from 8 linear elements, it was found two successive $h$-refinements to 128 linear elements achieved a high level of accuracy compared to Monte Carlo while incurring a 16.3-fold increase in baseline computation time. Although two successive $p$-refinements to 8 cubic elements incurred only a 2.9-fold increase in baseline computation time, the dose was not quite as accurate in the air region. Ultimately it was decided a combination
of one $h$-refinement and one $p$-refinement to 32 quadratic elements struck a good balance with accuracy comparable to 128 linear elements, while reducing computation time 2.4-fold. Further comparison to Monte Carlo employed 32 quadratic elements in angle (figures 7–12).

For the 3D gamma analysis, over 99.96% (96.22%) of points analyzed passed the 2%/2 mm (1%/1 mm) criterion. Notably these test scenarios are numerically challenging due to the configuration of material inhomogeneities. A larger $10 \times 10 \text{ cm}^2$ radiotherapy field with the same angular discretization of 32 angular elements and quadratic basis functions in a larger phantom geometry was also tested in the presence of a 1.5 T parallel magnetic field as shown in figures 9 and 10.

In this case, 99.97% (96.56%) of points analyzed passed a 2%/2 mm (1%/1 mm) gamma criterion. The agreement achieved with 32 angular elements and quadratic basis functions is comparable to previously published results (St-Aubin et al 2016) which utilized 520 linear elements on a flattened angular domain. In the context of the current framework, results using 32 quadratic elements were approximately 12 times more efficient than what was published previously requiring 520 linear angular finite elements.

It should be noted, despite achieving similar accuracy in the presented cases relevant to radiotherapy, this framework does not resolve issues observed in an extreme case of a 3 T perpendicular magnetic field, and exhibits the same numerical artifact distal to the bone region as observed previously (St-Aubin et al 2016), thus will be a subject for future investigation. However, for radiotherapy applications such a case is non-clinical, and this artifact in the dose calculation is not expected to have a major impact since it is localized to a small region of air.

### 3.3. Simulating oblique orientations of magnetic field

To test accuracy when simulating oblique fields in the most general way which leverages the full flexibility of this framework, a 1.5 T magnetic field oriented at $\chi = 37^\circ$ in the $y$-$z$ plane was chosen as a representative rotation. Figure 11 presents the depth dose and profiles, while the 2D slice comparison is shown in figure 12.

A gamma analysis for the rotated magnetic field calculation had over 99.42% (95.45%) of points analyzed pass the 2%/2 mm (1%/1 mm) criterion. Defining angular elements directly on the unit sphere enables the rotational transformation applied in the spatial domain to easily be applied in the angular domain. When coupled to spatial elements of a Cartesian grid aligned to the octant boundaries of the angular mesh, the framework preserves the spatial sweep ordering over all angles, thus requires minimal additional computational complexity to simulate oblique magnetic fields. The flattened angular domain used previously (St-Aubin et al 2016) does not allow for a simple rotation of its angular elements due to the Cartesian nature of the flattened angular space, requiring the underlying patient geometry to be rotated independent of the angular mesh. Consequently, a new spatial Cartesian mesh must be generated for each new patient orientation, along with recalculation of spatial sweep ordering, adding substantial additional complexity to the problem. In this newly developed formalism (section 2.9), the spatial meshing, element connectivities, and the transport sweep ordering remain unchanged for every orientation of magnetic field.

### 4. Conclusion

A novel angular framework was developed to accommodate upwind stabilization of the magnetic field operator on the unit-sphere. By partitioning each angular finite element edge into segments of exclusively upwind or
down-wind contribution, and iteratively updating down-wind boundary sections using the connected upwind angular element from the previous iteration, boundary conditions in angle are respected.

Correctness of this framework and its implementation are verified using the method of manufactured solutions which provided confidence through an order of convergence within 6% of the expected order. By comparing different discretization parameters using MMS, higher order basis functions were found to more accurately model anisotropy. This was especially true when the magnetic field streaming operator dominates relative to particle interactions with the medium.

This new angular framework applied to a deterministic dose calculation was validated against the Monte Carlo code GEANT4 for computationally challenging scenarios involving air, bone, and a strong 1.5 T magnetic field. With spatial elements on a Cartesian grid, and angular elements respecting octant boundaries on the unit
sweep ordering was achieved. The net result was a high level of accuracy achieved using 32 angular elements with quadratic basis functions. A gamma comparison exceeded 99% (95%) for the 2%/2 mm (1%/1 mm) criterion for every case tested. Finally, a computationally efficient method to simulate oblique angles of magnetic field was presented which does not require spatial remeshing. These developments form important building blocks towards a fast, clinically feasible deterministic dose calculation in magnetic fields.

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Conflicts of interest

Dr B G Fallone is a CEO and Co-founder of MagnetTx Oncology Solutions.

Appendix

Calculation of angular gradient term.

\[ \hat{\tau} \left( \vec{B}, \hat{\Omega} \right) \cdot \vec{\nabla}_\Omega \gamma_q \left( \hat{\Omega} \right) = \frac{1}{\sqrt{1 - \left( \cos \theta \right)^2}} \left[ \left( \hat{\Omega} \times \left( \hat{\Omega} \times \vec{B} \right) \right)_z \hat{\phi} - \left( \hat{\Omega} \times \vec{B} \right)_z \hat{\theta} \right] \left( \frac{1}{\sqrt{1 - \left( \cos \theta \right)^2}} \frac{\partial}{\partial \phi} \hat{\phi} + \frac{\partial}{\partial \theta} \hat{\theta} \right) \gamma_q \left( \hat{\Omega} \right). \]  

(A.1)

In our problem setup, the magnetic field is along the z-axis \( (B_x = B_y = 0) \), resulting in a well-defined azimuthal flow:

\[ \hat{\tau} \left( \hat{\Omega} \right) = B_z \sin \theta \hat{\phi}. \]  

(A.2)

Equation (A.1) simplifies to:

\[ \hat{\tau} \left( \hat{\Omega} \right) \cdot \vec{\nabla}_\Omega \gamma_q \left( \hat{\Omega} \right) = B_z \sin \theta \frac{1}{\sqrt{1 - \left( \cos \theta \right)^2}} \frac{\partial}{\partial \phi} \gamma_q \left( \hat{\Omega} \right) = B_z \frac{\partial}{\partial \phi} \gamma_q \left( \hat{\Omega} \right). \]  

(A.3)

Angular basis functions are initially defined with respect to canonical coordinates as \( \gamma \left( \epsilon, \eta \right) \). Using the chain rule, equation (A.3) becomes:

\[ B_z \left( \frac{\partial \epsilon}{\partial \phi} \frac{\partial}{\partial \epsilon} + \frac{\partial \eta}{\partial \phi} \frac{\partial}{\partial \eta} \right) \gamma_q \left( \epsilon, \eta \right) = B_z \frac{\partial}{\partial \phi} \gamma_q \left( \epsilon, \eta \right). \]  

(A.4)

For example when \( \gamma \left( \epsilon, \eta \right) \) are quadratic basis functions,

\[ \gamma_1 \left( \epsilon, \eta \right) = (1 - \epsilon - \eta) (1 - 2 \epsilon - 2 \eta). \]  

(A.5)

It can easily be shown

\[ \frac{\partial \gamma_1}{\partial \epsilon} = 4 \epsilon + 4 \eta - 3. \]  

(A.6)

The other chain rule terms \( \frac{\partial \epsilon}{\partial \phi}, \frac{\partial \eta}{\partial \phi}, \frac{\partial \epsilon}{\partial \theta}, \frac{\partial \eta}{\partial \theta} \) are uniquely derived for each element using the inverse mappings of equations (10) and (11).

In the context of the finite element integral in equation (8a),

\[ \int_{\Omega_u} d\Omega \int_{\Omega_u} \gamma \left( \hat{\Omega} \right) \hat{\tau} \left( \vec{B}, \hat{\Omega} \right) \cdot \vec{\nabla}_\Omega \gamma_q \left( \hat{\Omega} \right) d\phi d\theta = B_z \int_{\epsilon, \eta} d\epsilon d\eta \left| J \right| \gamma \left( \epsilon, \eta \right) \left( \frac{\partial \epsilon}{\partial \phi} \frac{\partial}{\partial \epsilon} + \frac{\partial \eta}{\partial \phi} \frac{\partial}{\partial \eta} \right) \gamma_q \left( \epsilon, \eta \right) \]  

(A.7)

where

\[ \left| J \right| = \sin \theta \left| \begin{array}{cc} \frac{\partial \epsilon}{\partial \phi} & \frac{\partial \epsilon}{\partial \theta} \\ \frac{\partial \eta}{\partial \phi} & \frac{\partial \eta}{\partial \theta} \end{array} \right| \]  

(A.8)

is the Jacobian used to preserve area when integrating over the unit sphere with respect to canonical coordinates, also uniquely derived for each angular element.
References


Geant4 Collaboration 2011 Geant4 User’s Guide for Application Developers, Geant4 version 9.5.0 (http://geant4.cern.ch/)

Ghia A, Stéciw S, Fallon B G and Rathee S 2017 Experimental verification of EGSnrc Monte Carlo calculated depth doses within a realistic parallel magnetic field in a polystyrene phantom Med. Phys. 44 4804–15

Hennink A 2015 A discontinuous Galerkin method for charged particle transport in the Fokker–Planck limit MSc Thesis Technical University of Delft


Jin J M 2014 The Finite Element Method in Electromagnetics (Los Alamos, NM: Sandia National Laboratory)


Lewis E F and Miller W F Jr 1993 Computational Methods of Neutron Transport (La Grange Park, IL: American Nuclear Society, Inc.)


Pautz S D 2001 Verification of Transport Codes by the Method of Manufactured Solutions: The ATITLA Experience (Los Alamos, NM: Los Alamos National Laboratory)


Raaymakers B W et al 2009 Integrating a 1.5 T MRI scanner with a 6 MV accelerator: proof of concept Phys. Med. Biol. 54 N229–37

Raymond M, Fallon B G and Rathee S 2013 Dose response of selected ion chambers in applied homogeneous transverse and longitudinal magnetic fields Med. Phys. 40 041202

Salarie K and Knupp P 2000 Code Verification by the Method of Manufactured Solutions (Albuquerque, NM: Sandia National Laboratory)


Pautz S D 2001 Verification of Transport Codes by the Method of Manufactured Solutions: The ATITLA Experience (Los Alamos, NM: Los Alamos National Laboratory)


Raaymakers B W et al 2009 Integrating a 1.5 T MRI scanner with a 6 MV accelerator: proof of concept Phys. Med. Biol. 54 N229–37

Reynolds M, Fallon B G and Rathee S 2013 Dose response of selected ion chambers in applied homogeneous transverse and longitudinal magnetic fields Med. Phys. 40 041202

Salarie K and Knupp P 2000 Code Verification by the Method of Manufactured Solutions (Albuquerque, NM: Sandia National Laboratory)


