# Development of an Efficient Algorithmic Framework for Deterministic Patient Dose Calculation in MRI-guided Radiotherapy 

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#### Abstract

Accurate and efficient patient dose calculation for Magnetic Resonance Imaging (MRI)-guided Radiotherapy is pursued based on a deterministic solution to the Linear Boltzmann Transport Equation (LBTE) with magnetic fields, as a technique which does not suffer from statistical uncertainty, and presents an emerging alternative to Monte Carlo. In this framework, magnetic fields are modeled by an angular advection operator which introduces unique challenges and a new frontier to devise accurate and efficient solution techniques.

Key innovations in this work include, (i) the development of conventions to discretize the 6dimensional phase-space permitting harmonious interplay between space and angle, while retaining an acyclic space-angle discontinuous finite element solution sweep graph for all magnetic field orientations, (ii) the development of a novel angular advection upwind stabilization framework for curvilinear finite elements on the unit-sphere with flexibility energy adaptive forward-peaked angular meshing for parallel and perpendicular magnetic fields, and (iii) a novel runtime approach which ray-traces primary fluence using underlying continuous densities, while secondary scatter is reasonably approximated using a limited set of bulk material densities parameterized by $k$-means clustering. This enables an efficient transport sweep architecture leveraging batched multiplication by pre-inverted matrices and hierarchical batched assembly of the iterative scatter source.


Through the development of these novel mathematical frameworks and algorithms, overall computational complexity is greatly reduced, with the flexibility to compute multi-beam treatment plans on patient anatomies in the presence of strong magnetic fields parallel or
perpendicular to the radiation beam. At anatomical sites including lung, liver, and brain, over $99 \%(94 \%)$ of points pass a stringent $2 \% / 2 \mathrm{~mm}(1 \% / 1 \mathrm{~mm})$ gamma criterion validated against GEaNT4 reference Monte Carlo calculations in the presence of clinical magnetic field configurations. Runtimes of approximately 10 minutes per beam were achieved on a nonparallelized workstation implementation.

The algorithmic building blocks and prototype code developed in this work demonstrate feasibility for highly accurate patient dose calculations in clinical magnetic field configurations, and serves as a robust launching point for further investigation towards realtime adaptive MRIgRT.

## Preface

Patient datasets on which dose calculations are performed were obtained with ethics approval by the Health Research Ethics Board of Alberta Cancer Committee (HREBA.CC), under the Project Name: "Evaluation of novel dose calculation formalism for Linac-MR treatment planning," Project Number: HREBA.CC-15-0040, April 20, 2018.

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In all publications I was responsible for the design, mathematical development, software implementation, troubleshooting, and validation of novel algorithmic techniques, as well as writing the manuscript and revisions. Discussions with Dr. Zelyak helped clarify the role of Jacobians in mathematics. A GEANT4 user-code for radiotherapy in magnetic fields, along with computational cluster queuing system were written by Dan Michael Santos, and used for validation studies against Monte Carlo. Dr. Fallone provided project oversight, access to computational resources in the department, and contributed to manuscript review and revisions. Dr. St-Aubin provided key troubleshooting insight through numerous discussions, guidance on the scope and direction of possible investigations, early validation datasets from his proof of concept code, as well as major contributions to manuscript preparation and revision.

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## List of Abbreviations

| AAA | Anisotropic Analytic Algorithm |
| :---: | :---: |
| AAPM | American Association of Physicists in Medicine |
| BLAS | Basic Linear Algebra Subroutine |
| CBCT | Cone Beam Computed Tomography |
| CCC | Collapsed Cone Superposition Algorithm |
| CDF | Cumulative Probability Distribution |
| CEPXS | Coupled Electron Photon Cross Section |
| CFEM | Continuous Finite Element Method |
| CG | Conjugate Gradients |
| CHT | Condensed History Technique |
| CNR | Contrast to Noise Ratio |
| CPE | Charged Particle Equilibrium |
| CPU | Central Processing Unit |
| CSD | Continuous Slowing Down |
| CSDA | Continuous Slowing Down Approximation |
| CSR | Compressed Sparse Row |
| CT | Computed Tomography |
| CUDA | Compute Unified Device Architecture |
| DFEM | Discontinuous Finite Element Method |
| DO | Discrete Ordinates |
| DSA | Diffusion Synthetic Acceleration |
| DVH | Dose Volume Histogram |
| ECD | Electron Collimation Deflector |
| EEDL | Evaluated Electron Data Library |
| EPDL | Evaluated Photon Data Library |
| ERE | Electron Return Effect |
| FEM | Finite Element Method |
| FSDS | First Scattered Distributed Source |
| GBBS | Grid Based Boltzmann Solver |
| GPU | Graphics Processing Unit |
| GQ | Gaussian Quadrature |
| HSF | Head Scatter Factor |
| HU | Hounsfield Unit |
| ICF | Inhomogeneity Correction Factor |
| ICRU | International Commission on Radiological Units and Measurements |
| IGRT | Image Guided Radiotherapy |
| IM | Internal Margin |


| IRB | Institutional Review Board |
| :--- | :--- |
| IS | Inverse Square |
| KBA | Koch-Baker-Alcouffe |
| LBTE | Linear Boltzmann Transport Equation |
| MC | Monte Carlo |
| MMS | Method of Manufactured Solutions |
| MPF | Mean Free Path |
| MRI | Magnetic Resonance Imaging |
| MRIgRT | Magnetic Resonance Imaging Guided Radiotherapy |
| MU | Monitor Units |
| MV | Mega-Voltage |
| NIST | National Institute for Standards and Technology |
| OAF | Off-Axis Ratio |
| OAR | Organ at Risk |
| PDD | Percentage Depth Dose |
| PDF | Probability Distribution Function |
| PSF | Phantom Scatter Factor |
| PTV | Planning Target Volume |
| RF | Radio-Frequency |
| SI | Source Iteration |
| SAD | Source to Axis Distance |
| SIMD | Single Instruction Multiple Data |
| SM | Setup Margin |
| SNR | Signal to Noise Ratio |
| SPD | Symmetric Positive Definite |
| SSD | Source to Surface Distance |
| TERMA | Total Energy Released to Medium |
| TI | Therapeutic Index |
| TPR | Tissue Phantom Ratio |
| VRT | Variance Reduction Technique |
| WCSS | Within Cluster Sum of Squares |
|  |  |

## Chapter 1 Introduction

### 1.1 Cancer Control using Radiation Therapy

In both developing and developed countries, cancer ranks among the leading causes of mortality, and a growing healthcare burden, with more than 18 million new cases and 9.5 million deaths worldwide in $2018^{1}$. The lifetime risk of being diagnosed with cancer is estimated between 1 in 3 and 1 in 2 in developed countries including Canada ${ }^{2}$, the $\mathrm{UK}^{3}$, and the United States ${ }^{4}$. With increasing life expectancy and our interaction with complex modern environments of carcinogens, the genetic and physiochemical basis of each cancer is unique, thus no universal cure or vaccine ${ }^{5}$.

Shortly after the discovery of X-rays ${ }^{6}$ and radioactivity ${ }^{7}$ at the end of the $19^{\text {th }}$ century, the therapeutic application of ionizing radiation to treat cancer began showing promising results ${ }^{8}$, leading to Holthusen's hypothesis on the differential response between tumor cells and normal tissue ${ }^{9}$. Ionizing radiation sets in motion a cascade of physics interactions, resulting in the deposition of energy within the patient, quantified per unit mass as physical dose:

$$
\begin{equation*}
D=\frac{d E}{d m}, \text { units: }[G y]=\left[\frac{J}{k g}\right] . \tag{1.1}
\end{equation*}
$$

As illustrated in Figure 1.1, dose delivered within a certain range can achieve effective tumor control while sparing healthy tissue, leading to a beneficial therapeutic outcome.


Figure 1.1: Illustrating Holthusen's hypothesis on differential response of tumor and normal tissue cells to ionizing radiation dose.

Therapeutic Index (TI) is formally defined as the ratio between dose to normal tissue and dose to tumor to reach the same biological endpoint, usually $50 \%$ tumor kill and $50 \%$ normal tissue toxicity ${ }^{10}$ :

$$
\begin{equation*}
T I=\left.\frac{D_{N}}{D_{T}}\right|_{50 \% \text { tumor kill, } 50 \% \text { normal tissue toxicity }} \tag{1.2}
\end{equation*}
$$

Advances in the scientific understanding of ionizing radiation and biological response, along with technological progress in beam generation, modulation, and image guidance have enabled delivery of the optimal dose to ever tighter tolerances.

In the present day, more than half of cancer patients undergo radiation therapy, either as a primary treatment modality, or adjuvant to surgery and chemotherapy ${ }^{11}$. The focus herein will concern Mega-Voltage (MV) external beam photon radiotherapy, which is non-invasive, has sufficient depth penetration to reach deep seated tumors, and utilizes sophisticated technologies facilitating the generation, beam-forming, and delivery of the MV X-rays.

Radiation delivered to a living patient intersects a complex heterogeneous distribution of anatomy, each region having distinct radio-sensitivity and deformable motion ${ }^{10}$. Towards the overarching goal of improving Therapeutic Index across the patient geometry and over the duration of treatment, uncertainties in patient positioning (setup margin, SM) and intra-fractional motion of tumors (internal margin, IM) must be minimized ${ }^{12}$. Current mainstream image guide radiotherapy (IGRT) utilizes kilo-voltage X-ray cone beam Computed Tomography (CBCT) which rotates with the gantry. This on-board CBCT technique deposits a non-therapeutic radiation dose to all tissues in the field of view and is not capable of real-time imaging during treatment. Magnetic resonance imaging (MRI) guided delivery systems have been developed to greatly reduce internal margins of healthy tissue irradiated, though also introducing unique challenges for dose calculation.

### 1.1.1 MRI-guided Radiotherapy

The nuclear magnetic resonance signal ${ }^{13,14}$ of hydrogen nuclei in water molecules can be leveraged as a diagnostic imaging modality which offers superior soft tissue contrast, flexible
pulse sequences to reconstruct arbitrary 3D volumes, and the ability to image continuously without depositing additional ionizing radiation ${ }^{15}$. When integrated with external beam delivery, this enables high contrast volumetric tracking of soft tissue anatomy during irradiation, such that by adapting the beam in real-time, internal margins irradiating healthy tissue is significantly reduced, especially at sites involving respiratory motion. With this adaptation, dose to the tumor can be escalated while sparing surrounding organs at risk, thus improving the Therapeutic Index of the treatment.

Decoupling of magnetic interference between a linear accelerator (Linac) and MRI has been resolved by several groups ${ }^{16-18}$, resulting in hybrid Linac-MR devices now being adopted in the clinic. Two broad categories can be characterized based on their geometry, specifically the orientation of the main magnetic field $\left(\mathrm{B}_{0}\right)$ relative to the radiation beam, as illustrated in Figure 1.2. Key specifications of available clinical systems, or systems undergoing regulatory clearance are summarized in Table 1.1.


Figure 1.2: Illustrating major classifications of Linac-MR geometries (a) Bi-planar open design with beam configured parallel to main magnetic field, (b) Cylindrical solenoid design, where beam always remains perpendicular to the main magnetic field (inset illustrates cylindrical geometry viewed from same perspective as (a)).

Table 1.1: Linac-MR Systems and Key Specifications

| Device | Linac Energy | Magnetic Field <br> Strength | Magnetic Field Relative to <br> Beam |
| :---: | :---: | :---: | :---: |
| Magnettx Aurora-RT ${ }^{19}$ | 6 MV | 0.5 T | Parallel $(\\|)$ |
| Viewray MRIdian | 6 MV | 0.35 T | Perpendicular $(\perp)$ |
| Elekta Unity ${ }^{21}$ | 7.2 MV | 1.5 T | Perpendicular $(\perp)$ |

Traditional MRI scanners are based on a cylindrical solenoid geometry producing a magnetic field along its axis. Two systems are available where a linear accelerator radiation source rotates about the fixed $B_{0}$ axis of a stationary magnet, such that the beam remains perpendicular to a stationary magnetic field ${ }^{22,23}$ (Figure 1.2b). The MR imager in this classic configuration can easily achieve high $\mathrm{B}_{0}$ field strength, such as 1.5 T on the Elekta ${ }^{\mathrm{TM}}$ Unity ${ }^{\circledR}{ }^{\circledR}$ system, which has a high signal to noise ratio (SNR) equivalent to diagnostic grade images ${ }^{24}$. However, dosimetric perturbations of hot and cold spots inherent to the perpendicular configuration are present even at lower field strengths such as the 0.35 T Viewray ${ }^{\mathrm{TM}}$ MRIdian ${ }^{\circledR}{ }^{\circledR}$ system ${ }^{25}$. Cylindrical magnets are also limited in their bore diameter, resulting in a claustrophobic experience for patients ${ }^{26}$, while only able to achieve longitudinal couch motion to deliver optimal treatments along the central axis, and not anatomical extremities ${ }^{27}$.

A novel alternative is to integrate a compact linear accelerator in-line with an open bi-planar superconducting MRI magnet ${ }^{28,29}$ rotated together on the same gantry such that the magnetic field remains parallel to the irradiation beam at all gantry angles relative to the patient (Figure 1.2a). The research system which has developed into the Magnet $\tau x^{\text {TM }}$ Aurora-RT ${ }^{\circledR}$ was the world's first to produce MR images during irradiation ${ }^{30}$. This design utilizes the opening of the bobbin around which current carrying wires are wound to serve as an aperture for the linac beam to pass through, always parallel to $\mathrm{B}_{0}$. Despite falling short of diagnostic quality 1.5 T , studies have shown the 0.5 T range to be optimal for maximizing contrast to noise ratio (CNR) ${ }^{31}$ which is an important metric for contouring soft tissue anatomy ${ }^{32}$. The open setup allows for improved patient access, including the flexibility for lateral couch shift to treat anatomical extremities at isocenter. Moreover, this device does not require cryogens nor the radiation shielding complications of a quench-pipe, and is able to fit inside a standard vault without special renovations ${ }^{29}$. Most importantly, dosimetric perturbations in-vivo are less disruptive than in the perpendicular configuration ${ }^{33}$.

### 1.1.2 Dose Perturbation in a Strong Magnetic Field

The inevitable physics of irradiating the patient while immersed in a strong magnetic field is to cause deflection of dose depositing secondary electrons via the Lorentz force. Specifically we consider the main imaging magnetic field $\mathrm{B}_{0}$ which is orders of magnitude stronger than gradient or fringe fields ${ }^{34}$. The dominant dosimetric effect can be characterized based on whether $\mathrm{B}_{0}$ is parallel or perpendicular to the exteral beam, applicable to the systems in Table 1.1.


Figure 1.3: Schematic illustrating angular distribution of 6 MeV electrons in air for (a) No magnetic field, (b) $\mathrm{B}_{0}$ parallel to the beam, (c) No magnetic field, (d) $\mathrm{B}_{0}$ perpendicular to the beam. Figures generated using validated codebase ${ }^{35}$ of Chapter 4. Colormap used to facilitate depth perception.


Figure 1.4: Central axis depth dose in a heterogeneous phantom showing perturbation due to a magnetic field (red) compared to a baseline without magnetic fields (blue) for (a) $\mathrm{B}_{0}=1.5 \mathrm{~T}_{\text {perpendicular }}$ crossing heterogeneous slab of lung (b) $\mathrm{B}_{0}=$ $0.5 \mathrm{~T}_{\text {parallel }}$ crossing heterogeneous slab of lung, (c) $\mathrm{B}_{0}=0.5 \mathrm{~T}_{\text {parallel }}$ crossing heterogeneous slab of air. Plots generated using validated codebase ${ }^{35}$ of Chapter 4.


Figure 1.5: Dose distribution for a 6 MV photon beam directed downwards through a heterogeneous phantom in the presence of a 1.5 T magnetic field (a) parallel to the beam, (b) at $90^{\circ}$ to the beam, (c) at $37^{\circ}$ to the beam. Figures generated using validated codebase ${ }^{35}$ of Chapter 4.

When $\mathrm{B}_{0}$ is parallel to the beam, the dominant effect is increased collimation and reduction in dose penumbra due to electron confinement in tight helical trajectories along magnetic field lines ${ }^{33,36,37}$. As observed in Figures $1.4(b, c)$, increase to dose along the central axis is most pronounced for low density media, especially air, where the mean free path (MPF) of electrons is longest, allowing the magnetic field the greatest opportunity to induce cyclotron motion ${ }^{38}$ which complements electrons' forward momentum, effectively elongating the path length, and thus the opportunity to undergo interactions which deposit energy. In lung, the dose increase is only about $3 \%$, however in air, the difference approaches $35 \%$. As shown in Figure 1.3a, the overall direction of electrons in a parallel magnetic field remains unchanged, however near the beam edges, the angular distribution pinches slightly inward, indicative that electrons otherwise scattering away from the beam are confined by strong magnetic field guiding centers ${ }^{38}$. An important consequence for MRIgRT is the tendency for fringe fields to focus electron contaminants generated in the linac head to proceed under strong collimation by the parallel magnetic field to reach the patient surface, causing a substantial increase in skin dose, up to $1000 \%$ for $\mathrm{B}_{0}=1 \mathrm{~T}$ compared to no magnetic field ${ }^{39}$. Designs have been proposed of electron collimation deflector (ECD) ${ }^{40}$ systems where a permanent magnet assembly installed just below the linac head creates a perpendicular magnetic field to deflect electrons originating from the head away from the beam. In simulation studies, several of the proposed ECD designs efficiently
deflected nearly all electron contaminants originating from the head, while having minimal impact on MRI image quality ${ }^{41}$. Other sources of electron contamination enhanced by a parallel magnetic field arise when photons of a megavoltage beam ionize air as well as standard radiofrequency (RF) coils enroute to the patient ${ }^{42}$. Studies attempting to mitigate increased skin dose from these sources investigated substituting air with helium ${ }^{41}$, and the design of radiologically transparent RF coils which do not obstruct the beam path ${ }^{43}$. An alternative strategy to mitigate enhanced surface dose to the patient is to add a bolus to absorb any hotspots produced by electrons, however this brings the effective maximum dose to the surface, sacrificing the skin sparing benefits of megavoltage beams ${ }^{44}$. Approaches to manage skin dose remains an active area of research.

The potential benefits of a parallel magnetic field for lung treatment planning have been confirmed by multiple groups ${ }^{33,45-48}$. By reducing lateral scatter in low density media, more energy is preserved in the forward direction where multiple beams intersect at the tumor, accompanied by the characteristic dose increase to low density regions of the $\mathrm{PTV}^{45}$. Moreover, sharper beam edges enable a steeper dose gradient between the PTV and surrounding lung tissue, and thus overall dose to lung for a multi-field plan can be reduced by nearly $20 \%{ }^{46}$ However, realizing these benefit requires a dose calculation engine which accurately models the effect of magnetic fields ${ }^{49}$.

The impact of a perpendicular magnetic field relative to the beam presents potentially greater concern for avoiding gross errors in the resulting treatment plan ${ }^{46}$. As seen in Figure 1.3b, the angular distribution of electrons is deflected laterally, consistent with the Lorentz force. The degree of lateral deflection varies inversely with density (and MPF) of electrons in the medium. Within homogeneous water, the buildup to maximum dose is shallower (Figure 1.4a), with an asymmetric shift in the lateral profile (Figure 1.5b). These effects have been measured by various groups ${ }^{50,51}$. The greatest perturbation occurs at the boundary proximal to low density media, such as where the beam exits the patient into air, or at internal boundaries to air pockets (in lung, bowel, rectum, or stomach). Electrons, upon entering a low density medium, have sufficient mean free path length to be deflected $180^{\circ}$ by a perpendicular magnetic field, depositing dose on the proximal surface, with dose increases on the order of $40 \%$ (Figure 1.4a). This returning of electrons to the proximal surface has been termed the electron return effect (ERE). Exit skin dose
increases due to ERE while entrance skin dose decreases ${ }^{44}$. Meanwhile, dose decreases at the distal end of the low density region due to an absence of electrons to replace those swept upstream by the magnetic field. It is essential that dose calculations for Linac-MR systems of the perpendicular configuration accurately model these manifestations of the ERE to anticipate and mitigate hot and cold spots caused by the magnetic field ${ }^{52,53}$. Studies attempting to minimize the impact of ERE by optimizing beam configuration have achieved acceptable plan quality in terms of dose volume metrics ${ }^{47,54,55}$, however characteristic hotspots and coldspots cannot be eliminated completely, thus contribute to greater dose heterogeneity in irradiated regions. The technique of adding beams from multiple angles to spatially distribute ERE hotspots angles must consider that each beam passes through different organs at risk (OAR), with the spinal cord being particularly sensitive ${ }^{54}$. Ultimately, plan optimization is predicated on dose calculations which accurately model magnetic fields in heterogeneous media ${ }^{56,57}$.

### 1.2 Radiotherapy Dose Calculation

Accurate determination of the radiation dose delivered to a patient's anatomy provides essential information to predict the effectiveness and safety of a radiotherapy treatment plan. The international commission on radiological units and measurements (ICRU) recommends physical dose be delivered to within $5 \%$ of the planned distribution, establishing an action level for uncertainties across the entire treatment ${ }^{12}$. Considering sources of error in patient positioning, movement of internal anatomy, and variations in machine output, the accuracy of dose calculation is recommended to be kept within $2 \%$ of measurement in low gradient regions, and within 2 mm for high gradient regions ${ }^{58}$. Further detailed guidelines established in the AAPM Medical Physics Practice Guideline 5.a specify acceptance criteria for dose uncertainties during commissioning ${ }^{59}$. When deployed to heterogeneous media, AAPM report 85 recommends accuracy of computed dose distributions to be between $1 \%-2 \%$ of delivered dose ${ }^{60}$.

In addition to accuracy, another important consideration for clinical dose calculations is the runtime within a treatment workflow. The focus herein will concern external beam photon radiotherapy in the presence of strong magnetic fields, starting with an overview of historical dose calculation techniques and their limitations.

### 1.2.1 Correction-Based Framework

Early attempts to model patient dose distributions were derived from data repositories of standard commissioning measurements made in a homogeneous water phantom. Through the use of algebraic correction factors having well characterized physical origins, the dose to a point can be estimated. An approach for isocentric linac planning can be formulated as ${ }^{61}$ :

$$
\begin{equation*}
D\left(d_{p}, x\right)=\dot{D}_{r e f} \cdot M U \cdot T P R_{\left(d_{p}, f s @ z_{p}\right)} \cdot I S_{\left(z_{r f} \rightarrow z_{p}\right)} \cdot H S F_{\left(f_{\text {collimeted }}\right)} \cdot P S F_{\left(f s @ d_{r e f}\right)} \cdot O A F_{(x)} \tag{1.3}
\end{equation*}
$$

where dose delivered to a point of interest at depth $d_{p}$ from the phantom surface ( $z_{p}$ from the source) and lateral displacement $x$ from the central axis is a product of several factors, chief among them the Tissue Phantom Ratio (TPR) ${ }^{61}$ :

$$
\begin{equation*}
T P R=\frac{D\left(d_{p}\right)}{D\left(d_{r e f}\right)} \tag{1.4}
\end{equation*}
$$

which relates dose at the central axis depth of interest relative to a central axis reference depth where absolute dose is normalized. Monitor Units (MU) characterize the machine output of the linac. In TG- $51^{62}$, a linear accelerator is calibrated to deliver a dose rate $\dot{D}_{\text {ref }}=1 \mathrm{cGy} / \mathrm{MU}$ for a $10 \times 10 \mathrm{~cm}^{2}$ field size, typically at $d_{\text {ref }}=d_{\max }$. TPR is measured during commissioning for each output energy and standard field size. Inverse Square (IS) corrects for area over which the beam energy is spread, Head Scatter Factor (HSF) and Phantom Scatter Factor (PSF) correct for differences in relative dose at the reference point due to scatter from the linac head and from the patient medium respectively. Off Axis Factor (OAF) corrects for dose variations moving away from the central axis. The product of all these factors is a point dose assuming homogeneous water throughout.
Additional factors may correct for irregular surface topology, blocking due to beam modifiers (wedges), the presence of material inhomogeneities within the patient, and irregular field shape. Of these effects, inhomogeneities are the most interesting to consider, and highlights the ultimate limitations of correction based approaches in a medium not composed of pure water.

Most simplistically, an Equivalent Radiological Path Length can be defined ${ }^{60}$ :

$$
\begin{equation*}
d_{e f f}=\int_{0}^{d} \rho(\vec{r}) d l, \tag{1.5}
\end{equation*}
$$

where $d_{\text {eff }}$ is the effective depth of water which would attenuate the same amount as tracing through the actual density distribution along $d l$. The inhomogeneity correction factor is thus ${ }^{60}$ :

$$
\begin{equation*}
I C F_{e q u i v}=\frac{\operatorname{TPR}\left(d_{e f f}, f s\right)}{\operatorname{TPR}(d, f s)} \tag{1.6}
\end{equation*}
$$

where $f_{S}$ denotes square field edge dimension at the point of interest. Notably the location of inhomogeneity does not play a role. Improvements through the Batho Power Law ${ }^{63}$ accounts for relative location of slab inhomogeneities while Equivalent Tissue Phantom Ratio (ETPR) ${ }^{64}$ additionally weights the relative scatter contribution for arbitrarily shaped inhomogeneities. The effect of irregular field size can be approximated using Clarkson sector integration ${ }^{65}$ still used by some second-check codes ${ }^{50}$.

Ultimately, the system of correction factors fails to model scatter near material boundaries, with inaccuracies up to $70 \%$ in the sinus region and $20 \%$ in lung ${ }^{66}$. Magnetic fields pose further challenges as the Lorentz force may deflect the trajectory of electrons upstream (consider Figure 1.5), which cannot be predicted using effective path length scaling.

Correction based approaches require strict conditions of charged particle equilibrium (CPE) to qualify as an accurate measurement of dose. TPR provides relative dose with respect to the reference measurement of TG-51, which requires the stopping power ratio between water and air at other depths to approximately equal that at the reference point ${ }^{62}$. CPE is violated in the buildup region where far more high energy electrons are released as they start their tracks than are stopped ${ }^{67}$, resulting in a highly variable stopping power ratio ${ }^{68}$. Another limitation arises near field edges and for small field sizes, where the absence of lateral charged particle equilibrium (more particles stopping than set in motion) causes similar difficulties for normalization ${ }^{69}$. Moreover, volume averaging in the positioning of a finite size ion chamber near field edges causes the penumbra to broaden.

Due to the relative simplicity of algebraic correction factors and traceability to measured data, correction-based approaches still have relevance as an order of magnitude sanity check, often computed by hand or extremely rapidly by digital computers ${ }^{70}$.

### 1.2.2 Model-Based Framework

Advances in digital computers make it feasible to model certain aspects of radiation transport explicitly, and thus move away from the look-up table approach of correction-based methods. Point kernel superposition will be examined in terms of its mechanics and limitations with respect to inhomogeneities and magnetic fields. This method shares key attributes with other clinical workhorse algorithms like pencil beam superposition and collapsed cone superposition. The central challenge for model based approaches arises due to nonlocal energy deposition, where dose to a point is due to energy released from particles upstream.

Primary photons from the radiation source are explicitly transported by raytracing to points of interaction in the patient geometry. The total energy released into the medium (TERMA, $T(\vec{r})$ ) at the interaction site $\vec{r}$ is ${ }^{71}$ :

$$
\begin{equation*}
T(\vec{r})=\Psi(\vec{r})\left(\frac{\mu}{\rho}\right), \tag{1.7}
\end{equation*}
$$

where $\Psi$ refers to the energy fluence of primary photons having units of $J / \mathrm{m}^{2}$ (a different meaning will be given to $\Psi$ in the context of the LBTE for Chapter 2 and beyond). $\mu$ is the total linear attenuation coefficient for the material at the interaction site, and $\rho$ is the density of the medium at the point of interaction. For a realistic polyenergetic source, the entire spectrum is considered, often simplified as the expectation value of the full spectrum. TERMA includes all energy released to secondary particles from point of primary interaction (including radiative components). The downstream spatial distribution of dose deposition can be encoded by a kernel function $\Lambda\left(\vec{r}-\vec{r}^{\prime}\right)$ which depends only on relative displacement between the site of primary interaction $\vec{r}^{\prime}$ and site of dose consideration $\vec{r}$, resulting in the formulation:

$$
\begin{equation*}
D(\vec{r})=\int T\left(\vec{r}^{\prime}\right) \Lambda\left(\vec{r}-\vec{r}^{\prime}\right) d \vec{r}^{\prime} . \tag{1.8}
\end{equation*}
$$

Dose to a point is the result of upstream TERMA coupled to a kernel accounting for nonlocal energy deposition. Within homogeneous media, Eq. 1.8 can be treated as a linear shift-invariant system where the convolution operation can be done in the frequency domain by first invoking a Fast Fourier Transform ${ }^{72}$.

More generally, the kernel, which has been precalculated using more fundamental techniques such as Monte Carlo, can be parameterized by material at the point of interaction $\Lambda_{\text {mat }\left(\vec{r}^{\prime}\right)}\left(\vec{r}-\vec{r}^{\prime}\right) d \vec{r}^{\prime} .{ }^{70}$ Most implementations assume a kernel in water, parameterized by effective radiological path length (conceptually defined in Eq. 1.5) which involves scaling by mass density. This serves as a reasonable approximation in the Compton dominated energy regime where the effective atomic number for physiologic media does not differ significantly from water. These conventions can be formulated ${ }^{70}$ :

$$
\begin{equation*}
D(\vec{r})=\int T\left(\rho_{\vec{r}^{\prime}} \cdot \vec{r}^{\prime}\right) \Lambda\left(\rho_{\vec{r}-\vec{r}^{\prime}} \cdot\left(\vec{r}-\vec{r}^{\prime}\right)\right) d \vec{r}^{\prime} \tag{1.9}
\end{equation*}
$$

where the effective radiological path length $\rho_{r^{\prime}} \cdot \vec{r}^{\prime}$ is from source to primary interaction point, and $\rho_{\vec{r}-\vec{r}^{\prime}} \cdot\left(\vec{r}-\vec{r}^{\prime}\right)$ is from the primary interaction to dose deposition site. This approach addresses variable attenuation by inhomogeneities for primaries and scatter along the direct line of sight between point of interaction and point of dose deposition. However, this method is unable to correct for complex scenarios where sources of lateral scatter must also be considered ${ }^{70}$. Ultimately it is infeasible to pre-calculate kernels representing every complex configuration of material heterogeneity.

Nonlocal energy deposition presents further challenges in the presence of magnetic fields which alter the macroscopic angular distribution of electrons, as a function of material and magnetic field configuration.


Figure 1.6: Visualization of non-local energy deposition as scattering kernels for 6 MeV electrons in (a) pure water, (b) pure air, (c) crossing the boundary from water to air, where distal regions of the kernel upon reaching air are not correctly deflected in the presence of magnetic fields. Colormap used to facilitate depth perception.

As illustrated in Figure 1.6, if the material changes over the practical range of secondary electrons (on the order of centimeters for megavoltage energies), there is no mechanism in the superposition framework to correct for the altered behavior of scattering due to a magnetic field.

Pfaffenberger ${ }^{73}$ attempted to implement kernel warping to account for magnetic field dose perturbation within a superposition framework, however the approach was not sufficiently robust to account for the sheer variety of materials, magnetic field orientations and strengths which could occur in radiotherapy. Near material boundaries, charged particle equilibrium is perturbed, and magnetic fields can dramatically alter the scattering behavior, requiring particle transport to be modeled at a more fundamental level to ensure accurate patient dose calculations ${ }^{73}$.

Pencil beam superposition condenses point kernels along the depth axis, assuming an infinite water medium ${ }^{61}$. The resulting kernel is coupled to TERMA over a 2D plane where the beam enters the patient. This approach improves the efficiency of calculations, and is used as a clinical workhorse Varian's Anisotropic Analytic Algorithm (AAA) ${ }^{74}$. Collapsed cone superposition $(\mathrm{CCC})^{71}$ condenses the lateral spread of point kernels to the central axes of a set of cones distributed in orientation, emanating from each primary interaction site. Dose is only transported along these discrete directions, ignoring inverse square falloff, and resulting in ray-effect artifacts far from the source ${ }^{70}$. The aforementioned limitations (Figure 1.6) apply to both pencil
beam and collapsed cone approaches, thus a more sophisticated framework is needed for MRIguided radiotherapy.

### 1.2.3 Principle Based Framework

The most rigorous approach to dose calculation solves the underlying physics of radiation transport, as governed by the Linear Boltzmann Transport Equation (LBTE). Although computationally intensive, they simulate physics at a fundamental level including regions in the absence of charged particle equilibrium.

### 1.2.3.1 Monte Carlo

Stochastic integration of the LBTE using a Monte Carlo (MC) approach involves simulating the histories of a large number of particles and sampling their probabilistic interactions in traversing through heterogeneous media. A detailed theoretical overview is provided in $\S 2.5$.

The flexibility of MC and its relative simplicity in formulating particle transport as probabilistic sampling of microscopic processes paved the way for early development and maturation of MC to become the gold standard for accurate radiotherapy dose calculations. It had long been thought Monte Carlo offered the only feasible way to incorporate magnetic fields into radiotherapy dose calculations ${ }^{75}$. General purpose MC codes such as GEANT4 ${ }^{76}$, Penelope ${ }^{77}$, and EGSnrc ${ }^{78}$ have been adapted for radiotherapy regimes, with successful implementations of magnetic fields, validated against measurement ${ }^{79-81}$.

Historically, MC had been too computationally intensive to be deployed routinely in the clinic, and its results always involve a degree of statistical uncertainty. The central methodology for achieving faster runtimes in Monte Carlo is through variance reduction techniques (VRT) ${ }^{82}$, with the goal of minimizing statistical uncertainty (variance) in the region of interest, which scales inversely proportional to the number of statistically independent particles $N$.

Real variance reduction techniques (RVRT) alter the microscopic transport and sampling of physics in a way which increases efficiency, though with the property of converging to the true
expected value in the statistical limit of large number ${ }^{83}$. An example commonly deployed in radiotherapy codes is Directional Splitting with Russian Roulette ${ }^{84}$. In the event that a single particle generated by an interaction has sufficient probability of reaching the detector, it is split into a large number $N_{\text {split }}$ of 'meager' particles, each having a reduced weight $w=1 / N_{\text {split }}$, distributed according to a precalculated probability function. Russian Roulette is performed on meager particles having less probability of reaching the detector, with survival probability $1 / N_{\text {split }}$, with remaining particle weights adjusted accordingly. Applied to Bremstrahlung photons, this was shown to have the single greatest impact on efficiency, with a speedup factor of $\sim 150{ }^{85}$. Extra overhead is needed to keep track of particle weights as to not overestimate the number of statistically independent events contributing to variance in the final result.

Other RVRTs include interaction forcing, exponential transform, and Woodcock tracking ${ }^{83}$, the latter often the basis for fast implementations of photon transport ${ }^{84}$. A fictitious cross section which leaves the energy and direction of the photon unchanged is added in the correct proportion to every spatial element such that the total cross section perceived by the photon is uniform across the entire domain, enabling direct transport to the interaction site without raytracing ${ }^{84}$.

Another class of approximate variance reduction methods (AVRT) alter the treatment of physics in a way which does bias the final outcome ${ }^{83}$. Nevertheless, when applied judiciously, these methods can retain sufficient accuracy for the intended application while yielding substantial gains in efficiency. This includes the condensed history technique (CHT) ${ }^{86}$, a core methodology for electron Monte Carlo transport which treats soft collisions using the continuous slowing down (CSDA) formalism ${ }^{68}$. Other approximations which can be adapted into efficient tradeoffs involve the setting of various physics transport parameters and cutoffs; for example eliminating particles from being tracked once their energy falls below a certain threshold ${ }^{83}$. Moreover, sequences of quasi-random numbers can be used which more efficiently integrate the higher dimensional space under consideration ${ }^{84}$.

When multiple variance reduction techniques are applied, their interplay must be carefully managed to avoid biasing downstream results. Since Monte Carlo tracks the histories of
individual particles, the effect of various approximations on macroscopic dose is more difficult to anticipate.

Denoising comprises a family of post-processing techniques which smoothen the qualitative appearance of the dose distribution, and can reduce the number of particles needed to achieve a visual criterion of smoothness by up to a factor of $20^{87}$. These include the wavelet method ${ }^{88}$, diffusion based filtering ${ }^{89}$, and iterative smoothing techniques which minimize the spatial derivatives of dose ${ }^{90}$. Since filtering techniques are not aware of any of the underlying physics, they can increase both systematic and random error, thus are most useful for generating a visually smooth distribution for qualitative evaluation of adaptive plans to be rapidly calculated using a reduced number of histories ${ }^{87}$.

Various accelerated Monte Carlo codes including GPU implementations have introduced approximations such as aggressive variance reduction, coarser sampling of physics processes, and dose smoothing ${ }^{91-93}$ which can degrade the accuracy compared to reference-standard research codes such as GEANT4 ${ }^{94}$ and EGSnrc ${ }^{95}$. Moreover, due to the inherent statistical uncertainty of Monte Carlo dose distributions, AAPM TG-105 recommends they not be used to prescribe point dose, but rather through dose volume histogram (DVH) metrics ${ }^{82}$. Introduction of a magnetic field, especially in the perpendicular configuration, is known to cause heterogeneous dose distributions within the volume of interest ${ }^{55}$, thus the statistical uncertainty of MC limits the confident evaluation of dose distribution information not captured by DVH, but otherwise yielding valuable insight for MRIgRT planning.

### 1.2.3.2 Deterministic GBBS

Deterministic techniques directly discretize the 6-dimensional particle phase space (position and angular momentum distribution) of the LBTE, which is solved using a numerical framework such as the Finite Element Method (FEM). A deterministic solution implies that given the same discretization parameters, problem setup, and convergence criteria, every run will repeatedly converge to identical values for the discrete degrees of freedom within machine precision. Theoretical foundations have been established by the nuclear engineering community, in particular for neutron transport during the late $20^{\text {th }}$ century ${ }^{96,97}$.

A renaissance for radiotherapy applications was established by the Atilla code ${ }^{98,99}$, showing proof of concept the potential to achieve very high accuracy for calculating dose in heterogeneous media ${ }^{100,101}$, exhibiting far better agreement with Monte Carlo than model-based AAA or CCC algorithms ${ }^{102-105}$. Practical advantages of the deterministic approach include the ability to simulate all beams of an arc plan simultaneously ${ }^{102}$, whereas Monte Carlo requires independent histories at each beam angle. Moreover, the deterministic solution does not introduce statistical uncertainty ${ }^{106}$, enabling accurate evaluation of point doses, and even interpolation within a given spatial element.

The commercial code Acuros ${ }^{107}$, evolved from Attila, is based on a Discrete Ordinates (DO) model in angle, and currently deployed for patient dose calculation in clinics worldwide. In their whitepaper, it is stated that the approach in Acuros is only valid in the absence of external magnetic fields ${ }^{107}$. However, the closely related Vlasov equation had been used in linear accelerator design, explicitly to simulate the effect of charged particles in the presence of oscillating electric and magnetic fields ${ }^{108}$. Pioneering efforts by St-Aubin et al ${ }^{109}$ have successfully incorporated the Lorentz force operator into the Eulerian (deterministic) form of the LBTE as an advection operator in angle. Similar findings were also shown by Pautz et al ${ }^{110}$. Excellent agreement with Monte Carlo was demonstrated at the $2 \% / 2 \mathrm{~mm}$ and $1 \% / 1 \mathrm{~mm}$ gamma criteria ${ }^{109}$ for challenging heterogeneous geometries. However, the Source Iteration (SI) solution technique when applied to a Discrete Ordinates formalism in angle was found to have a limited regime of stability, and becomes unstable for low density media or strong magnetic fields ${ }^{111}$. Moreover, Discrete Ordinates exhibits known ray-effect artifacts consisting of non-physical variations in the directional distribution of fluence, distal to a scattering source ${ }^{96}$.

A more sophisticated scheme of angular discretization utilizes the Discontinuous Finite Element Method (DFEM) in angle, which had been successfully incorporated to transport codes in the absence of magnetic fields ${ }^{112-117}$, shown to mitigate ray-effects and improve accuracy. When angular DFEM was implemented with magnetic fields on a flattened domain ${ }^{118}$, the approach was shown to be unconditionally stable ${ }^{111}$.

An alternative deterministic approach incorporating magnetic fields is a low-order angularmoments approximation of the LBTE, which was shown to achieve reasonable passing rates at a $3 \% / 3 \mathrm{~mm}$ gamma criterion against Monte Carlo ${ }^{119}$, though it was also found to be sensitive to magnetic field orientation ${ }^{120}$, with constraints on stability which require careful setting of a relaxation parameter shown to impact accuracy ${ }^{121}$. Thus it is hypothesized that explicit modeling of the angular domain through DFEM preserves the highest levels of intrinsic accuracy and robustness, while offering fine control over the physics and discretization parameters to enable an efficient calculation.

Compared to MC, development of efficient deterministic dose calculation approaches for MRIgRT has received far less attention, representing a new area of science to be explored.

### 1.3 Research Motivation

Having established feasibility to include magnetic fields in the LBTE ${ }^{109,118}$, efforts shift to the development of accurate, more efficient, and flexible algorithmic techniques demonstrating feasibility for deterministic patient dose calculations in MRI-guided radiotherapy.

Early proof of concept calculations ${ }^{118}$ took days to run on a 48-CPU high performance server, with substantial room for improvement towards clinical applicability. Advection in angle, as a consequence of magnetic fields, presents unique computational challenges requiring a DFEM approach in angle which is more complex but offers greater flexibility compared to discrete ordinates. Interplay between space and angle, adaptations to anisotropic meshing, conventions for oblique beams, hierarchical assembly and runtime orchestration of scattering terms, and conventions for patient material distributions all have room for improvement through the development of new algorithms.

The focus herein concerns formulation of novel mathematical frameworks, algorithmic techniques, and physics adaptations which reduced runtime from days to minutes on a single workstation. These algorithms provide the flexibility to calculate on patient geometries and clinical magnetic field configurations, and validated to preserve the highest levels of accuracy.

This work contributes key algorithmic building blocks towards an efficient patient dose calculation in magnetic fields, specifically by developing:
(i) Conventions to discretize 6-dimensional phase-space permitting harmonious interplay between space and angle by retaining an acyclic space-angle DFEM sweep graph for oblique magnetic field orientations without regridding the underlying geometry.
(ii) A novel angular advection upwind stabilization framework for curvilinear DFEM on the unitsphere with flexibility to independently adapt and transfer fluence between forward and backscattering angular hemispheres, enabling energy adaptive meshing schemes tailored to problem anisotropy in parallel and perpendicular magnetic fields.
(iii) A novel transport sweep architecture leveraging batched multiplication of pre-inverted matrices with bulk material densities parameterized by $k$-means clustering of patient material densities. At runtime a hybrid approach ray-traced primary fluence using the full CT data, while secondary scatter was reasonably approximated using a limited set of bulk material densities.
(iv) A complete implementation codebase involving adaptive Cartesian mesh generation, raytracing of oblique beams, patient data pipeline, and hierarchical batched assembly of the iterative scatter-source. These results are compared against full Monte Carlo calculations using 3D gamma metrics for multi-field plans on anatomical sites encompassing lung, brain, and liver, for parallel and perpendicular magnetic fields.

As an alternative to accelerated Monte Carlo codes, we demonstrate feasibility of a novel deterministic approach to arrive at an accurate dose distribution through a completely different solution methodology, providing complementary perspective, for potential deployment as a primary dose calculation engine, or second check algorithm.

These developments contribute new insights to the emerging field of deterministic dose calculations in magnetic fields for which we show highly accurate patient dose calculations within a reasonable runtime and absence of statistical uncertainty.

### 1.4 Thesis Scope and Outline

Having introduced the context of radiotherapy dose calculations and the unique challenges of modeling magnetic fields for MRIgRT, aspects on the development of a novel deterministic codebase is detailed in upcoming chapters. Although many investigations were performed, only those yielding key insights or enduring algorithmic building blocks will be discussed.

Chapter 2 establishes theoretical foundations for a deterministic solution to particle transport by deriving the LBTE, describing the physics processes responsible for cross sections, and introducing the numerical techniques for discretization as well as convergence. Theoretical foundations of Monte Carlo and details of the research code GEANT4 are provided which was used as the validation tool to benchmark our novel algorithms.

Chapter 3 describes an initial attempt to reformulate the problem for maximum explicit parallelization using a second order least squares continuous finite element framework (LSCFEM). This enabled the development of novel algorithms which leverage the single instruction multiple data (SIMD) parallelism of GPU architectures. A full end-to-end dose calculation was developed, however the dosimetric limitations of continuous finite elements in modeling sharp material discontinuities are highlighted, requiring reformulation.

Chapter 4 revisits the discontinuous finite element method (DFEM), and establishes conventions for harmonious interplay between space and angle resulting in acyclic directed sweep graphs even for oblique magnetic field orientations.

Chapter 5 develops enabling algorithmic techniques for energy-adaptive forward-peaked angular FEM discretization conformed to the energy dependent fluence anisotropy in both parallel and perpendicular magnetic fields, as well as conventions for oblique beams.

Chapter 6 develops a novel spatial transport sweep architecture addressing the most computationally intensive aspect of the solution, through batched multiplication by pre-inverted matrices, with material densities ascertained by $k$-means clustering. Validation for multi-field plans on lung, brain, and liver anatomical sites are presented, in the presence of parallel and perpendicular magnetic fields.

Chapter 7 concludes with discussion on areas for future development and novel applications of deterministic dose calculations.

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## Chapter 2 Theory and Techniques

### 2.1 Linear Boltzmann Transport Equation

Deterministic principle-based dose calculations explicitly solve the Linear Boltzmann Transport Equation (LBTE) to obtain the distribution of angular fluence in a 6 -dimensional phase space as a precursor to dose. The basic terms and overall structure of the LBTE will be derived from principles of differential particle balance. Interaction cross sections will be decomposed into selected relevant physics processes.

### 2.1.1 Phase Space

The Lagrangian and Eulerian formulations provide complementary perspectives on particle transport ${ }^{1}$. Microscopically, the position $\vec{r}=\{x, y, z\}$ and momentum $\vec{p}=\left\{p_{x}, p_{y}, p_{z}\right\}$ can be tracked for each particle in a Lagrangian formulation of the LBTE such as Monte Carlo ${ }^{2}$.

Alternatively, a macroscopic function quantifying the density of particles for each position and momentum state can be solved through a Eulerian formulation of the LBTE.

The density of particles in phase-space as a function of position, angle, and energy can be specified as:

$$
\begin{equation*}
N(\vec{r}, \hat{\Omega}, E, t) \tag{2.1}
\end{equation*}
$$

where momentum has been equivalently expressed in terms of energy $E$, and direction of propagation $\hat{\Omega}=\{\sin \theta \cos \varphi, \sin \theta \sin \varphi, \cos \theta\}$, with $\varphi$ being the azimuthal angle and $\theta$ the polar angle in spherical coordinates.

For radiotherapy contexts it is more convenient to consider angular fluence:

$$
\begin{equation*}
\Psi(\vec{r}, \hat{\Omega}, E, t)=v N(\vec{r}, \hat{\Omega}, E, t) \tag{2.2}
\end{equation*}
$$

where $v$ denotes the local speed of particles.

Dose at a point is obtained by integrating the steady state angular fluence of energy depositing particles over all angles, and energies, coupled to the energy macroscopic deposition cross section $\sigma_{E D}(\vec{r}, E)$ :

$$
\begin{equation*}
D(\vec{r})=\int_{0}^{E} d E \frac{\sigma_{E D}(\vec{r}, E)}{\rho(\vec{r})} \int_{4 \pi} d \hat{\Omega} \Psi(\vec{r}, \hat{\Omega}, E) \tag{2.3}
\end{equation*}
$$

where $\rho(\vec{r})$ is the material density. The LBTE, as a governing equation for the underlying physics of particle transport, provides the mathematical framework to solve for angular fluence.

### 2.1.2 Derivation by Differential Particle Balance

For simplicity in deriving the basic structure and key terms of the LBTE, we consider a system having only one type of particle with phase space density $N(\vec{r}, \hat{\Omega}, E, t)$. At a microscopic level, the LBTE considers particle dynamics, including sources and sinks which alter $N(\vec{r}, \hat{\Omega}, E, t)$ at each differential compartment of phase space, illustrated in Figure 2.1 as a differential cylinder.


Figure 2.1: Geometric parameters for a differential cylinder in phase space with its base centered at position $\vec{r}$, having height $d u$, endcap area $d A$, and oriented in the direction $\hat{\Omega}$ along which particles under consideration are transported within a range of solid angles $d \hat{\Omega}$, within an energy interval $d E$ centered at $E$.

Accounting for aggregate influx and outflux, in a generic sense (without specifying underlying physics), follows the balance equation formalism ${ }^{3}$. The net influx of particles during a time differential $d t$ is:

$$
\begin{equation*}
[N(\vec{r}, \hat{\Omega}, E, t+\Delta t)-N(\vec{r}, \hat{\Omega}, E, t)] d u d A d \hat{\Omega} d E . \tag{2.4}
\end{equation*}
$$

Processes responsible for influx and outflux include: (i) particle streaming, (ii) collisional interactions, and (iii) an explicit source.
(i) Streaming quantifies particle flow due to a density gradient between faces of the cylinder. For each cylindrical sector of phase space, particles are assumed to drift along its axis at speed $v$ over time interval $d t$, covering an axial distance $d u=v d t$. The number of particles entering the surface at $\vec{r}$ is $N(\vec{r}, \hat{\Omega}, E, t) v d t d A d \hat{\Omega} d E$, while the number exiting at face $\vec{r}+\hat{\Omega} d u$ is $N(\vec{r}+\hat{\Omega} d u, \hat{\Omega}, E, t) v d t d A d \hat{\Omega} d E$. Therefore the net influx of particles streaming into the cylinder is:

$$
\begin{equation*}
[N(\vec{r}, \hat{\Omega}, E, t)-N(\vec{r}+\hat{\Omega} d u, \hat{\Omega}, E, t)] v d t d A d \hat{\Omega} d E \tag{2.5}
\end{equation*}
$$

(ii) Particles interact through various physical processes, some leaving, others entering the differential cylinder of phase space, with each process governed by its respective probability of interaction. The sum of all interaction probabilities by which particles leave the cylinder is modeled by the macroscopic total removal cross section $\sigma_{T}(\vec{r}, E)$, expressed per unit path length, which varies with the underlying material and energy. The net outflux of particles by collisional removal is the product of this probability and the total number of particles traversing the cylinder:

$$
\begin{equation*}
\sigma_{T}(\vec{r}, E) N(\vec{r}, \hat{\Omega}, E, t) d u d A d \hat{\Omega} d E v d t \tag{2.6}
\end{equation*}
$$

Meanwhile, interactions in other sectors of phase space (having energy $E^{\prime}$, travelling in direction $\hat{\Omega}^{\prime}$ ) may result in particles transferred or emerging in the current cylinder under consideration. This probability is modeled by the macroscopic differential scattering cross section $\sigma_{S}\left(\vec{r}, \hat{\Omega}^{\prime} \cdot \hat{\Omega}, E^{\prime} \rightarrow E\right)$ such that the net influx can be expressed by the integral:

$$
\begin{equation*}
\left[\int_{0}^{\infty} d E^{\prime} \int_{4 \pi} d \hat{\Omega}^{\prime} \sigma_{S}\left(\vec{r}, \hat{\Omega}^{\prime} \cdot \hat{\Omega}, E^{\prime} \rightarrow E\right) N\left(\vec{r}, \hat{\Omega}^{\prime}, E^{\prime}, t\right)\right] d u d A d \hat{\Omega} d E v d t \tag{2.7}
\end{equation*}
$$

(iii) An explicit source of particles in radiotherapy is modeled by $S(\vec{r}, \hat{\Omega}, E, t)$ which specifies the rate at which particles are emitted into a system, its contribution to the differential volume given by:

$$
\begin{equation*}
S(\vec{r}, \hat{\Omega}, E, t) d u d A d \hat{\Omega} d E d t \tag{2.8}
\end{equation*}
$$

Processes of influx and outflux are summarized in Figure 2.2.


Figure 2.2: Terms responsible for particle influx and outflux within differential sector of phase space, where $v N(\vec{r})$ and $v N(\vec{r}+\hat{\Omega} d u)$ represent streaming influx and outflux respectively, $\sigma_{T}$ represents collisional outflux, $\sigma_{S}$ represents scattering influx, and $S$ denotes an explicit particle source.

Eq. 2.4 is balanced with Eqs. 2.5-2.8, with a sign convention of net particle influx, resulting in:

$$
\begin{align*}
& {[N(\vec{r}, \hat{\Omega}, E, t+\Delta t)-N(\vec{r}, \hat{\Omega}, E, t)] d u d A d \hat{\Omega} d E} \\
& =-[N(\vec{r}+\hat{\Omega} d u, \hat{\Omega}, E, t)-N(\vec{r}, \hat{\Omega}, E, t)] v d A d \hat{\Omega} d E d t \\
& -\sigma_{T}(\vec{r}, E) N(\vec{r}, \hat{\Omega}, E, t) v d u d A d \hat{\Omega} d E d t  \tag{2.9}\\
& +\left[\int_{0}^{\infty} d E^{\prime} \int_{4 \pi} d \hat{\Omega}^{\prime} \sigma_{S}\left(\vec{r}, \hat{\Omega}^{\prime} \cdot \hat{\Omega}, E^{\prime} \rightarrow E\right) N\left(\vec{r}, \hat{\Omega}^{\prime}, E^{\prime}, t\right) v\right] d u d A d \hat{\Omega} d E d t \\
& +S(\vec{r}, \hat{\Omega}, E, t) d u d A d \hat{\Omega} d E d t
\end{align*}
$$

The differentials ( $d u d A d \hat{\Omega} d E d t$ ) are divided in every term of Eq. 2.9, and angular fluence $\Psi(\vec{r}, \hat{\Omega}, E, t)=v N(\vec{r}, \hat{\Omega}, E, t)$ is substituted, resulting in:

$$
\begin{align*}
& \frac{1}{v} \frac{d \Psi(\vec{r}, \hat{\Omega}, E, t)}{d t}= \\
& -\frac{d \Psi(\vec{r}, \hat{\Omega}, E, t)}{d u}-\sigma_{T}(\vec{r}, E) \Psi(\vec{r}, \hat{\Omega}, E, t)  \tag{2.10}\\
& +\left[\int_{0}^{\infty} d E^{\prime} \int_{4 \pi} d \hat{\Omega}^{\prime} \sigma_{S}\left(\vec{r}, \hat{\Omega}^{\prime} \cdot \hat{\Omega}, E^{\prime} \rightarrow E\right) \Psi\left(\vec{r}, \hat{\Omega}^{\prime}, E^{\prime}, t\right)\right]+S(\vec{r}, \hat{\Omega}, E, t) .
\end{align*}
$$

By considering a steady state solution, the time derivative is 0 on the left hand side of Eq. 2.10, and $\Psi(\vec{r}, \hat{\Omega}, E)$ is no longer a function of time. Rearranging terms of outflux to the left, and influx to the right, the steady state balance equation becomes:
$\hat{\Omega} \cdot \vec{\nabla} \Psi(\vec{r}, \hat{\Omega}, E)+\sigma_{T}(\vec{r}, E) \Psi(\vec{r}, \hat{\Omega}, E)=\left[\int_{0}^{\infty} d E^{\prime} \int_{4 \pi} d \hat{\Omega}^{\prime} \sigma_{S}\left(\vec{r}, \hat{\Omega}^{\prime} \cdot \hat{\Omega}, E^{\prime} \rightarrow E\right) \Psi\left(\vec{r}, \hat{\Omega}^{\prime}, E^{\prime}\right)\right]+S(\vec{r}, \hat{\Omega}, E)$,
where the directional derivative $\frac{d}{d u}$ has been re-expressed in Cartesian coordinates as $\hat{\Omega} \cdot \nabla$ It is customary to combine the collisional and removal terms in operator notation as:

$$
\begin{equation*}
\boldsymbol{L}=\left[\hat{\Omega} \cdot \vec{\nabla}+\sigma_{T}(\vec{r}, E)\right], \tag{2.12}
\end{equation*}
$$

and express the Boltzmann scattering integral as:

$$
\begin{equation*}
\boldsymbol{Q}(\vec{r}, \hat{\Omega}, E)=\int_{0}^{\infty} d E^{\prime} \int_{4 \pi} d \hat{\Omega}^{\prime} \sigma_{S}\left(\vec{r}, \hat{\Omega}^{\prime} \cdot \hat{\Omega}, E^{\prime} \rightarrow E\right) \Psi\left(\vec{r}, \hat{\Omega}^{\prime}, E^{\prime}\right) \tag{2.13}
\end{equation*}
$$

In condensed notation, the Linear Boltzmann Transport Equation becomes:

$$
\begin{equation*}
\boldsymbol{L} \Psi(\vec{r}, \hat{\Omega}, E)=\boldsymbol{Q}(\vec{r}, \hat{\Omega}, E)+S(\vec{r}, \hat{\Omega}, E) \tag{2.14}
\end{equation*}
$$

### 2.1.3 Physics Processes and Approximations

Having established the overall form and key terms of the LBTE, physics interactions are considered which give rise to cross sections. For particles of type $v$, the LBTE is formulated:

$$
\begin{equation*}
\boldsymbol{L}_{v} \Psi_{v}(\vec{r}, E, \hat{\Omega})=\sum_{u} \boldsymbol{Q}^{u \rightarrow v}(\vec{r}, E, \hat{\Omega})+S_{v}(\vec{r}, E, \hat{\Omega}) \tag{2.15}
\end{equation*}
$$

where the scattering integral includes particle sources from all other types $u$. An underlying assumption of the LBTE is that particles interact with the medium, but not each other. Moreover, particle fluence is considered sufficiently low to not alter the surrounding medium. Therefore, the steady state (time invariant) particle fluence is solved for.

The scope of particle interactions in photon beam radiotherapy involves the coupling between primary photons from the source which interact to generate scattered secondary electrons ultimately responsible for depositing dose in a patient. A photon-electron system of equations with partial coupling is employed in this work. This coupling is outlined in Figure 2.3, and is further explained Tables 2.1-2.2. The physics cross section data used in this work is generated with the multi-group Legendre CEPXS (Coupled Electron Photon Cross Section) code ${ }^{4}$.


Figure 2.3: Schematic of the photon-electron partial coupled system. Solid lines denote processes which are explicitly modeled by cross-sections, while dashed lines represent effects which are approximated, thus not explicitly modeled.

Table 2.1: Photon Processes and Implementation in CEPXS ${ }^{4}$

| Label | Photon Process | CEPXS Implementation |
| :---: | :---: | :---: |
| $\gamma . i$ | Incoherent Scattering and <br> Electron Production | Klein-Nishina cross section, binding effects ignored <br> due to photoelectric dominance at lower energies |
| $\gamma . i i$ | Photoelectric | Biggs-Lighthill ${ }^{5}$ cross sections |
| $\gamma . i i i$ | Pair Production | Bethe-Heitler ${ }^{6}$ energy distribution, <br> positrons treated as electrons |
| $\gamma . i v$ | Coherent Scattering | (not implemented due to negligible contribution) |

Table 2.2: Electron Processes and Implementation in CEPXS ${ }^{4}$

| Label | Electron Process | CEPXS Implementation |
| :---: | :---: | :---: |
| $e . i$ | Inelastic Scattering: Collisional Loss <br> and Knock-on Production | Møller cross section ${ }^{7}$ |
| e.ii | Elastic Scattering | Riley cross section $(<256 \mathrm{keV})^{8}$, Mott cross <br> section w/ Moliere screening $(>256 \mathrm{keV})^{7}$ |
| e.iii | Radiative Loss, including <br> Bremsstrahlung Production | Berger-Seltzer cross sections ${ }^{9}$ |
| e.iv | Impact Ionization (causing | Gryzinski ${ }^{10}$ cross sections |

Simplifying approximations to the physics model are justified by the tradeoff between (i) complexity saved in mathematical formulation, and (ii) order-of-magnitude contribution to dose, within the context of photon-beam MR-guided radiotherapy.

As depicted in Figure 2.3, particle types are limited to photons and electrons. Positrons arising from pair and triplet production are treated as electrons. This is a reasonable approximation as most of the photon fluence in a polyenergetic spectrum falls below 1 MeV , where positrons are not produced. For photons from 1 MeV to 6 MeV , incoherent scattering remains the dominant contribution by nearly an order of magnitude (Table 2.3).


Figure 2.4: Relative contributions of photon processes to interaction cross sections from 1 keV to 10 MeV for (a) water, (b) lung, (c) bone. Data from NIST XCOM ${ }^{11}$.

Table 2.3: Percentage contribution to cross section of photon processes at selected energies in water (based on data from NIST XCOM ${ }^{11}$ )

| Photon Process | $\mathbf{1 0 k e V}$ | $\mathbf{3 0 k e V}$ | $\mathbf{1 0 0 k e V}$ | $\mathbf{5 0 0 k e V}$ | $\mathbf{2 M e V}$ | $\mathbf{6 M e V}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Incoherent | $2.9 \%$ | $48.7 \%$ | $95.3 \%$ | $99.8 \%$ | $99.2 \%$ | $88.6 \%$ |
| Photoelectric | $92.8 \%$ | $38.8 \%$ | $1.6 \%$ | $0.0 \%$ | $0.0 \%$ | $0.0 \%$ |
| Pair Production | $0.0 \%$ | $0.0 \%$ | $0.0 \%$ | $0.0 \%$ | $0.8 \%$ | $10.8 \%$ |
| Triplet Production | $0.0 \%$ | $0.0 \%$ | $0.0 \%$ | $0.0 \%$ | $0.0 \%$ | $0.6 \%$ |
| Coherent | $4.3 \%$ | $12.5 \%$ | $3.1 \%$ | $0.2 \%$ | $0.0 \%$ | $0.0 \%$ |

Not having to explicitly formulate a Boltzmann equation for positrons presents a fundamental reduction in complexity at the outset by (i) eliminating the need to solve the phase space for a third type of particle, and (ii) neglecting annihilation interactions which produce photons, thereby removing cyclic dependencies in particle coupling. Treating positrons as electrons invokes an approximation affecting only a small proportion of events, avoiding undesirable complexity in particle coupling, while not completely ignoring the process of pair production.
Likewise, radiative processes involving secondary electrons (including Bremsstrahlung and fluorescence following impact ionization) are assumed to deposit their energy locally. By examining the modes of energy loss, radiative processes contribute orders of magnitude less to the total stopping power than collisional interactions over the scope of materials and energies under consideration, as shown in Figure 2.5 and Table 2.4.


Figure 2.5: Relative contribution of electron collisional and radiative processes to total stopping power between 1 keV and 10 MeV for (a) water, (b) lung, (c) bone. Data from NIST ESTAR ${ }^{12}$.

Table 2.4: Percentage contribution to total stopping power of electron processes at selected energies in water (based on data from NIST ESTAR ${ }^{12}$ )

| Electron Process | $\mathbf{1 0 k e V}$ | $\mathbf{3 0 k e V}$ | $\mathbf{1 0 0 k e V}$ | $\mathbf{5 0 0 k e V}$ | $\mathbf{2 M e V}$ | $\mathbf{6 M e V}$ |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Collisional | $100.0 \%$ | $100.0 \%$ | $99.9 \%$ | $99.7 \%$ | $98.6 \%$ | $95.1 \%$ |
| Radiative | $0.0 \%$ | $0.0 \%$ | $0.1 \%$ | $0.4 \%$ | $1.4 \%$ | $4.9 \%$ |

Characteristic x-rays for biological media typically fall below 1 keV , thus an assumption of local energy deposition is reasonable given its limited probability of occurrence.
Physics interactions compatible with allowed modes of coupling can be unified into aggregate macroscopic cross sections: (i) total removal $\sigma_{T}$ on the left hand side, and (ii) differential scattering influx $\sigma_{S}$ on the right hand side.

In the photon LBTE, processes of adequate significance include the photoelectric effect, incoherent scatter (Compton effect), and pair production with the aforementioned approximations. Incoherent scattering dominates across most of the energy range considered, and is modeled using the Klein-Nishina cross section ${ }^{4}$. Binding effects at lower energies are ignored because photoelectric interactions typically dominate this range ${ }^{13}$. Coherent (Rayleigh) scattering, triplet production, and photodisintegration are neglected as photon processes having negligible probability in the energy range under consideration.

Secondary electrons produced through photon interactions proceed to lose their energy and deposit dose in the medium through coulombic exchange with atomic electrons and nuclei in the medium. Given the long range of the Coulomb force and abundant surroundings of charged entities in any medium, the probability of interaction is practically $100 \%$, thus a more informative metric is the electronic stopping power, quantifying average energy loss per path length travelled by the electron. As shown in Figure 2.5, stopping power contains both collisional and radiative components. When a relativistic electron passes near an atomic nucleus, it may undergo sharp deflection, accompanied by the emission of photons. The radiative stopping power formulated by Bethe and Heitler ${ }^{14}$, and extensively tabulated by Berger and Seltzer ${ }^{9}$, is used in CEPXS to formulate the differential radiative cross sections. Radiative processes (including soft radiative losses, Bremsstrahlung, and fluorescence following impact ionization) undergo the aforementioned approximation of depositing their energy locally in keeping with a partial-coupling assumption for sufficiently rare occurrences in radiotherapy (radiative stopping power typically less than $5 \%$, as shown in Table 2.4).

By far the predominant mode of interaction for fast electrons in the energy range of MRIgRT are collisions with bound electrons in the medium (Figure 2.5 and Table 2.4), classified as either soft collisions (distant coulomb interactions) as well as catastrophic collisions which ionize the atom giving rise to knock-on electrons. Cumulative energy loss through the mass collisional stopping power is given by the Bethe-Bloch theory, expressed in Eq. 2.16 for electrons ${ }^{15}$ as:

$$
\begin{equation*}
\frac{S_{c o l}}{\rho}=2 \pi r_{e}^{2} \frac{Z}{A} N_{A} \frac{m_{e} c^{2}}{\beta^{2}}\left[\ln \left(\frac{T^{2}}{I^{2}}\right)+\ln \left(1+\frac{\tau}{2}\right)+\left(1-\beta^{2}\right)\left(1+\frac{\tau^{2}}{8}-(2 \tau+1) \ln 2\right)-\delta\right], \tag{2.16}
\end{equation*}
$$

where $T$ is the electron's kinetic energy, $\tau=T / m_{e} c^{2}$ is kinetic energy normalized to electron mass units, $\beta=v / c$ is the relativistic factor, $I$ is the mean ionization energy, $r_{e} \approx 2.818 \mathrm{fm}$ is the classical electron radius, $N_{A}=6.022 \cdot 10^{23}$ is Avogadro's number, and $\delta$ is the density correction factor which dampens soft collisions by polarization of the medium.

While stopping power is useful in a microscopic Lagrangian formulation where particle trajectories are individually tracked, the LBTE is a macroscopic Eulerian formulation which deals with differential cross sections. In the case of inelastic collisional losses, the differential

Møller scattering cross section (Eq. 2.17) ${ }^{4}$ describes the predominant interaction of incident electrons having kinetic energy $T$ with bound electrons in the medium, resulting in a scattered energy $T_{p}$ :

$$
\begin{equation*}
\frac{d \sigma_{\text {moller }}}{d \varepsilon}=\left(\frac{Z}{A}\right)_{\text {eff }} N_{A} \frac{2 \pi r_{e}^{2}}{\beta^{2}}\left[\frac{1}{\left(\tau-\tau_{p}\right)^{2}}+\frac{1}{\tau_{p}^{2}}+\frac{1}{(\tau+1)^{2}}-\frac{2 \tau+1}{(\tau+1)^{2}\left(\tau-\tau_{p}\right) \tau_{p}}\right] \tag{2.17}
\end{equation*}
$$

where $\tau=T / m_{e} c^{2}$ and $\tau_{p}=T_{p} / m_{e} c^{2}$ are normalized to electron mass units, $r_{e}$ is the classical electron radius, and $\varepsilon=\tau-\tau_{p}$ is the energy lost, normalized to the electron rest mass. Eq. 2.17 is plotted for electrons up to 6 MeV in Figure 2.6, below.


Figure 2.6: Møller cross section differential in energy loss, as a function of incident electron kinetic energy $T$ and scattered energy $T_{p}$ in water.

As seen in Figure 2.6, the Møller cross section increases rapidly (several orders of magnitude) for small energy losses ( $T_{p} \approx T$ ). These correspond to soft collisions which account for nearly half of the total energy lost by an electron. In anticipation of a discretized formulation to the electron LBTE for which Møller scattering is the dominant contribution, the extreme variation in the differential cross section $\sigma_{S, \text { moller }}\left(\vec{r}, \hat{\Omega}^{\prime} \cdot \hat{\Omega}, E^{\prime} \rightarrow E\right)$ as $E^{\prime} \approx E$ would require an unfeasibly high number of narrowly spaced energy intervals to model accurately. An approximation invoked for the electron LBTE to accommodate this behavior is described in the next section.

### 2.1.4 Boltzmann-CSD Equations

Soft collisions responsible for the sharply increasing component of the differential Møller cross section involve small energy losses (below a threshold $\left(E-E^{\prime}\right)<\Delta E_{\text {threshold }}$ ) with minimal angular deflection $\left(\hat{\Omega} \approx \hat{\Omega}^{\prime}\right)$. In such regimes, the Boltzmann scattering operator can be approximated through a Taylor expansion about the incident particle direction, yielding terms of the Fokker-Planck scattering equation ${ }^{16}$ where the dominant contribution is the continuous slowing down (CSD) operator ${ }^{17}$ as shown in Eq. 2.18:

$$
\begin{equation*}
\int_{0}^{\infty} d E^{\prime} \int_{4 \pi} d \hat{\Omega}^{\prime} \sigma_{S, \text { moller }}^{\text {soft }}\left(\vec{r}, \hat{\Omega}^{\prime} \cdot \hat{\Omega}, E^{\prime} \rightarrow E\right) \Psi_{e}\left(\vec{r}, \hat{\Omega}^{\prime}, E^{\prime}\right) \approx \frac{\partial}{\partial E}\left(\beta_{r}(\vec{r}, E) \Psi_{e}(\vec{r}, \hat{\Omega}, E)\right) . \tag{2.18}
\end{equation*}
$$

$\beta_{r}(\vec{r}, E)$ is the restricted mass stopping power, characterizing small energy losses capped at $\left(E-E^{\prime}\right)<\Delta E_{\text {threshold }}$, without deflection in angle, presenting a suitable physics approximation for electron soft collisions. Catastrophic collisions involving energy losses exceeding $\Delta E_{\text {treshold }}$, accompanied by large angular deflection and generation of secondary electrons (knock-on or delta-rays) continue to be encoded by the differential Møller cross section.

The Boltzmann-CSD equation (Eq. 2.19) models electron energy losses on different scales using distinct mathematical formalisms: catastrophic collisions using the Boltzmann scattering operator and soft collisions by the CSD operator:

$$
\begin{align*}
& {\left[\hat{\Omega} \cdot \vec{\nabla}+\sigma_{T, e}(\vec{r}, E)\right] \Psi_{e}(\vec{r}, \hat{\Omega}, E)-\underbrace{\frac{\partial}{\partial E} \beta_{r}(\vec{r}, E)}_{\begin{array}{c}
\text { CSD operator for } \\
\text { electron soft collisions }
\end{array}} \Psi_{e}(\vec{r}, \hat{\Omega}, E)=} \\
& \int_{E}^{E_{\max }} d E^{\prime} \int_{4 \pi} d \hat{\Omega}^{\prime} \sigma_{S}^{\gamma e}\left(\vec{r}, \hat{\Omega}^{\prime} \cdot \hat{\Omega}, E^{\prime} \rightarrow E\right) \Psi_{\gamma}\left(\vec{r}, \hat{\Omega}^{\prime}, E^{\prime}\right)  \tag{2.19}\\
& +\underbrace{\int_{E}^{E_{\max }} d E^{\prime} \int_{4 \pi} d \hat{\Omega}^{\prime} \sigma_{S}^{e e}\left(\vec{r}, \hat{\Omega}^{\prime} \cdot \hat{\Omega}, E^{\prime} \rightarrow E\right) \Psi_{e}\left(\vec{r}, \hat{\Omega}^{\prime}, E^{\prime}\right)}_{\text {Boltzmann scattering operator for electron catastrophic collisions }} .
\end{align*}
$$

The restricted mass stropping power is determined by energy losses not attributed to catastrophic collisions, can be written ${ }^{13,18,19}$ :

$$
\begin{equation*}
\beta_{r}(E)=\frac{S_{c o l}(E)}{\rho}-\int_{\Delta E_{\text {tresesold }}}^{\Delta E_{\max }} \Delta E \frac{d \sigma_{\text {moller }}}{d(\Delta E)} d(\Delta E) \tag{2.20}
\end{equation*}
$$

where $\Delta E_{\text {threshold }}$ and $\Delta E_{\max }$ both vary depending on the energy $E$ under consideration ${ }^{13}$. Elastic scattering also contributes to $\sigma_{S}^{e e}$ through the Mott cross section, where an electron exchanges coulomb interactions with an atomic nucleus (at a distance on the order of the impact parameter) such that the nucleus recoils with negligible velocity, while deflecting the incident electron in angle with essentially no loss in kinetic energy. The differential cross section component $\sigma_{S}^{\gamma e}$ accounts for electrons generated by photoelectric, Compton, and pair production processes.

### 2.1.5 Magnetic Field Operator

To see how external forces can be formulated into the LBTE requires a more rigorous derivation based on Liouville's Theorem ${ }^{20}$. Consider again particle phase space (Eq. 2.21) in terms of position, momentum, and time:

$$
\begin{equation*}
N(\vec{r}, \vec{p}, t)=N\left(x, y, z, p_{x}, p_{y}, p_{z}, t\right) . \tag{2.21}
\end{equation*}
$$

In the context of transport theory, Liouville's Theorem enforces conservation of the total number of particles in each differential phase-space volume: $\frac{d N}{d t}=0$. That is, terms in the total derivative sum to 0 :

$$
\begin{equation*}
\frac{d N}{d t}=\frac{\partial N}{\partial t}+\left(\frac{\partial N}{\partial x} \frac{d x}{d t}+\frac{\partial N}{\partial y} \frac{d y}{d t}+\frac{\partial N}{\partial z} \frac{d z}{d t}\right)+\left(\frac{\partial N}{\partial p_{x}} \frac{d p_{x}}{d t}+\frac{\partial N}{\partial p_{y}} \frac{d p_{y}}{d t}+\frac{\partial N}{\partial p_{z}} \frac{d p_{z}}{d t}\right)=\frac{\partial N}{\partial t}+\vec{\nabla} \cdot\left(N \frac{\partial \vec{r}}{\partial t}\right)+\vec{\nabla}_{p} \cdot\left(N \frac{\partial \vec{p}}{\partial t}\right) . \tag{2.22}
\end{equation*}
$$

By definition $\frac{\partial \vec{r}}{\partial t}=\vec{v}$, and $\frac{\partial \vec{p}}{\partial t}=\vec{F}$ by the impulse relation $\Delta \vec{p}=\vec{F} \Delta t$.
Rewriting Eq. 2.22 while imposing Liouville's Theorem yields:

$$
\begin{equation*}
0=\frac{\partial N}{\partial t}+\vec{\nabla} \cdot(N \vec{v})+\vec{\nabla}_{p} \cdot(N \vec{F}) \tag{2.23}
\end{equation*}
$$

At steady state (enforcing time independence), $\frac{\partial N}{\partial t}=0$, yielding:

$$
\begin{equation*}
\vec{\nabla} \cdot(N \vec{v})+\vec{\nabla}_{p} \cdot(N \vec{F})=0 . \tag{2.24}
\end{equation*}
$$

Eq. 2.24 takes the form of the Vlaslov equation ${ }^{1}$ where particles interact amongst themselves, but not with the surrounding media. One context where such model applies is for electron packets in a RF linear accelerator. If external forces are assumed absent $(\vec{F} \equiv 0)$, then $\vec{\nabla} \cdot(N \vec{v})=0$ reduces to the streaming term of the LBTE derived earlier, $\hat{\Omega} \cdot \vec{\nabla} \Psi=0$.

However, including forces and collisions with the surrounding media yields Eq. 2.25:

$$
\begin{equation*}
\vec{\nabla} \cdot(N \vec{v})+\vec{\nabla}_{p} \cdot(N \vec{F})=(\delta N)_{\text {coll }}, \tag{2.25}
\end{equation*}
$$

where $(\delta N)_{\text {coll }}$ includes all sources and sinks, including the Boltzmann scattering integral, total removal cross section, and explicit source. In this precursor form to the LBTE, we see explicit provision to include a force term:

$$
\begin{equation*}
\vec{\nabla}_{p} \cdot(N \vec{F}) . \tag{2.26}
\end{equation*}
$$

Expressing Eq. 2.26 as a velocity derivative, and using angular fluence, yields:

$$
\begin{equation*}
\vec{\nabla}_{v} \cdot\left(\vec{a} \frac{\Psi}{v}\right) \tag{2.27}
\end{equation*}
$$

It can be shown ${ }^{21}$ that for relativistic electrons,

$$
\begin{equation*}
\vec{a}=\frac{1}{m_{0} \gamma}\left(\vec{F}-\beta^{2}(\vec{F} \cdot \hat{\Omega}) \hat{\Omega}\right), \tag{2.28}
\end{equation*}
$$

where the usual relativistic definitions apply: $\gamma(v)=\frac{1}{\sqrt{1-v^{2} / c^{2}}}, m_{0}$ denotes the particle's rest mass, $v$ its speed, and $\beta=v / c$, where $c$ is the speed of light.

Substituting the Lorentz force $\vec{F}=q(\vec{E}+\vec{v} \times \vec{B})$, into Eq. 2.28 and assuming an absence of electric fields ( $\vec{E}=0$ ), the acceleration becomes:

$$
\begin{equation*}
\vec{a}=\frac{q}{\gamma m_{0}}[\vec{v} \times \vec{B}]=\frac{q v}{\gamma m_{0}}[\hat{\Omega} \times \vec{B}] . \tag{2.29}
\end{equation*}
$$

After numerous simplifying vector calculus relations, and substituting 2.29 into 2.27 , it can be shown ${ }^{21}$ :

$$
\begin{equation*}
\vec{\nabla}_{v} \cdot\left(\vec{a} \frac{\Psi}{v}\right)=\frac{q}{|\vec{p}|}(\hat{\Omega} \times \vec{B})_{z} \frac{\partial \Psi}{\partial \mu}+\frac{q}{|\vec{p}|\left(1-\mu^{2}\right)}(\hat{\Omega} \times(\hat{\Omega} \times \vec{B}))_{z} \frac{\partial \Psi}{\partial \varphi} \tag{2.30}
\end{equation*}
$$

where $\vec{p}$ denotes particle momentum, and $\mu=\cos \theta$, with $\theta$ corresponding to the global polar angle in spherical coordinates. Likewise $\varphi$ is the global azimuthal angle in spherical coordinates.

Eq. 2.30 can be factored into the following components:

$$
\begin{gather*}
\vec{\tau}(\vec{B}, \hat{\Omega})=\frac{1}{\sqrt{1-\mu^{2}}}\left[(\hat{\Omega} \times(\hat{\Omega} \times \vec{B}))_{z} \hat{\boldsymbol{\varphi}}-(\hat{\Omega} \times \vec{B})_{z} \hat{\boldsymbol{\theta}}\right]  \tag{2.31a}\\
\vec{\nabla}_{\Omega}=\frac{1}{\sqrt{1-\mu^{2}}} \frac{\partial}{\partial \varphi} \hat{\boldsymbol{\varphi}}+\frac{\partial}{\partial \theta} \hat{\boldsymbol{\theta}} \tag{2.31b}
\end{gather*}
$$

such that the magnetic field operator can be compactly expressed as ${ }^{22}$ :

$$
\begin{equation*}
\frac{q}{|\vec{p}|} \vec{\tau}(\vec{B}, \hat{\Omega}) \cdot \vec{\nabla}_{\Omega} \tag{2.32}
\end{equation*}
$$

Eq. 2.32 is added to the left hand side of the electron Boltzmann-CSD equation, with the assumption that magnetic fields do not modify the underlying cross sections.

### 2.1.6 Coupled Boltzmann System of Equations

For photon beam MRIgRT, the LBTE coupled system with magnetic fields becomes:

$$
\begin{gather*}
{\left[\hat{\Omega} \cdot \vec{\nabla}+\sigma_{T, \gamma}(\vec{r}, E)\right] \Psi_{\gamma}(\vec{r}, \hat{\Omega}, E)=\boldsymbol{Q}^{\gamma \rightarrow \gamma}(\vec{r}, \hat{\Omega}, E)+S_{\gamma}(\vec{r}, \hat{\Omega}, E),}  \tag{2.33a}\\
{\left[\hat{\Omega} \cdot \vec{\nabla}+\sigma_{T, e}(\vec{r}, E)+\frac{q}{|\vec{p}|} \vec{\tau}(\vec{B}, \hat{\Omega}) \cdot \vec{\nabla}_{\Omega}\right] \Psi_{e}(\vec{r}, \hat{\Omega}, E)-\frac{\partial}{\partial E} \beta_{r}(\vec{r}, E) \Psi_{e}(\vec{r}, \hat{\Omega}, E)=\boldsymbol{Q}^{\gamma \rightarrow e}(\vec{r}, \hat{\Omega}, E)+\boldsymbol{Q}^{\varrho \rightarrow e}(\vec{r}, \hat{\Omega}, E)} \tag{2.33b}
\end{gather*}
$$

with vacuum boundary conditions:

$$
\begin{align*}
& \Psi_{\gamma}(\vec{r}, \hat{\Omega}, E)=0, \hat{\Omega} \cdot \hat{n}<0, \\
& \Psi_{e}(\vec{r}, \hat{\Omega}, E)=0, \hat{\Omega} \cdot \hat{n}<0 . \tag{2.33c}
\end{align*}
$$

Eq. 2.33c enforces zero incoming fluence from outside the spatial problem geometry. Equivalently, all fluence originates from within the domain, either through raytracing of primary photons, or scattered photons and electrons.

An analytic solution to the LBTE with magnetic fields is not possible in general, owing to the variety of patient geometries and source configurations. Numerical techniques unlock a far grander scope of engineering designs and research simulations which ultimately reduce to a matrix formulation able to leverage the incredible switching speeds and parallelism of silicon transistors. A deterministic solution implies that given the same discretization parameters, problem setup, and convergence criterion, every run will repeatedly converge to identical values for the discretized degrees of freedom within machine precision. Discretization techniques will be introduced for each phase space variable, culminating in a matrix formulation for a numerical system of equations.

### 2.2 Energy Discretization and Inscatter Iteration

Energy is discretized as the outermost variable of the solution technique, such that for each discrete energy interval, space and angle are solved iteratively to convergence.

### 2.2.1 Multigroup Method in Energy

The energy domain can be partitioned into discrete intervals denoted by group index $g$, over which energy dependence is assumed to be piecewise constant. By convention, $g$ is enumerated with increasing index going from high energy to low energy, reflecting the general order the groups must be solved given the specified interactions only cause energy degradation or energy or downscatter.


Figure 2.7: Schematic of partitioning the energy spectrum into discrete intervals enumerated by $g$, and representation of an energy dependent function $f(E)$ by a piecewise constant approximation $f_{g}$.

The multigroup angular fluence becomes:

$$
\begin{equation*}
\Psi_{g}(\vec{r}, \hat{\Omega})=\int_{E_{g+1}}^{E_{g}} d E \Psi(\vec{r}, \hat{\Omega}, E) \tag{2.34}
\end{equation*}
$$

with the multigroup total cross sections defined as:

$$
\begin{equation*}
\sigma_{T, g}(\vec{r})=\frac{\int_{E_{g+1}}^{E_{g}} d E \sigma_{T}(\vec{r}, E)}{E_{g}-E_{g+1}}, \tag{2.35}
\end{equation*}
$$

and multigroup differential scattering cross section defined as:

$$
\begin{equation*}
\sigma_{S, g^{\prime} \rightarrow g}\left(\vec{r}, \hat{\Omega}^{\prime} \cdot \hat{\Omega}\right)=\frac{\int_{E_{g+1}}^{E_{g}} d E \int_{E_{g^{\prime}+1}}^{E_{g^{\prime}}} d E^{\prime} \sigma_{S}\left(\vec{r}, \hat{\Omega}^{\prime} \cdot \hat{\Omega}, E^{\prime} \rightarrow E\right)}{E_{g}-E_{g+1}} \tag{2.36}
\end{equation*}
$$

In a one-way coupled photon-electron Boltzmann system (Eq. 2.33), the nature of scattering dependencies (downscatter only, electrons forbidden to create photons) paves the way for
discretization of a unified Multigroup equation (Eq. 2.37) solved first for $N_{p g}$ photon groups (from high to low energy), followed by $N_{e g}$ electron groups (again from high to low energy each depending only on previously solved photon groups and electron groups of higher energy).

$$
\begin{equation*}
\left[\hat{\Omega} \cdot \vec{\nabla}+\kappa_{g} \vec{\tau}(\vec{B}, \hat{\Omega}) \cdot \vec{\nabla}_{\Omega}+\sigma_{T, g}(\vec{r})\right] \Psi_{g}(\vec{r}, \hat{\Omega})=\sum_{g^{\prime}=1}^{g} \sigma_{S, g^{\prime} \rightarrow g}\left(\vec{r}, \hat{\Omega}^{\prime} \cdot \hat{\Omega}\right) \Psi_{g^{\prime}}\left(\vec{r}, \hat{\Omega}^{\prime}\right)+S_{g}(\vec{r}, \hat{\Omega}) \tag{2.37}
\end{equation*}
$$

Photon and electron group structures are concatenated to form a single series, as illustrated in Figure 2.8, solved in sequence $g=1, . ., N_{p g}+N_{e g}$.


Figure 2.8: Concatenated energy group structure of photons and electrons, applied to unified multigroup equation.

Particle type is implicitly classified based on group index. Only photons have an explicit source whereas only electrons are subject to the influence of magnetic fields. These consequences are summarized in Table 2.5 below:

Table 2.5: Conventions for Unified Multigroup Equation

| Particle Type | $g$ | $S_{g}$ | $\kappa_{g}$ |
| :--- | :---: | :---: | :---: |
| Photon $(\gamma)$ | $1, . ., N_{p g}$ | $\neq 0$ | $\equiv 0$ |
| Electron $(e)$ | $\left(N_{p g}+1\right), \ldots,\left(N_{p g}+N_{e g}\right)$ | $\equiv 0$ | $\neq 0$ |

The multigroup parameter in Eq. 2.37 pertaining to magnetic fields is given $\mathrm{as}^{22}$ :

$$
\begin{equation*}
\kappa_{g}=\frac{q c}{E_{g}-E_{g+1}} \ln \left(\frac{E_{g}+E_{0}+\sqrt{\left(E_{g}+E_{0}\right)^{2}-\left(E_{0}\right)^{2}}}{E_{g+1}+E_{0}+\sqrt{\left(E_{g+1}+E_{0}\right)^{2}-\left(E_{0}\right)^{2}}}\right), \tag{2.38}
\end{equation*}
$$

where $E_{0}=m_{0} c^{2}$ is the rest mass of the electron.

Also noteworthy upon energy discretization, the action of the energy CSD operator in Eq. 2.33b is absorbed into the scattering cross sections $\sigma_{T, g}$ and $\sigma_{S, g^{\prime} \rightarrow g}$ through a diamond-difference formalism ${ }^{23}$. The CSD component can be written:

$$
\begin{equation*}
\hat{\Omega} \cdot \vec{\nabla} \psi=\frac{\partial}{\partial E}\left(\beta_{r} \psi\right), \tag{2.39}
\end{equation*}
$$

expressed in discrete terms of edge fluences in a diamond difference form:

$$
\begin{equation*}
\hat{\Omega} \cdot \vec{\nabla} \psi_{g}=\frac{\beta_{r, g-1 / 2} \psi_{g-1 / 2}-\beta_{r, g+1 / 2} \psi_{g+1 / 2}}{\Delta E_{g}}, \tag{2.40}
\end{equation*}
$$

where

$$
\begin{equation*}
\psi_{g}=\frac{1}{2}\left(\psi_{g-1 / 2}+\psi_{g+1 / 2}\right) \tag{2.41}
\end{equation*}
$$

related to the multigroup fluence by:

$$
\begin{equation*}
\Psi_{g}=\psi_{g} \Delta E_{g} \tag{2.42}
\end{equation*}
$$

Applying Eq. 2.41 to Eq. 2.40 recursively, it can be shown:

$$
\begin{align*}
& \hat{\Omega} \cdot \vec{\nabla} \psi_{g}+\left(2 \beta_{r, g+1 / 2} / \Delta E_{g}\right) \psi_{g} \\
& =2\left(\left(\beta_{r, g-1 / 2}+\beta_{r, g+1 / 2}\right) / \Delta E_{g}\right)  \tag{2.43}\\
& \left(\psi_{g-1}-\psi_{g-2}+\psi_{g-3}-\psi_{g-4}+\ldots+(-1)^{g} \psi_{1}\right)
\end{align*}
$$

such that applying multigroup fluences (Eq. 2.42), Eq. 2.43 can be expressed in terms of standard multigroup cross sections:

$$
\begin{equation*}
\hat{\Omega} \cdot \vec{\nabla} \Psi_{g}+\sigma_{T, C S D} \Psi_{g}=\sum_{g^{\prime}=1}^{g} \sigma_{S, C S D, g^{\prime} \rightarrow g} \Psi_{g^{\prime}}, \tag{2.44}
\end{equation*}
$$

where

$$
\begin{gather*}
\sigma_{T, C S D}=\left(2 \beta_{r, g+1 / 2} / \Delta E_{g}\right)  \tag{2.45a}\\
\sigma_{S, C S D, g^{\prime} \rightarrow g}=(-1)^{g-g^{\prime}+1} 2\left(\left(\beta_{r, g-1 / 2}+\beta_{r, g+1 / 2}\right) / \Delta E_{g^{\prime}}\right) \tag{2.45b}
\end{gather*}
$$

These conventions eliminate the need of an explicit CSD operator in Eq. 2.37. Nevertheless, the separation of catastrophic from soft collisions is preserved in the physics representation, enabling accurate discretization of the energy domain without requiring an excessive number of intervals.

The group structure (number and spacing of discrete energy intervals) impacts solution accuracy and numerical degrees of freedom in the problem. Tradeoffs are explored, in consideration of how cross sections and source spectrum vary with energy to settle on an appropriate parameterization for photon beam MRIgRT. Logarithmic spacing of energy bins are employed, with narrower spaced bins at lower energies where cross section values increase more rapidly. We had investigated more sophisticated models of a linear-discontinuous ${ }^{24}$ approximation in energy in the presence of magnetic fields, with the hope of reducing the number of intervals. However, it was found that this more computationally intensive form offered no tangible benefit over the multigroup method with diamond differenced CSDA, while requiring increased calculation time.

Discrete values of multigroup cross sections are generated using CEPXS ${ }^{4}$. Since angular variation in $\sigma_{S, g^{\prime} \rightarrow g}\left(\vec{r}, \hat{\Omega}^{\prime} \cdot \hat{\Omega}\right)$ depends only on the relative scattering angle $\left(\mu=\hat{\Omega}^{\prime} \cdot \hat{\Omega}=\cos \theta\right)$, symmetry can be invoked to compactly encode differential cross sections as a series of coefficients to Legendre polynomials which form an orthonormal basis with respect to $\mu$, as given in Eq. 2.46:

$$
\begin{equation*}
\sigma_{S, g^{\prime} \rightarrow g}\left(\vec{r}, \hat{\Omega}^{\prime} \cdot \hat{\Omega}\right) \approx \sum_{l=0}^{L} \frac{2 l+1}{4 \pi} \sigma_{S, g^{\prime} \rightarrow g, l}(\vec{r}) P_{l}(\mu)=\sum_{l=0}^{L} \sigma_{S, g^{\prime} \rightarrow g, l}(\vec{r}) \sum_{m=-l}^{l} Y_{l, m}\left(\hat{\Omega}^{\prime}\right) Y_{l, m}(\hat{\Omega}), \tag{2.46}
\end{equation*}
$$

where $P_{l}(\mu)$ is the Legendre polynomial of order $l$, and the expansion in Eq. 2.46 is practically truncated at order $L=5$, determined to be sufficient to model the scattering anisotropy in MRIgRT ${ }^{21}$. Much of the highly forward-peaked anisotropy due to soft collisional scattering has been offloaded to the CSD operator through a Fokker-Planck approximation (§2.14).

In this work, real form spherical harmonics are considered,

$$
Y_{l, m}(\hat{\Omega})=\left\{\begin{array}{cc}
\sqrt{2} \cdot c_{l, m} \cdot \sin (|m| \varphi) & m<0  \tag{2.47}\\
c_{l, m} & m=0 \\
\sqrt{2} \cdot c_{l, m} \cdot \cos (m \varphi) & m>0
\end{array} \quad, \quad c_{l, m}=\sqrt{\frac{(2 l+1)}{4 \pi} \frac{(l-|m|)!}{(l+|m|)!}} P_{l}^{|m|}(\mu),\right.
$$

where $P_{l}^{|m|}(\mu)$ are the associated Legendre polynomials. The variation of angular fluence over direction $\hat{\Omega}$ can be approximated by a summation over spherical harmonics as:

$$
\begin{equation*}
\Psi_{g}(\vec{r}, \hat{\Omega})=\sum_{l=0}^{L} \sum_{m=-l}^{l} \Phi_{g, l, m}(\vec{r}) Y_{l, m}(\hat{\Omega}), \tag{2.48}
\end{equation*}
$$

where the coefficients are scalar flux moments, derived as:

$$
\begin{equation*}
\Phi_{g l, m}(\vec{r})=\int d \hat{\Omega} Y_{l, m}(\vec{\Omega}) \Psi_{g}(\vec{r}, \hat{\Omega}), \tag{2.49}
\end{equation*}
$$

requiring far fewer degrees of freedom than angular fluence itself.

### 2.2.2 Establishing an Iterative Source Model

Source Iteration (SI) as applied to the multigroup equations serves to converge on the solution of inscatter (interactions where particles remain in the same energy interval), by decoupling the angular dependence of inscatter in the Boltzmann scattering integral (Eq. 2.13), which is reformulated as an expansion over spherical harmonics. This introduces an iteration index $(t)$ for which the update equation for angular fluence to $(t+1)$ is:

$$
\begin{align*}
& {\left[\hat{\Omega} \cdot \vec{\nabla}+\kappa_{g} \vec{\tau}(\vec{B}, \hat{\Omega}) \cdot \vec{\nabla}_{\Omega}+\sigma_{T, g}(\vec{r})\right] \Psi_{g}^{(t+1)}(\vec{r}, \hat{\Omega})} \\
& =\underbrace{\sum_{l=0}^{L} \sum_{m=-l}^{l} \Phi_{g, l, m}^{(t)}(\vec{r}) \sigma_{S, g \rightarrow g, l}(\vec{r}) Y_{l, m}(\hat{\Omega})}_{\text {inscatter }}+\underbrace{\sum_{g^{\prime}=1}^{g-1} \sum_{l=0}^{L} \sum_{m=-l}^{l} \Phi_{g^{\prime}, l, m}(\vec{r}) \sigma_{S, g^{\prime} \rightarrow g, l}(\vec{r}) Y_{l, m}(\hat{\Omega})}_{\text {downscater }}+\underbrace{S_{g}(\vec{r}, \hat{\Omega})}_{\text {source }} . \tag{2.50}
\end{align*}
$$

The angular dependence of inscatter on the right hand side of Eq. 2.50 is expressed as a summation over spherical harmonics (Eq. 2.48), with coefficients derived using Eq. 2.49 from angular fluence of the previous iteration $(t)$. The same formalism applies to downscatter, whose scalar flux moments have been derived from the converged angular fluence of upstream energy groups $g^{\prime}<g$.

The source term can be formulated in an analogous way as:

$$
\begin{equation*}
\boldsymbol{S}_{\gamma_{p r i m a r y}, g}=\left(\sum_{g^{\prime}=1}^{\max \left(g, N_{p g}\right)} \sum_{l=0}^{L} \sum_{m=-l}^{l} \Phi_{F S D S, g^{\prime} l, m}(\vec{r}) \sigma_{S, g^{\prime} \rightarrow g, l}(\vec{r}) Y_{l, m}(\hat{\Omega})\right)_{\text {photon source }} . \tag{2.51}
\end{equation*}
$$

The primary fluence $W_{\gamma, g^{\prime}}$ is raytraced to points of the geometry within the beam, then expanded in terms of scalar flux moments for a First Scattered Distributed Source (FSDS):

$$
\begin{equation*}
\Phi_{F S D S, g^{\prime} l, m}(\vec{r})=\int d \hat{\Omega} \frac{W_{\gamma, g^{\prime}} \cdot e^{-\int \sigma_{T, g^{\prime}(\vec{r}) d r}}}{4 \pi\left(\vec{r}_{p}-\vec{r}_{0}\right)^{2}} Y_{l, m}\left(\hat{\Omega}_{r p}\right), \tag{2.52}
\end{equation*}
$$

where $\hat{\Omega}_{r p}$ is the direction vector from the source location $\vec{r}_{0}$ to point $\vec{r}_{p}$ in the geometry, and $W_{\gamma, g^{\prime}}$ is the weighting given to the source spectrum over the energy group $g^{\prime}$. Both the downscatter and source terms remain static during SI.

$$
\begin{equation*}
\boldsymbol{S}_{\text {static }, g}=\boldsymbol{S}_{\gamma_{\text {primany }}, g}+\boldsymbol{S}_{D S, g} . \tag{2.53}
\end{equation*}
$$

In contrast, inscatter interactions need be iterated upon for the current group $g$ :

$$
\begin{equation*}
\boldsymbol{S}_{S l, g}^{(t)}=\left(\sum_{l=0}^{L} \sum_{m=-l}^{l} \Phi_{g, l, m}^{(t)}(\vec{r}) \sigma_{S, g \rightarrow g, l}(\vec{r}) Y_{l, m}(\hat{\Omega})\right)_{\mathrm{in}-\text { scatter }}, \tag{2.54}
\end{equation*}
$$

where $\Phi_{g, l, m}^{(t)}(\vec{r})=\int d \hat{\Omega} \Psi_{g}^{(t-1)}(\vec{r}, \hat{\Omega}) Y_{l, m}(\hat{\Omega})$, with the initial guess $\Psi_{g}^{(0)}(\vec{r}, \hat{\Omega})=0$ (assume no inscatter on the first iteration). The left hand of Eq. 2.50 in operator notation is:

$$
\begin{equation*}
\boldsymbol{L}_{g}=\left[\hat{\Omega} \cdot \vec{\nabla}+\kappa_{g} \vec{\tau}(\vec{B}, \hat{\Omega}) \cdot \vec{\nabla}_{\Omega}+\sigma_{T, g}(\vec{r})\right] . \tag{2.55}
\end{equation*}
$$

With these conventions, Source Iteration involves solving

$$
\begin{equation*}
\boldsymbol{L}_{g} \Psi_{g}^{(t+1)}(\vec{r}, \hat{\Omega})=\boldsymbol{S}_{S l, g}^{(t)}+\boldsymbol{S}_{\text {static }, g} \tag{2.56}
\end{equation*}
$$

until the relative change in the L2 norm of scalar flux moments falls below a given threshold:

$$
\begin{equation*}
\frac{\left\|\Phi_{l m, g}^{(t+1)}-\Phi_{l m, g}^{(t)}\right\|_{2}}{\left\|\Phi_{l m, g}^{(t)}\right\|_{2}}<e p s . \tag{2.57}
\end{equation*}
$$

Often, eps $\approx 10^{-4}$ yields a suitably accurate solution.

### 2.3 Finite Element Analysis

Among the most versatile family of numerical techniques to solve partial differential equations is Finite Element Analysis (FEA), which provides the means to (i) discretize the problem domain, and (ii) mechanism to converge on the best approximation.

### 2.3.1 Domain Discretization

FEA partitions the continuous domain under consideration into local subdomains (elements), each having discrete degrees of freedom (nodes) often at the corners or along edges of an element's geometry. Each node is coupled to a respective basis function whose analytic form allows for interpolation within the element's domain.

For the LBTE, finite element discretization is applied to both spatial and angular domains, some examples are shown in Figure 2.9.


Figure 2.9: Examples of FEA partitioning of space into (a) structured hexahedral elements, (b) unstructured tetrahedral elements, as well as angle into (c) curvilinear elements on the sphere, and (d) mapping onto flattened space.

The interplay between conventions in space and angle will play a significant role for an efficient solution technique. The consequences of interdependencies between element geometry, spaceangle coupling, and special solution techniques often require careful consideration of tradeoffs, a key theme in Chapter 4. Algorithmic partitioning of each domain into constituent elements is performed through mesh generation, which typically allows adaptive resolution to refine regions expected to experience greater variation in the solution. The resulting mesh can be described by two data structures, the $P$ array which encodes node positions, and $T$ array which enumerate indices of nodes which form an element ${ }^{25}$.

After a mesh has been generated, functional variation of the solution within each element needs to be considered, and thereafter the problem becomes finding a function to approximate the partial integro-differential equation at a finite number of nodal degrees of freedom.

### 2.3.2 Basis Functions

Within each element, the approximate solution can be reconstructed as a linear combination of polynomials, each associated with a node, and formally denoted as basis functions. Having a functional form within the element enables interpolation of the solution at any location not explicitly defined by a node, while allowing differential operators to be applied analytically to the basis functions. A space-angle FEM discretization of angular fluence over a given element can be expanded as:

$$
\begin{equation*}
\Psi(\vec{r}, \hat{\Omega}) \approx \sum_{i=1}^{I} \sum_{p=1}^{p} \psi_{i, p} \lambda_{i}(\vec{r}) \gamma_{p}(\hat{\Omega}), \tag{2.58}
\end{equation*}
$$

where $\lambda_{i}(\vec{r})$ corresponds to the $i$-th spatial basis function of $I$ total spatial nodes, and $\gamma_{p}(\hat{\Omega})$ is the $p$-th angular basis function of $P$ total angular nodes (example in Figure 2.10), and $\psi_{i p}$, are the node coefficients representing numerical degrees of freedom to be solved.
Lagrange basis functions satisfy specific properties which maximize independence of each node while retaining a consistent scheme of normalization:

$$
\begin{align*}
& \lambda_{i}(\vec{r})=\left\{\begin{array}{lc}
1 & \vec{r}=\vec{r}_{i} \\
0 & \text { every other node }
\end{array} \quad \sum_{i} \int_{V^{e}} \lambda_{i}(\vec{r}) d V=1,\right.  \tag{2.59a}\\
& \gamma_{p}(\hat{\Omega})=\left\{\begin{array}{lc}
1 & \hat{\Omega}=\hat{\Omega}_{p} \\
0 & \text { every other node }
\end{array} \quad \sum_{p} \int_{\Omega_{\alpha}} \gamma_{p}(\hat{\Omega}) d \hat{\Omega}=1 .\right. \tag{2.59b}
\end{align*}
$$

Implicit to the definitions in Eq. $2.59(\mathrm{a}, \mathrm{b})$ is the property of Compact Support, where basis functions are defined locally over their respective element and zero in all other elements, such that the global domain is represented by a piecewise polynomial approximation.


Figure 2.10: Example illustrating cubic Lagrange basis functions at each of the 10 nodes of a triangular element.

For a chosen element $e l_{s}$ in space and $e l_{a}$ in angle, substituting the finite element expansion of angular fluence into the left hand side of Eq. 2.56 yields:

$$
\begin{equation*}
[\underbrace{\hat{\Omega} \cdot \vec{\nabla}}_{\text {streaming }}+\underbrace{\kappa_{g} \vec{\tau}(\vec{B}, \hat{\Omega}) \cdot \vec{\nabla}_{\Omega}}_{\text {magnetic field }}+\underbrace{\sigma_{T, g}\left(e l_{s}\right)}_{\text {removal }}] \sum_{i=1}^{I} \sum_{p=1}^{P} \underbrace{\psi_{g, i, p}^{(t+1)}}_{\text {node coefficient spatial basis angular basis }} \underbrace{\lambda_{i}(\vec{r})}_{i} \gamma_{p}(\hat{\Omega}) . \tag{2.60}
\end{equation*}
$$

Evident in Eq. 2.60, the streaming operator can be applied directly to the spatial basis function, while the magnetic field gradient can be applied to the angular basis function. Material parameterization is assumed to be constant over each spatial element, indexed $\mathrm{el}_{s}$. Having established a discretized representation in terms of nodes and basis functions, the process of determining optimal coefficient values is a second major component of FEA.

### 2.3.3 Residual Error Minimization through Galerkin Approach

A partial differential equation in operator notation can be expressed as:

$$
\begin{equation*}
\hat{\mathbf{A}} \boldsymbol{u}=\boldsymbol{f}, \tag{2.61}
\end{equation*}
$$

where $\boldsymbol{u}$ is a continuous function representing the solution, $\boldsymbol{f}$ is a source function, and $\hat{\mathbf{A}}$ is a differential operator which applies a transformation from the vector space of $\boldsymbol{u}$ to the vector space of $\boldsymbol{f}$.

For simplicity, consider a 1D domain where the solution can be approximated as:

$$
\begin{equation*}
\tilde{\boldsymbol{u}}(x)=\sum_{i=1}^{I} u_{i} \lambda_{i}(x) . \tag{2.62}
\end{equation*}
$$

The continuous function of the true solution $\boldsymbol{u}$ and its FEA approximation $\tilde{\boldsymbol{u}}$ are illustrated in the vector space of the solution (Figure 2.11).


Figure 2.11: Approximation of the true solution function $\boldsymbol{u}$ by an expansion over basis functions $\tilde{\boldsymbol{u}}$ in the solution vector space, where $\lambda_{i}(x)$ are linear basis functions about the respective node $i$, having compact support.

Applying the differential operator $\hat{\mathbf{A}}$ to $\tilde{\boldsymbol{u}}(x)$ yields an approximation in the vector space of the source which deviates from the true source function $\boldsymbol{f}$ as quantified by a residual:

$$
\begin{equation*}
\tilde{\boldsymbol{R}}=\hat{\boldsymbol{A}} \tilde{\boldsymbol{u}}-\boldsymbol{f} \tag{2.63}
\end{equation*}
$$

Integrating the squared L2-norm of the residual over the domain yields a representation of the error in the vector space of the source:

$$
\begin{equation*}
\|\tilde{\boldsymbol{R}}\|_{2}^{2}=\int_{x \in L}(\hat{\boldsymbol{A}} \tilde{\boldsymbol{u}}-\boldsymbol{f})^{2} d x \tag{2.64}
\end{equation*}
$$

Minimizing Eq. 2.64 in the vector space of the source is sought by adjusting coefficients $u_{i}$ in the vector space of the solution to obtain the best approximation $\tilde{\boldsymbol{u}}$. Although the goal is to minimize the error ( $\tilde{\boldsymbol{u}}-\boldsymbol{u})$ in the solution's own vector space, the squared L2 norm of the residual (Eq. 2.64) serves as a proxy metric in the vector space of the source. The degree to which the residual is proportional to error of the solution depends on the resolution of discretization and how the operator shifts and scales individual degrees of freedom between the two vector spaces.


Figure 2.12: The operator $\hat{\boldsymbol{A}}$ transforms the approximation $\tilde{\boldsymbol{u}}$ from (a) the vector space of the solution into (b) the vector space of the source where the residual $\|\tilde{\boldsymbol{R}}\|_{2}^{2}$ is evaluated as a proxy metric of solution error.

The goal of determining optimal coefficient values for limited degrees of freedom to approximate the true continuous solution is geometrically analogous to representing a higher dimensional vector in a lower dimensional subspace. The process is made rigorous through the projection operator, where the best possible coefficients are established for each degree of freedom in the subspace, such that any remaining error relative to the true solution is due to inherent limitation in the degrees of freedom available as opposed to poor choice of coefficients. In vector calculus terminology, this is achieved by enforcing that the residual is orthogonal to the approximation subspace. A geometric analogy of this reasoning is illustrated in Figure 2.13 for the projection of a 3D vector (with components in $x, y$, and $z$ ) to a 2D subspace spanning the $x-y$ plane.


Figure 2.13: Geometric depiction of Galerkin method, where a 3D vector $\vec{V}_{3}=[A \hat{x}+B \hat{y}+C \hat{z}]$ (representing true solution) is optimally projected onto a 2 D plane (representing the approximation subspace) as $\vec{V}_{2}=[A \hat{x}+B \hat{y}]$ such that the difference between the true solution and its projection is orthogonal to the plane.

In this trivial case, $\vec{V}_{3}=[A \hat{x}+B \hat{y}+C \hat{z}] \rightarrow \vec{V}_{2}=[A \hat{x}+B \hat{y}]$, involves simply replicating $x$ and $y$ components of the 3D vector, such that the components in the $x-y$ plane are the best that can possibly be chosen, and any residual $\vec{V}_{2}-\vec{V}_{3}=-C \hat{z}$ is due to inherently lacking a degree of freedom in $\hat{z}$. There are no components $\hat{x}$ or $\hat{y}$ in the residual, therefore the projection is optimal. For vector geometries, this condition is formally encoded by the dot product expression:

$$
\begin{equation*}
\overrightarrow{\text { residual }} \cdot \overrightarrow{\text { projection }}=0 . \tag{2.65}
\end{equation*}
$$

The dot product quantifies the degree of similarity between two vectors. In Eq. 2.65, the projection is optimal when it shares no overlap with the residual. The analogy can be made to functions, which reside in an abstract higher dimensional vector space. The degree of similarity between two functions is characterized by their inner product, involving an integral quantifying overlap over the problem domain:

$$
\begin{equation*}
\langle f(x), g(x)\rangle=\int_{x \in L} f(x) g(x) d x . \tag{2.66}
\end{equation*}
$$

The Galerkin approach proceeds in the spirit of optimal projection (Figure 2.13), though applied to functions instead of vectors.

The approximation subspace is assumed to be spanned by the set of basis functions $\left\{\lambda_{j}\right\}$, each associated with a nodal degree of freedom, running over index $j$, which spans the same range, but distinct from the index $i$ used in the finite element expansion of $\tilde{\boldsymbol{u}}$ in calculating the residual. Setting the residual to be orthogonal to the approximation subspace (in the spirit of Eq. 2.65), the inner product expression is:

$$
\begin{equation*}
\left\langle\boldsymbol{A} \tilde{\boldsymbol{u}}-\boldsymbol{f}, \lambda_{j}\right\rangle=0 . \tag{2.67}
\end{equation*}
$$

Invoking the linearity property of integration, Eq. 2.67 can be separated:

$$
\begin{equation*}
\left\langle\boldsymbol{A} \tilde{\boldsymbol{u}}, \lambda_{j}\right\rangle=\left\langle\boldsymbol{f}, \lambda_{j}\right\rangle . \tag{2.68}
\end{equation*}
$$

Eq. 2.68 is the foundational statement of Galerkin's method, providing a mathematical rationale to choose optimal discrete coefficients and is a member of the method of weighted residuals. Formally $\lambda_{j}$ are the weighting functions which have the same form as the approximation functions of Eq. 2.62. Other criteria can arise from alternative choices of weighting functions such as the Least Squares Finite Element Method (explored in Chapter 3), or the collocation method ${ }^{25}$. Ultimately these criteria enable the discrete problem to be cast into a matrix of linear equations.

### 2.3.4 Elemental Matrix Assembly

Galerkin's method (Eq. 2.68) applied to the multigroup LBTE, results in:

$$
\begin{equation*}
\left\langle\boldsymbol{L}_{g} \Psi_{g}^{(t+1)}, \Upsilon\right\rangle=\left\langle\mathbf{S}_{S I, g}^{(t)}+\mathbf{S}_{\text {static }, g}, \Upsilon\right\rangle \tag{2.69}
\end{equation*}
$$

where the operator $\boldsymbol{L}_{g}$ is:

$$
\begin{equation*}
\boldsymbol{L}_{g}=\left[\hat{\Omega} \cdot \vec{\nabla}+\kappa_{g} \vec{\tau}(\vec{B}, \hat{\Omega}) \cdot \vec{\nabla}_{\Omega}+\sigma_{T, g}\left(e l_{s}\right)\right] . \tag{2.70}
\end{equation*}
$$

The finite element expansion of angular fluence is:

$$
\begin{equation*}
\Psi_{g}^{(t+1)}(\vec{r}, \hat{\Omega}) \approx \sum_{i=1}^{I} \sum_{p=1}^{P} \psi_{g, i, p}^{(t+1)} \lambda_{i}(\vec{r}) \gamma_{p}(\hat{\Omega}), \tag{2.71}
\end{equation*}
$$

and the weighting function is:

$$
\begin{equation*}
\Upsilon(\vec{r}, \hat{\Omega})=\lambda_{j}(\vec{r}) \gamma_{q}(\hat{\Omega}) \tag{2.72}
\end{equation*}
$$

composed as a product of spatial and angular basis functions, enumerated over independent indices $j$, and $q$.

For a given spatial element $e l_{s}$, coupled to a given angular element $e l_{a}$, the left hand side inner product of Eq. 2.69 with respective definitions of the LBTE yields:

$$
\begin{align*}
& \left\langle\boldsymbol{L}_{g} \Psi_{g}^{(t+1)}, r\right\rangle=\underbrace{\text { Term 1: Streaming }}_{\Omega_{\Omega_{\alpha}} d \hat{\Omega} \int_{V^{e}} d V \hat{\Omega} \cdot \vec{\nabla}\left(\sum_{i=1}^{I} \sum_{p=1}^{p} \psi_{g, i, p}^{(t+1)} \lambda_{i}(\vec{r}) \gamma_{p}(\hat{\Omega})\right)\left(\lambda_{j}(\vec{r}) \gamma_{q}(\hat{\Omega})\right)} \\
& +\underbrace{\int_{\Omega_{\alpha}} d \hat{\Omega} \int_{V^{e}} d V \kappa_{g} \vec{\tau}(\vec{B}, \hat{\Omega}) \cdot \vec{\nabla}_{\Omega}\left(\sum_{i=1}^{I} \sum_{p=1}^{p} \psi_{g, i, p}^{(t+1)} \lambda_{i}(\vec{r}) \gamma_{p}(\hat{\Omega})\right)\left(\lambda_{j}(\vec{r}) \gamma_{q}(\hat{\Omega})\right)}_{\text {Term 2: Magnetic Field }}  \tag{2.73}\\
& +\underbrace{\int_{\Omega_{\alpha}} d \hat{\Omega} \int_{V^{e}} d V \sigma_{T, g}\left(e l_{s}\right)\left(\sum_{i=1}^{I} \sum_{p=1}^{p} \psi_{g, i, p}^{(t+1)} \lambda_{i}(\vec{r}) \gamma_{p}(\hat{\Omega})\right)\left(\lambda_{j}(\vec{r}) \gamma_{q}(\hat{\Omega})\right)}_{\text {Term 3:Removal }},
\end{align*}
$$

where $V^{e}$ denotes the volume domain encompassed by spatial element $e l_{s}$, and $\Omega_{\alpha}$ denotes the range of directions encompassed by angular element $e l_{a}$.

Applying the FEM approximation to the angular fluence and extracting the summation over nodal coefficients $\psi_{g, i, p}^{(t+1)}$ (common to all terms and not a function of space or angle), Eq. 2.73 can be re-expressed:

$$
\begin{array}{|l|}
\begin{array}{|l}
\sum_{i=1}^{I} \sum_{p=1}^{P} \psi_{g, i, p}^{(t+1)} \\
+\sum_{i=1}^{I} \sum_{p=1}^{P} \psi_{g, i, p}^{(t+1)} \\
+\sum_{i=1}^{I} \sum_{p=1}^{P} \psi_{g, i, p}^{(t+1)} \\
\text { forms elemental } \vec{\psi}_{g, e_{s, a}}^{(t+1)}
\end{array}  \tag{2.74}\\
\underbrace \begin{array} { c } 
{ \int _ { \Omega _ { \alpha } } d \hat { \Omega } _ { p } ( \hat { \Omega } ) \gamma _ { q } ( \hat { \Omega } ) \int _ { V ^ { e } } d V \hat { \Omega } \cdot \vec { \nabla } ( \lambda _ { \mathrm { i } } ( \vec { r } ) ) \lambda _ { \mathrm { j } } ( \vec { r } ) } \\
{ \kappa _ { g } \int _ { \Omega _ { \alpha } } d \hat { \Omega } \vec { \tau } ( \vec { B } , \hat { \Omega } ) \cdot \vec { \nabla } _ { \Omega } ( \gamma _ { p } ( \hat { \Omega } ) ) \gamma _ { q } ( \hat { \Omega } ) \int _ { V ^ { e } } d V \lambda _ { \mathrm { i } } ( \vec { r } ) \lambda _ { \mathrm { j } } ( \vec { r } ) } \\
{ \sigma _ { T , g } ( e l _ { s } ) \int _ { \Omega _ { \alpha } } d \hat { \Omega } \gamma _ { p } ( \hat { \Omega } ) \gamma _ { q } ( \hat { \Omega } ) \int _ { V ^ { e } } d V \lambda _ { \mathrm { i } } ( \vec { r } ) \lambda _ { \mathrm { j } } ( \vec { r } ) }
\end{array}, \\
\text { forms elemental matrix operator }[A]_{g, e l_{s, a}}
\end{array}
$$

where the degrees of freedom $p=1,2, . ., P$ in angle, nested within each degree of freedom $i=1,2, . . I$ in space can be unwrapped to form a vector $\vec{\psi}_{g, e_{s, a}}^{(t+1)}$. The remaining integrals form a
square matrix $[A]_{g, l_{s, a}}$ representing the operator, with indices of the basis functions ( $i$ and $p$ ) indexed horizontally over each row, and indices over the weighting functions ( $j$ and $q$ ) indexed vertically over each column, such that when multiplied to $\vec{\psi}_{g, e e_{s, a}}^{(t+1)}$, it transforms the degrees of freedom in the solution vector space to degrees of freedom in the source vector space. After applying a spatial FEM expansion to the spherical harmonic moments $\Phi$, the inner product on the right hand side of Eq. 2.69 becomes:

$$
\begin{gather*}
\left\langle S_{s t a t i c, g}, \Upsilon\right\rangle=\sum_{g^{\prime}=1}^{g} \sum_{l=0}^{L} \sum_{m=-l}^{l} \sum_{i=1}^{I}\left(\phi_{F S D S, g^{\prime}, l, m, i}+\phi_{g^{\prime}, l, m, i}\right) \sigma_{s, g^{\prime} \rightarrow g, l}\left(e l_{s}\right) \int_{\Omega_{\alpha}} d \hat{\Omega} Y_{l, m}(\hat{\Omega}) \gamma_{q}(\hat{\Omega}) \int_{V^{e}} d V \lambda_{i}(\vec{r}) \lambda_{j}(\vec{r}),  \tag{2.75a}\\
\left\langle S_{S I, g}^{(t)}, \Upsilon\right\rangle=\sum_{l=0}^{L} \sum_{m=-l}^{l} \sum_{i=1}^{I} \phi_{g, l, m, i}^{(t)} \sigma_{s, g \rightarrow g, l}\left(e l_{s}\right) \int_{\Omega_{\alpha}} d \hat{\Omega} Y_{l, m}(\hat{\Omega}) \gamma_{q}(\hat{\Omega}) \int_{V^{e}} d V \lambda_{i}(\vec{r}) \lambda_{j}(\vec{r}) . \tag{2.75b}
\end{gather*}
$$

Notably, scalar flux moments are expanded in terms of spherical harmonics, defined globally over the entire angular domain, while the weighting function pertains to the angular element under consideration. Equation 2.75a need only to be calculated once at the start of each energy group, remaining constant during source iteration, while Eq. 2.75 b is updated for successive estimations of inscatter. Their sum collapses to a source vector of known values $\vec{b}_{g, e l_{s, a}}^{(t)}$. The elemental matrix form is depicted in Figure 2.14, below:


Figure 2.14: Schematic of elemental matrix system and index enumerations.

Steps to a discretized solution over the entire domain are summarized in Schematic 2.1, where the notation []$_{g b l}$ indicates a repository of the enclosed entity over the entire problem domain.
(a) For $g=1, . ., N_{g} \%$ iterate over Multigroup intervals
(b) While $\delta_{\text {resid }}^{t+1}>$ eps $\%$ perform Source Iteration to update solution for index $t+1$
(c) For $e l_{a}=1, . ., N_{\text {angElem }} \%$ iterate over angular elements
(d) For $e l_{s}=1, . ., N_{\text {spaElem }} \%$ iterate over spatial elements
(e) Assemble elemental matrix $[A]_{g, e l_{s, a}}$ and elemental source $\vec{b}_{g, e l_{s, a}}^{(t)}$
(f) Solve the system

Update $\left[\vec{\phi}_{g}^{t}\right]_{g b l}$ using $\left[\vec{\psi}_{g}^{t}\right]_{g b l}$, and evaluate $\delta_{\text {resid }}^{t}$ over the entire domain.
If $\delta_{\text {resid }}^{t} \leq e p s$, integrate $\left[\vec{\psi}_{g}^{t}\right]_{g b l}$ over angle, and store in $\left[\psi_{g, \text { converged }}\right]_{g b l}$
Obtain dose per fluence: $[D]_{g b l}=\sum_{g=1}^{G}\left[\sigma_{E D} / \rho\right]_{g b l} . *\left[\psi_{g, \text { converged }}\right]_{g b l}$
Schematic 2.1: Outline of steps for solution to entire domain.

Typical problems in photon beam radiotherapy involve 52 to 72 energy groups, 8 to 520 angular elements, and 50,000 to 200,000 spatial elements. This amounts to many millions and occasionally billions of elemental matrix systems needing to be solved. Moreover, the presence of strong magnetic fields can require many source iterations to converge.

Novel techniques to facilitate such immense degrees of computational complexity are explored in upcoming chapters.

### 2.4 Deterministic Numerical Integration

A powerful functionality of numerical techniques is the versatility to integrate complicated expressions often spanning multiple dimensions and having no analytic anti-derivative. Newton Cotes techniques (including the Trapezoid rule and Simpson's rules) evaluate the function at equally spaced intervals ${ }^{26}$. While conceptually straightforward, the accuracy of integration given a highly oscillatory function is sensitive to which specific points are sampled as well as their spacing. A more robust family of Gaussian Quadrature (GQ) techniques ${ }^{27}$ strategically chooses $N$ unequally spaced points at which to evaluate the function, and determines their respective weighting providing integration over the entire interval with accuracy on the order of $2 \mathrm{~N}-1$ :

$$
\begin{equation*}
\int_{-1}^{1} f(x) d x \approx \sum_{i=1}^{N} w_{i} f\left(x_{i}\right) \tag{2.76}
\end{equation*}
$$

For example, 2-point GQ in 1-dimension can be written:

$$
\begin{equation*}
\int_{-1}^{1} f(x) d x=w_{1} f\left(x_{1}\right)+w_{2} f\left(x_{2}\right), \tag{2.77}
\end{equation*}
$$

expected to yield exact integration of $x^{0}, x^{1}, x^{2}, x^{3}$, such that:

$$
\begin{align*}
& f(x)=1 \rightarrow \int_{-1}^{1} 1 d x=2=w_{1}+w_{2} \\
& f(x)=x \rightarrow \int_{-1}^{1} x d x=0=w_{1} x_{1}+w_{2} x_{2}  \tag{2.78}\\
& f(x)=x^{2} \rightarrow \int_{-1}^{1} x^{2} d x=2 / 3=w_{1} x_{1}^{2}+w_{2} x_{2}^{2} \\
& f(x)=x^{3} \rightarrow \int_{-1}^{1} x^{3} d x=0=w_{1} x_{1}^{3}+w_{2} x_{2}^{3} .
\end{align*}
$$

Solving this nonlinear system of Eq. 2.78 yields:

$$
\begin{equation*}
w_{1}=1, w_{2}=1, x_{1}=-\frac{1}{\sqrt{3}}, x_{2}=\frac{1}{\sqrt{3}} . \tag{2.79}
\end{equation*}
$$

Thus Eq. 2.77 becomes:

$$
\begin{equation*}
\int_{-1}^{1} f(x) d x=f\left(-\frac{1}{\sqrt{3}}\right)+f\left(\frac{1}{\sqrt{3}}\right), \tag{2.80}
\end{equation*}
$$

providing exact integration of polynomials up to degree 3. Higher order rules can be generated noting that the abscissa are located at the roots of the corresponding Legendre polynomial of
order $N$, hence the name Gauss-Legendre Quadrature rules ${ }^{27}$. For example, $x_{1}=-\frac{1}{\sqrt{3}}, x_{2}=\frac{1}{\sqrt{3}}$ are roots of $P_{2}(x)=\frac{1}{2}\left(3 x^{2}-1\right)$, for which determination of weighting coefficients reduces to solving a linear system. The domain of canonical coordinates is defined as:

$$
\begin{equation*}
\eta_{i} \sim[-1,1], \tag{2.81}
\end{equation*}
$$

which can be mapped to arbitrary bounds $\xi_{i} \sim[a, b]$ by:

$$
\begin{equation*}
\xi_{i}=(b-a) \eta_{i}+a . \tag{2.82}
\end{equation*}
$$

The generalization to multiple dimensions requires a tensor product such that the number of function evaluations increases exponentially with dimension, a reason that deterministic frameworks were initially hypothesized as infeasible to solve particle transport through 6dimensional phase space, and early developments favored Monte Carlo.

### 2.5 Monte Carlo

### 2.5.1 Stochastic Sampling Techniques

Monte Carlo (MC) techniques provide a generalized stochastic framework to integrate functions of arbitrary complexity, involving sampling with random numbers. Consider a 1-demensional integral over the domain $[a, b]$ :

$$
\begin{equation*}
I=\int_{a}^{b} f(x) d x \tag{2.83}
\end{equation*}
$$

An estimate $I_{1}$ using a single random sample $x_{1}$ uniformly distributed in $[a, b]$ yields:

$$
\begin{equation*}
I_{1}=(b-a) f\left(x_{1}\right) \tag{2.84}
\end{equation*}
$$

Increasing the number of samples yields a better estimate, as illustrated in Figure 2.15.


Figure 2.15: Estimating integral over polyenergetic photon source spectrum by evaluating function at 4 points: $I_{4}=\frac{b-a}{4}\left(f\left(x_{1}\right)+f\left(x_{2}\right)+f\left(x_{3}\right)+f\left(x_{4}\right)\right)$.

Sampling at a large number points $N$,

$$
\begin{equation*}
I_{N}=\frac{b-a}{N} \sum_{i=1}^{N} f\left(x_{i}\right)=(b-a)\langle f(x)\rangle, \tag{2.85}
\end{equation*}
$$

where the expectation value of the function over $N$ samples is:

$$
\begin{equation*}
\langle f\rangle=\frac{1}{N} \sum_{i=1}^{N} f\left(x_{i}\right) . \tag{2.86}
\end{equation*}
$$

According to the Central Limit Theorem ${ }^{28}$, the probability distribution of the estimate $\langle f\rangle$ approaches the true value $f_{\text {True }}$ as:

$$
\begin{equation*}
p(\langle f\rangle)=\frac{1}{\sigma \sqrt{2 \pi}} \exp \left(\frac{-\left(\langle f\rangle-f_{\text {True }}\right)^{2}}{2 \sigma^{2}}\right) \tag{2.87}
\end{equation*}
$$

where variance can be reduced by increasing the number of samples:

$$
\begin{equation*}
\boldsymbol{\sigma}^{2}=\frac{\left\langle f^{2}\right\rangle-\langle f\rangle^{2}}{N-1} \tag{2.88}
\end{equation*}
$$

such that in the limit of large $N$, a practical estimate can be obtained. Crucially, Eq. 2.88 does not depend on the number of dimensions, whereas the number of points required for Gaussian quadratures compounds multiplicatively with dimension. This theoretical foundation was among the reasons Monte Carlo was hypothesized as more computationally tractable for particle transport through 6-dimensional phase space, hence received more attention and early development than deterministic techniques ${ }^{2}$.

Equation 2.85 can be generalized to higher dimensions, such as a volume integral ${ }^{27}$ :

$$
\begin{equation*}
\int_{V} f d V \approx V\langle f\rangle \pm V \sqrt{\frac{\left\langle f^{2}\right\rangle-\langle f\rangle^{2}}{N-1}} \tag{2.89}
\end{equation*}
$$

Monte Carlo techniques can be adapted beyond integration to sample the functions of interest in particle transport: differential cross sections for scattering, absorption, secondary production, and annihilation, often complicated fits of empirical data taking the form of a probability distribution function (PDF), $p(x) \geq 0$, normalized over the domain $\left[x_{\min }, x_{\max }\right]$ such that:

$$
\begin{equation*}
\int_{x_{\min }}^{x_{\max }} p\left(x^{\prime}\right) d x^{\prime}=1 . \tag{2.90}
\end{equation*}
$$

Integrating the PDF yields the cumulative distribution function (CDF) $0 \leq P(x) \leq 1$ :

$$
\begin{equation*}
P(x)=\int_{x_{\min }}^{x} p\left(x^{\prime}\right) d x^{\prime} \tag{2.91}
\end{equation*}
$$

whose output monotonically increases over the range $\eta_{i} \sim[0,1]$, conveniently sampled by a random number generator to determine an abscissa, for example the scattering angle. The most direct approach to sampling an input parameter $x_{i}$ given a random number $\eta_{i} \sim[0,1]$ is by mapping through the inverse function of the CDF:

$$
\begin{equation*}
x_{i}=P^{-1}\left(\eta_{i}\right) . \tag{2.92}
\end{equation*}
$$

In most cases, determination of the inverse CDF is infeasible, or computationally burdensome given experimental data fit with a complicated piecewise PDF. Moreover, calculation of the CDF can require computationally intensive numerical integration. An alternative to sampling Eq. 2.92 is to invoke a simpler Rejection Method ${ }^{27}$, which operates directly on the PDF.


Figure 2.16: Example illustrating Rejection Sampling where (a) sample is accepted, (b) sample is rejected.

A much simpler bounding function $M(x)$ is defined whose inverse is easy to obtain such that given a random number $\xi_{1} \sim[0, \max (M)]$, an abscissa is proposed $x_{1}=M^{-1}\left(\xi_{1}\right)$, where an additional sample $\xi_{2} \sim\left[0, M\left(x_{1}\right)\right]$ determines whether $x_{1}$ is accepted $\left(\xi_{2} \leq p\left(x_{1}\right)\right)$ or rejected $\left(\xi_{2}>p\left(x_{1}\right)\right)$ as illustrated in Figure 2.16. Notably, two random numbers are required, and the bounding function $M(x)$ if chosen poorly can lead to a high rejection rate, thus degrading efficiency. Nevertheless the flexibility of rejection sampling is leveraged as a core technique in most Monte Carlo frameworks such as GEANT4 (described in §2.5.2).

The paradigm of decomposition into multiple sampling steps can be used to accommodate multi dimensional PDFs often encountered in differential cross sections of particle transport ${ }^{29}$.

$$
\begin{gather*}
p(x, y)=p(x \mid y) q(y),  \tag{2.93a}\\
q(y)=\int_{x_{\min }}^{x_{\max }} d x p(x, y)  \tag{2.9.9b}\\
p(x \mid y)=\frac{p(x, y)}{q(y)} . \tag{2.93c}
\end{gather*}
$$

In Eq. 2.93, $q(y)$ is the marginal PDF representing the projection onto variable $y$ for any value of $x$, and $p(x \mid y)$ is a conditional PDF for $x$ given a fixed value of $y$. Therefore Eq. 2.93a is
decomposed as the product of univariate distributions and can be applied recursively to sample even higher dimensions.

### 2.5.2 Particle Transport in magnetic fields using GEANT4

A framework for modeling particle transport using Monte Carlo comprises 4 key steps ${ }^{30}$, termed as analog simulation:
(i) Determine the distance to next site of interaction by random sampling,
(ii) Transportation of particle to site of interaction, respecting geometric boundary crossings and magnetic fields,
(iii) Determine type of interaction and parameters pertaining to interaction,
(iv) Simulate the interaction: change to particle energy, trajectory, and any secondaries produced. This conceptually simple framework can be adapted to problems of variable difficulty, modular in its inclusion of physics processes. Specifically, we consider the general purpose Monte Carlo research code GEANT4, accommodating high energy physics as well as medical applications. Geant4 uses a combination of rejection (Figure 2.16) and composition techniques (Eq. 2.93) to sample differential cross sections of various physical processes.

### 2.5.2.1 Geant4 Photon Transport

The linac source spectrum is sampled (as shown in Figure 2.16) to yield primary photons incident on the detector geometry ${ }^{31}$.
The probability of photon interaction in a medium at a distance $s$ from the current position is ${ }^{31}$ :

$$
\begin{equation*}
p(s) d s=\mu(E) e^{-\mu(E) s} d s \tag{2.94}
\end{equation*}
$$

where $\mu(E)$ is the linear attenuation coefficient for a given material at the energy $E$ under consideration, having the same meaning as the total interaction cross section $\sigma_{T}(E)$ in the LBTE. The concept of mean free path length (MPF) is introduced to facilitate the transport step through heterogeneous media, defined as the expectation value to distance travelled ${ }^{31}$ :

$$
\begin{equation*}
\langle s\rangle=\int_{0}^{\infty} d s s p(s)=\int_{0}^{\infty} d s \mu(E, s) s e^{-\mu(E, s) s} \tag{2.95}
\end{equation*}
$$

where $\mu(E, s)$ can vary based on the material traversed along $s$.

The number of MFP traversed over a distance $s$ can be defined:

$$
\begin{equation*}
n_{\langle s\rangle}=\frac{s}{\langle s\rangle} \approx \sum_{\text {start }}^{\text {end }} \mu_{i}(E) s_{i}, \tag{2.96}
\end{equation*}
$$

where the summation over differential path segments $s_{i}$ through heterogeneous media $\mu_{i}(E)$ proceeds until the number of mean free path lengths has been expended, defining the endpoint. The cumulative distribution function can be written in terms of $n_{\langle s\rangle}$ as $^{31}$ :

$$
\begin{equation*}
P\left(n_{\langle s\rangle}\right)=\int_{0}^{n_{(s\rangle}} d n_{\langle s\rangle}^{\prime} p\left(n_{\langle s\rangle}^{\prime}\right)=\int_{0}^{n_{(s\rangle}} d n_{\langle s\rangle}^{\prime} e^{-n_{\langle s\rangle}^{\prime}}=1-e^{-n_{\langle s\rangle}}, \tag{2.97}
\end{equation*}
$$

for which inverse sampling given a random number $\eta_{i} \sim[0,1)$ is simply:

$$
\begin{equation*}
n_{\langle s)_{i}}=P^{-1}\left(\eta_{i}\right)=-\ln \left(1-\eta_{i}\right) . \tag{2.98}
\end{equation*}
$$

The photon is transported a corresponding number of MPFs, losing the appropriate amount of energy to terminate at a location approximated in Eq. 2.96 which accounts for traversal through heterogeneous materials.

A resulting interaction is randomly sampled ( $\eta_{i} \sim[0,1]$ ) based on the relative cross section of various processes given the particle's energy and surrounding material.


Figure 2.17: Example of sampling processes for 40 keV photons in water.
Within each process are further PDFs, usually multivariable semi-empirical fitting of experimental data, in the case of GEANT4 based on the Livermore Evaluated Photon Data Library (EPDL) ${ }^{32}$. Rejection sampling and composition are used.

### 2.5.2.2 Geant4 Electron Transport

Unlike photons, electrons possess a charge, thus undergo abundant coulombic interactions with the surrounding medium, unfolding as a torturous path which ultimately deposits energy in the
patient. Compared to photons which have an MPF on the order of 10 cm in the therapeutic range, electrons interact far more abundantly, with an MPF on the order of $10^{-5} \mathrm{~cm}$, thus $10^{5}$ interactions occur for every cm of media traversed ${ }^{33}$. Analog simulation would be computationally exhaustive to account for every electron interaction explicitly. Noting that the vast majority of electron interactions involve small energy losses and minimal change in trajectory, the cumulative effect of soft collisions can be approximated by a single bulk step with a net deflection and energy loss drawn from the probability distribution of multiple-scattering theory. This approach of condensed history (CH) transport introduced by Berger ${ }^{34}$ made possible the practical realization of electron transport using Monte Carlo. GEANT4 employs the Urban95 model ${ }^{35}$, shown to exhibit the best agreement with measurement ${ }^{36}$, and based on the Lewis theory of coulomb multiple scattering at small angles ${ }^{37}$ which provides the effective spatial and angular distributions after each step. Energy loss is modeled by the CSDA approximation which uses the restricted stopping power traversed over the true path length, corrected from the geometric path length.

As a mixed simulation, the threshold between catastrophic and soft collisions must be chosen judiciously to balance calculation efficiency and accuracy. GEANT4 employs a range cutoff for the production of secondary particles below which interactions are modeled using condensed histories. For example, setting this to $10 \mu \mathrm{~m}$ ascribes an effective maximum range of secondary particles produced by electron soft collisions.

Catastrophic collisions involving energy losses above this threshold have a MFP several orders of magnitude longer, which makes it feasible to model each interaction discretely using analog simulation, while modifying each transport step for the displacement, energy loss, and deflection caused by soft collisions. Step size is limited based on a percentage of maximum energy loss, distance to material boundary crossing, and error considerations in modeling the magnetic field trajectory, whichever is the minimum.

At the end of each transport step, the catastrophic interaction is sampled from differential cross sections of the Livermore Evaluated Electron Data Library (EEDL) ${ }^{38}$, resulting in changes to the parent particle and initiation of tracks for any secondaries produced. GEANT4 employs no
tracking cutoff, meaning particles are simulated until they are absorbed or exit the geometry. To avoid introducing systematic bias in modeling the underling physics, variance reduction techniques other than condensed histories are not used, therefore simulations in GEANT4 take relatively longer than other Monte Carlo frameworks.

### 2.5.2.3 Geant4 Magnetic Field Implementation

Magnetic fields are incorporated into GEANT4 through the transportation step, where equations of motion in a Lorentz force are approximated by chord segments using Runge-Kutta (RK) integration techniques ${ }^{39}$.

The principles of this numerical technique can be illustrated using the equation:

$$
\begin{equation*}
\frac{d y}{d t}=f(y, t) . \tag{2.99}
\end{equation*}
$$

The update equation is:

$$
\begin{equation*}
y_{i+1}=y_{i}+\lambda h, \tag{2.100}
\end{equation*}
$$

where $\lambda$ represents the slope, and $h$ is the step size ${ }^{26}$. The classic Euler Method directly uses the first derivative (Eq. 2.99) to estimate the slope at the current point:

$$
\begin{equation*}
\lambda=f\left(y_{i}, t_{i}\right) . \tag{2.101}
\end{equation*}
$$

This simple approach is prone to error when the slope changes greatly over the step size. Various refinements including Huen's Method and the Midpoint Rule improve the estimate of the slope, as precursors to Runge Kutta method in which truncation error is modeled of the Taylor series, though without needing to evaluate higher derivatives ${ }^{26}$.

The classic 4-point RK used to track magnetic field trajectories in Geant4 follows the update equation:

$$
\begin{equation*}
y_{i+1}=y_{i}+\frac{h}{6}\left(k_{1}+2 k_{2}+2 k_{3}+k_{4}\right), \tag{2.102}
\end{equation*}
$$

with the constants defined as ${ }^{26}$ :

$$
\begin{align*}
& k_{1}=f\left(y_{i}, t_{i}\right) \\
& k_{2}=f\left(y_{i}+h k_{1} / 2, t_{i}+h / 2\right) \\
& k_{3}=f\left(y_{i}+h k_{2} / 2, t_{i}+h / 2\right)  \tag{2.103}\\
& k_{4}=f\left(y_{i}+h k_{3}, t_{i}+h\right) .
\end{align*}
$$

Specifically the G4NystromRK4 stepping routine provides integration to $4^{\text {th }}$ order accuracy along with error estimate of the attempted step ${ }^{39}$.

The step size when navigating 3-dimensional curved trajectories is parameterized by the miss_distance, defined as the maximum deviation between the true trajectory and chord segment approximation, in addition to delta_intersection, the accuracy to which boundary crossings are computed ${ }^{39}$. Incorporation of magnetic fields is often the limiting factor in the step size. Energy loss is approximated using the condensed history approach.

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# Chapter 3 Second Order Least Squares Continuous Finite Element Formulation and GPU Implementation: Feasibility Study 

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solution to the linear Boltzmann transport equation, " Med. Phys. 43, 3655 (2016).

### 3.1 Purpose and Hypothesis

Presented with the need solve millions of elemental matrix systems over multiple source iterations for each energy group, we attempt to leverage highly parallel Single Instruction Multiple Data (SIMD) architectures of Graphics Processing Units (GPU) to efficiently solve a novel mathematical formulation that maximizes explicit parallelization. Specifically we investigate feasibility of a Second Order Least Squares Continuous Finite Element Method (LSCFEM) approach and develop novel algorithms to implement on GPU.

Adopting continuous finite elements permits the assembly of a global matrix encompassing the entire spatial domain. A given node receives contributions from all elements overlapping at its location, and a sparse global matrix is assembled from the contributions of each elemental matrix system. Moreover, a tight-coupling formalism is invoked between space and angle, using the Kronecker tensor product, eliminating explicit need for Source Iteration. Large sparse matrices are amenable to highly parallelized iterative approaches involving Basic Linear Algebra Subroutines (BLAS), which the GPU can provide as a high throughput solution.

The Galerkin formalism applied to first order systems containing advection are not stable when solved in the standard way, and require special techniques ${ }^{1}$. One such technique is the use of a second order Least Squares Continuous Finite Element Method (LS-CFEM) formulation that results in a Symmetric Positive Definite (SPD) system matrix amenable to a highly efficient Conjugate Gradients solver. In this feasibility study, unstructured tetrahedral elements are used in space, while angle uses a Discrete Ordinates (DO) method. The overarching hypothesis is that
a formulation maximizing explicit parallelization and leveraging implementation on SIMD computational architecture achieves progress towards a real-time dose calculation.

### 3.2 Theory and Techniques

### 3.2.1 Explicit Parallelism through Continuous-FEM Formulation

Many computationally intensive operations in artificial intelligence, computer graphics, and the Finite Element Method can be characterized as Basic Linear Algebra Subroutines (BLAS). These include i) vector-vector dot product, ii) matrix-vector multiplication, and iii) matrix-matrix multiplication ${ }^{2}$. Crucially they can be performed in parallel. Consider matrix-vector multiplication which is the main operation when iteratively solving a large system of equations.


Figure 3.1: Schematic of matrix-vector multiplication and its constituent operations.

As illustrated in Fig. 3.1, each element of the output vector is the dot product between a row of the matrix and the same vector multiplicand. These operations are independent thus can be performed concurrently. Moreover the dot product itself is the element-wise multiplication between two vectors (parallel operation), followed by summation. Matrix-matrix multiplication can be conceptualized as a set of matrix-vector multiplications, similarly parallelizable.

BLAS operations are ideally suited for Single Instruction Multiple Data (SIMD) computing architectures where a large number of threads perform the same logical or arithmetic operation, each on a different piece of data, all in lock-step. Among these SIMD architectures is the Graphical Processing Unit (GPU), offering massive hardware parallelism and among the highest throughput per unit area, power consumption, and cost ${ }^{3}$. One attempt to leverage their performance would be to maximize data-level parallelism by solving as much of the domain at
once (in as large of a matrix as possible), while minimizing serial dependencies in the mathematical framework.

The FEM system of equations applies to each element in isolation, providing no stipulation on how to solve the entire problem domain. While conceptually straightforward to solve one element at a time, this is a serial approach, unable to leverage the potential of GPUs and other SIMD architectures to perform large BLAS operations. Alternatively, by recognizing each element as part of the entire problem domain, where a given node can be shared by several neighboring elements, it is possible to assemble a Global Finite Element Matrix.


Figure 3.2: (a) Test geometry meshed using unstructured tetrahedral elements, (b) corresponding global finite element matrix system showing sparsity structure.

This is known as the Continuous FEM formalism since a node can be shared between neighboring elements. The resulting matrix (Figure 3.2b) is sparse because coupling only occurs between directly adjacent elements due to the compact support of the basis functions. Typically only $0.25 \%$ of elements being non-zero, thus efficiently stored in Compressed Sparse Row (CSR) format ${ }^{2}$.

A special class of symmetric positive definite (SPD) matrices satisfy the properties of symmetry (Eq. 3.1a) and positive definiteness (Eq. 3.1b).

$$
\begin{gather*}
\boldsymbol{A}=\boldsymbol{A}^{T},  \tag{3.1a}\\
\vec{x}^{T} \boldsymbol{A} \vec{x}>0 \text { for all } \vec{x} . \tag{3.1b}
\end{gather*}
$$

It can be shown ${ }^{4}$ the LSFEM residual can be cast in the form:

$$
\begin{equation*}
f(\vec{x})=\frac{1}{2} \vec{x}^{T} \boldsymbol{A} \vec{x}-\vec{b}^{T} \vec{x}+c . \tag{3.2}
\end{equation*}
$$

Applying the definitions of SPD (Eq. 3.1) it can be shown in Eq. 3.2 that the problem takes the form of a paraboloid, having a global minimum which corresponds to the solution of the system. The Conjugate Gradient (CG) method efficiently descends this paraboloid along mutually orthogonal vectors found using Arnoldi iteration, and can be efficiently parallelized as BLAS operations. However for the matrix to be SPD, the operator formulation must be self-adjoint ${ }^{1}$.


Figure 3.3: Depiction of conjugate gradients converging to the global minimum of a paraboloid error function arising from a symmetric positive definite matrix.

### 3.2.2 Reformulation of first order LBTE into second order Least Squares Finite Element system of Equations

The LBTE when formulated with the Galerkin method is not self-adjoint due to the presence of first order derivatives. Consider off-diagonal terms of the streaming operator:

$$
\begin{align*}
& A_{2,5} \sim \int_{V_{e_{s}}} d V \hat{\Omega} \cdot \vec{\nabla}\left(\lambda_{5}(\vec{r})\right) \lambda_{2}(\vec{r}),  \tag{3.3a}\\
& A_{5,2} \sim \int_{V_{e_{s}}} d V \hat{\Omega} \cdot \vec{\nabla}\left(\lambda_{2}(\vec{r})\right) \lambda_{5}(\vec{r}) . \tag{3.3b}
\end{align*}
$$

Evidently $A_{2,5} \neq A_{5,2}$ since the derivative is applied to different basis functions. When the elemental system is not symmetric, neither will the global FEM matrix.

The least squares finite element method (LSFEM) provides a way to construct an SPD matrix by design ${ }^{1}$. First it is instructive to develop the LSFEM optimization criteria and contrast it with the Galerkin method. Recall the residual is a proxy measure for error in the vector space of the source and is written:

$$
\begin{equation*}
\tilde{\boldsymbol{R}}=A \tilde{\boldsymbol{u}}-\boldsymbol{f} \tag{3.4}
\end{equation*}
$$

which can be negative or positive depending on how the approximation deviates from the source function. A convenient metric is to integrate the squared residual over the domain ( $\Omega$ ), and denote it by the functional:

$$
\begin{equation*}
I(\tilde{\boldsymbol{u}})=\int_{\Omega}(\boldsymbol{A} \tilde{\boldsymbol{u}}-\boldsymbol{f})^{2} d \Omega \tag{3.5}
\end{equation*}
$$

which takes the function $\tilde{\boldsymbol{u}}$ as input, and returns a scalar representation of the error. The terminology 'Least Squares' conveys the objective of minimizing the functional of a similar metric (squared residual), often used in curve fitting.

To see how the FEA equations arise, $\tilde{\boldsymbol{u}}$ is perturbed by a weighting function $\boldsymbol{v}$ multiplied by a scalar $t$. This results in the first-variation of the functional, as a directional derivative over infinite dimensional function spaces ${ }^{1}$ :

$$
\begin{equation*}
(\delta I(\tilde{\boldsymbol{u}}))_{t}=\lim _{t \rightarrow 0} \frac{I(\tilde{\boldsymbol{u}}+t \boldsymbol{v})-I(\tilde{\boldsymbol{u}})}{t}=\left.\frac{d}{d t} I(\tilde{\boldsymbol{u}}+t \boldsymbol{v})\right|_{t=0}, \tag{3.6}
\end{equation*}
$$

where the perturbed functional reads:

$$
\begin{equation*}
I(\tilde{\boldsymbol{u}}+t \boldsymbol{v})=\int_{\Omega}(\boldsymbol{A}\{\tilde{\boldsymbol{u}}+t \boldsymbol{v}\}-\boldsymbol{f})^{2} d \Omega \tag{3.7}
\end{equation*}
$$

Therefore the first variation becomes:

$$
\begin{equation*}
\frac{d}{d t} I(\tilde{\boldsymbol{u}}+t \boldsymbol{v})=\int_{\Omega} 2(\boldsymbol{A}\{\tilde{\boldsymbol{u}}+t \boldsymbol{v}\}-\boldsymbol{f})(\boldsymbol{A} \boldsymbol{v}) d \Omega \tag{3.8}
\end{equation*}
$$

The condition for $\tilde{\boldsymbol{u}}$ to be the best approximation is when the first variation vanishes:

$$
\begin{equation*}
\lim _{t \rightarrow 0} \frac{d}{d t} I(\tilde{\boldsymbol{u}}+t \boldsymbol{v})=0 \tag{3.9}
\end{equation*}
$$

which results in:

$$
\begin{equation*}
\int_{\Omega}(\hat{\boldsymbol{A}} \tilde{\boldsymbol{u}}-\boldsymbol{f})(\hat{\boldsymbol{A}} \boldsymbol{v}) d \Omega=0 . \tag{3.10}
\end{equation*}
$$

Using linearity to split the terms,

$$
\begin{equation*}
\int_{\Omega}(\boldsymbol{A} \tilde{\boldsymbol{u}})(\boldsymbol{A} \boldsymbol{v}) d \Omega-\int_{\Omega}(\boldsymbol{f})(\boldsymbol{A} \boldsymbol{v}) d \Omega=0 . \tag{3.11}
\end{equation*}
$$

Expressed using inner-product notation, the fundamental statement of LSFEM becomes:

$$
\begin{equation*}
\langle\boldsymbol{A} \tilde{\boldsymbol{u}}, \boldsymbol{A} \boldsymbol{v}\rangle=\langle\boldsymbol{f}, \boldsymbol{A} \boldsymbol{v}\rangle . \tag{3.12}
\end{equation*}
$$

Contrasted with the Galerkin system, the operator $\boldsymbol{A}$ is additionally applied to the weighting functions $\boldsymbol{v}$.

### 3.2.3 LSFEM applied to discretized LBTE

As a proof of concept study, we initially neglect magnetic fields, and consider a simpler Discrete Ordinates (DO) method in angle ${ }^{5}$ where the solution is only defined along specified transport vectors defined by Gaussian Quadrature rules as opposed to angular finite elements. Integration over angle is approximated as the summation over discrete directions and their associated weights:

$$
\begin{equation*}
\int_{4 \pi} f(\hat{\Omega}) d \hat{\Omega} \approx \sum_{n=1}^{2 N^{2}} w_{n} f\left(\hat{\Omega}_{n}\right) . \tag{3.13}
\end{equation*}
$$

A square symmetric quadrature set is chosen based on the $\mathrm{S}_{\mathrm{N}}$ formalism, consisting of $2 N^{2}$ directions ( $N$ polar chosen based on roots of Legendre polynomials, $2 N$ azimuthal chosen based on roots of the Chebyshev polynomials) ${ }^{6}$. Examples of the $S_{4}$ and $S_{6}$ set are illustrated in Figure 3.4, below.


Figure 3.4: Discrete Ordinate transport directions visualized on the surface of the sphere for (a) $\mathrm{S}_{4}$, and (b) $\mathrm{S}_{6}$ square-symmetric quadrature sets.

Tight coupling between space and angle eliminates the need for source iteration such that the global CFEM space-angle matrix is directly solved using conjugate gradients. Specifically, the Boltzmann scattering integral is displaced to the left hand side of the multigroup $S_{N}$ equation:

$$
\begin{equation*}
\left[\hat{\Omega}_{n} \cdot \vec{\nabla}+\sigma_{T, g}(\vec{r})-\sum_{n^{\prime}=1}^{2 N^{2}} w_{n^{\prime}} \sigma_{S, g \rightarrow g}\left(\vec{r}, \hat{\Omega}_{n^{\prime}} \cdot \hat{\Omega}_{n}\right)\right] \Psi_{g}\left(\vec{r}, \hat{\Omega}_{n}\right)=S_{g}\left(\vec{r}, \hat{\Omega}_{n}\right)+\sum_{g^{\prime}=1}^{g-1} \sum_{n=1}^{2 N^{2}} w_{n} \sigma_{S, g^{\prime} \rightarrow g}\left(\vec{r}, \hat{\Omega}_{n^{\prime}} \cdot \hat{\Omega}_{n}\right) \Psi_{g^{\prime}}\left(\vec{r}, \hat{\Omega}_{n^{\prime}}\right), \tag{3.14}
\end{equation*}
$$

with vacuum boundary conditions:

$$
\begin{equation*}
\Psi_{g}(\vec{r}, \hat{\Omega})=0, \hat{\Omega} \cdot \hat{n}<0 . \tag{3.15}
\end{equation*}
$$

Applying Eq. 3.12, the LBTE is reformulated as:

$$
\begin{equation*}
\left\langle\boldsymbol{L}_{g, n} \Psi_{g, n}, \boldsymbol{L}_{g, n} \lambda\right\rangle=\left\langle\boldsymbol{S}_{\text {static, }, n, n}, \boldsymbol{L}_{g, n} \lambda\right\rangle \tag{3.16}
\end{equation*}
$$

where the multigroup spatial FEM, angular $\mathrm{S}_{\mathrm{N}}$ expansion of angular fluence is:

$$
\begin{equation*}
\Psi_{g}\left(\vec{r}, \hat{\Omega}_{n}\right) \approx \sum_{i=1}^{I} \psi_{g, i, n} \lambda_{i}(\vec{r}) . \tag{3.17}
\end{equation*}
$$

The tightly-coupled operator for inscatter is:

$$
\begin{equation*}
\boldsymbol{L}_{g, n}=\underbrace{\hat{\Omega}_{n} \cdot \vec{\nabla}}_{\text {term 1: :streaming }}+\underbrace{\sigma_{T, g}\left(e l_{s}\right)}_{\text {term 2: removal }}-\underbrace{\sum_{l=0}^{L} \sum_{n^{\prime}=1}^{2 N^{2}} w_{n^{\prime}} \frac{2 l+1}{4 \pi} \sigma_{s, g \rightarrow g, l}\left(e l_{s}\right) P_{l}\left(\hat{\Omega}_{n^{\prime}} \cdot \hat{\Omega}_{n}\right)}_{\text {term 3: inscatter }}, \tag{3.18}
\end{equation*}
$$

where terms are numbered as indicated.

As with the Galerkin method, the weighting functions are chosen to be the set spanned by spatial basis functions, though running over an independent index:

$$
\begin{equation*}
\lambda=\left\{\lambda_{j}(\vec{r})\right\} . \tag{3.19}
\end{equation*}
$$

Carrying out the inner product on the left-hand side of Eq. 3.16 using the definitions of Eqs. 3.17-3.19, and factoring out the summation $\sum_{i=1}^{I} \psi_{g, i, n}$ in anticipation of a matrix formulation (in analogy to Eq. 2.77), the matrix-vector coupling for spatial element $e l_{s}$ over the global angular $\mathrm{S}_{\mathrm{N}}$ ordinate set of directions becomes:

$$
\begin{align*}
& \sum_{i=1}^{I} \psi_{g, i, n} \underbrace{\int_{V^{e}} d V \hat{\Omega}_{n} \cdot \vec{\nabla}\left\{\lambda_{i}(\vec{r})\right\} \hat{\Omega}_{n} \cdot \vec{\nabla}\left\{\lambda_{j}(\vec{r})\right\}}_{\text {Tem } 1,1} \\
& +\sum_{i=1}^{I} \psi_{g, i, n} \underbrace{\int_{V^{d}} d V \sigma_{T, g}\left(e l_{s}\right)\left\{\lambda_{i}(\vec{r})\right\} \sigma_{T, g}\left(e l_{s}\right)\left\{\lambda_{j}(\vec{r})\right\}}_{\operatorname{Tem} 2,2} \\
& +\sum_{i=1}^{I} \psi_{g, i, n} \int_{V^{2}} d V\left(-\sum_{l=0}^{L} \sum_{n=1}^{2 N^{2}} w_{n^{\prime}} \frac{2 l+1}{4 \pi} \sigma_{s, g \rightarrow g, l}\left(e l_{s}\right) P_{l}\left(\hat{\Omega}_{n^{\prime}} \cdot \hat{\Omega}_{n}\right)\left\{\lambda_{i}(\vec{r})\right\}\right) \\
& \underbrace{\left(-\sum_{l=0}^{L} \sum_{n=1}^{2 N^{2}} w_{n} \frac{2 l+1}{4 \pi} \sigma_{s, g \rightarrow g, l}\left(e l_{s}\right) P_{l}\left(\hat{\Omega}_{n} \cdot \hat{\Omega}_{n}\right)\left\{\lambda_{j}(\vec{r})\right\}\right)}_{\text {Term } 3,3} \\
& +\sum_{i=1}^{I} \psi_{g, i, n} \underbrace{\int_{V^{2}} d V \hat{\Omega}_{n} \cdot \vec{\nabla}\left\{\lambda_{i}(\vec{r})\right\} \sigma_{T, g}\left(e l_{s}\right)\left\{\lambda_{j}(\vec{r})\right\}}_{\text {Tem } 1,2} \\
& +\underbrace{\sum_{i=1}^{I} \psi_{g, i, n} \int_{V^{d}} d V \sigma_{T, g}\left(e l_{s}\right)\left\{\lambda_{i}(\vec{r})\right\} \hat{\Omega}_{n} \cdot \vec{\nabla}\left\{\lambda_{j}(\vec{r})\right\}}_{\text {Tem } 2,1}  \tag{3.20}\\
& +\sum_{i=1}^{I} \psi_{g, i, n} \underbrace{\int_{V^{2}} d V \hat{\Omega}_{n} \cdot \vec{\nabla}\left\{\lambda_{i}(\vec{r})\right\}\left(-\sum_{l=0}^{L} \sum_{n=1}^{2 N^{2}} w_{n} \frac{2 l+1}{4 \pi} \sigma_{s, g \rightarrow g, l}\left(e e_{s}\right) P_{l}\left(\hat{\Omega}_{n^{\prime}} \cdot \hat{\Omega}_{n}\right)\left\{\lambda_{j}(\vec{r})\right\}\right)}_{\text {Temm } 1,3} \\
& +\sum_{i=1}^{I} \psi_{g, i, n} \underbrace{\int_{V^{e}} d V\left(-\sum_{l=0}^{L} \sum_{n^{\prime}=1}^{2 N^{2}} w_{n^{\prime}} \frac{2 l+1}{4 \pi} \sigma_{s, g \rightarrow g, l}\left(e l_{s}\right) P_{l}\left(\hat{\Omega}_{n^{\prime}} \cdot \hat{\Omega}_{n}\right)\left\{\lambda_{i}(\vec{r})\right\}\right) \hat{\Omega}_{n} \cdot \vec{\nabla}\left\{\lambda_{j}(\vec{r})\right\}}_{\text {Tem } 3,1} \\
& +\sum_{i=1}^{I} \psi_{g, i, n} \underbrace{\int_{V^{2}} d V \sigma_{T, g}\left(e l_{s}\right)\left\{\lambda_{i}(\vec{r})\right\}\left(-\sum_{l=0}^{L} \sum_{n=1}^{2 N^{2}} w_{n} \frac{2 l+1}{4 \pi} \sigma_{s, g \rightarrow g, l}\left(e l_{s}\right) P_{l}\left(\hat{\Omega}_{n^{\prime}} \cdot \hat{\Omega}_{n}\right)\left\{\lambda_{j}(\vec{r})\right\}\right)}_{\text {Tem } 2,3} \\
& +\underbrace{\sum_{i=1}^{I} \psi_{g, i, n} \int_{V^{e}} d V\left(-\sum_{l=0}^{L} \sum_{n^{\prime}=1}^{2 N^{2}} w_{n^{\prime}} \frac{2 l+1}{4 \pi} \sigma_{s, g \rightarrow g, l}\left(e l_{s}\right) P_{l}\left(\hat{\Omega}_{n^{\prime}} \cdot \hat{\Omega}_{n}\right)\left\{\lambda_{i}(\vec{r})\right\}\right) \sigma_{T, g}\left(e e_{s}\right)\left\{\lambda_{j}(\vec{r})\right\}}_{\text {Tem } 3,2} .
\end{align*}
$$

Since the operator is applied to both basis functions and weighting functions, the LSFEM system matrix contains $3^{2}=9$ terms (Eq. 3.20), with pairs $(1,2 \mid 2,1)(1,3 \mid 3,1)(2,3 \mid 3,2)$ formulated as mirror images about the main diagonal, preserving symmetry.

### 3.2.4 LSFEM Global Matrix Formulation

The tight coupling of the entire angular domain (encompassing $2 N^{2}$ directions) at each spatial node is implemented through the Kronecker tensor product:

$$
[A] \otimes[B]=\left[\begin{array}{ccc}
a_{11}[B] & a_{11}[B] & \cdots  \tag{3.21}\\
a_{11}[B] & a_{11}[B] & \cdots \\
\vdots & \vdots & \ddots
\end{array}\right] .
$$

Shown for simplicity is the angular matrix formulation of $\boldsymbol{L}_{g} \Psi_{g}$ at spatial node $i=1$,

$$
\begin{align*}
& \underbrace{\left[\begin{array}{cccc}
\hat{\Omega}_{1} \cdot \vec{\nabla} & 0 & \cdots & 0 \\
0 & \hat{\Omega}_{2} \cdot \vec{\nabla} & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \cdots & \hat{\Omega}_{2 N^{2}} \cdot \vec{\nabla}
\end{array}\right]}_{\text {tem } 1} \cdot\left[\begin{array}{c}
\psi_{g, 1,1} \lambda_{1}(\vec{r}) \\
\psi_{g, 1,2,} \lambda_{1}(\vec{r}) \\
\vdots \\
\psi_{g, 1,2 N^{2}} \lambda_{1}(\vec{r})
\end{array}\right]+\underbrace{\sigma_{T, g}\left(e l_{s}\right)}_{\text {term } 2}\left[\begin{array}{cccc}
1 & 0 & \cdots & 0 \\
0 & 1 & \cdots & 0 \\
\vdots & \vdots & \ddots & \vdots \\
0 & 0 & \cdots & 1
\end{array}\right] \cdot\left[\begin{array}{c}
\psi_{g, 1,1} \lambda_{1}(\vec{r}) \\
\psi_{g, 1,2} \lambda_{1}(\vec{r}) \\
\vdots \\
\psi_{g, 1,2 N^{2}} \lambda_{1}(\vec{r})
\end{array}\right] \\
& -\underbrace{-\sum_{l=0}^{L}\left(\frac{2 l+1}{4 \pi} \sigma_{s, g \rightarrow g, l}\left(e l_{s}\right)\left[\begin{array}{cccc}
w_{1} \cdot P_{l}\left(\hat{\Omega}_{1} \cdot \hat{\Omega}_{1}\right) & w_{2} \cdot P_{l}\left(\hat{\Omega}_{1} \cdot \hat{\Omega}_{2}\right) & \cdots & w_{2 N^{2}} \cdot P_{l}\left(\hat{\Omega}_{1} \cdot \hat{\Omega}_{2 N^{2}}\right) \\
w_{1} \cdot P_{l}\left(\hat{\Omega}_{2} \cdot \hat{\Omega}_{1}\right) & w_{2} \cdot P_{l}\left(\hat{\Omega}_{2} \cdot \hat{\Omega}_{2}\right) & \cdots & w_{2 N^{2}} \cdot P_{l}\left(\hat{\Omega}_{2} \cdot \hat{\Omega}_{2 N^{2}}\right) \\
\vdots & \vdots & \ddots & \vdots \\
w_{1} \cdot P_{l}\left(\hat{\Omega}_{N} \cdot \hat{\Omega}_{1}\right) & w_{2} \cdot P_{l}\left(\hat{\Omega}_{N} \cdot \hat{\Omega}_{2}\right) & \cdots & w_{2 N^{2}} \cdot P_{l}\left(\hat{\Omega}_{2 N^{2}} \cdot \hat{\Omega}_{2 N^{2}}\right)
\end{array}\right]\right)}_{\text {tem } 3}\left[\begin{array}{c}
\psi_{g, 1,1} \lambda_{1}(\vec{r}) \\
\psi_{g, 1,2} \lambda_{l}(\vec{r}) \\
\vdots \\
\psi_{g, 1,2 N^{2}} \lambda_{1}(\vec{r})
\end{array}\right] . \tag{3.22}
\end{align*}
$$

In the spatial domain, volume integrals appearing in each term of Eq. 3.20, for example $\int_{V^{e}} d V \lambda_{\mathrm{i}}(\vec{r}) \lambda_{\mathrm{j}}(\vec{r})$ quantify the amount of coupling between the basis function centered at the node $i$ under consideration and a weighting function centered at node $j$ of the same element. The result is subsequently mapped to the corresponding node location in the global matrix according to the $T$-array. For element index $e l_{s},(i, j) \rightarrow\left(T\left(e l_{s}, i\right), T\left(e l_{s}, j\right)\right)$. Similarly, the angular global matrix can be constructed and nested at each spatial node using the Kronecker product (Eq. 3.21), thereby creating a single large sparse SPD matrix, efficiently solved by the iterative Conjugate Gradients method based on BLAS primitives.

Terms 1 and 2 result in diagonal angular matrices, formulated separately for each angle, whereas term 3 results in a dense angular matrix on account of explicit tight-coupling introduced between all angles. Term 3,3 is tightly coupled in its angular operator to both the basis functions and weighting functions, formed as the matrix:

$$
\left[L_{3 T C}\right]=-\sum_{l=0}^{L}\left(\frac{2 l+1}{4 \pi} \sigma_{s, g \rightarrow g, l}\left(e l_{s}\right)\left[\begin{array}{cccc}
w_{1} \cdot P_{l}\left(\hat{\Omega}_{1} \cdot \hat{\Omega}_{1}\right) & w_{2} \cdot P_{l}\left(\hat{\Omega}_{1} \cdot \hat{\Omega}_{2}\right) & \cdots & w_{2 N^{2}} \cdot P_{l}\left(\hat{\Omega}_{1} \cdot \hat{\Omega}_{2 N^{2}}\right)  \tag{3.23}\\
w_{1} \cdot P_{l}\left(\hat{\Omega}_{2} \cdot \hat{\Omega}_{1}\right) & w_{2} \cdot P_{l}\left(\hat{\Omega}_{2} \cdot \hat{\Omega}_{2}\right) & \cdots & w_{2 N^{2}} \cdot P_{l}\left(\hat{\Omega}_{2} \cdot \hat{\Omega}_{2 N^{2}}\right) \\
\vdots & \vdots & \ddots & \vdots \\
w_{1} \cdot P_{l}\left(\hat{\Omega}_{N} \cdot \hat{\Omega}_{1}\right) & w_{2} \cdot P_{l}\left(\hat{\Omega}_{N} \cdot \hat{\Omega}_{2}\right) & \cdots & w_{2 N^{2}} \cdot P_{l}\left(\hat{\Omega}_{2 N^{2}} \cdot \hat{\Omega}_{2 N^{2}}\right)
\end{array}\right]\right) .
$$

Considering the inner product relation ${ }^{7}$ :

$$
\begin{equation*}
\left\langle\boldsymbol{L}_{3 T C} \Psi, \boldsymbol{L}_{3 T C} \lambda\right\rangle=\left\langle\boldsymbol{L}_{3 T C}^{\dagger} \boldsymbol{L}_{3 T C} \Psi, \lambda\right\rangle . \tag{3.24}
\end{equation*}
$$

The angular matrix operator can be calculated:

$$
\begin{equation*}
\left[L_{3 T C}\right]^{T}\left[L_{3 T C}\right], \tag{3.25}
\end{equation*}
$$

and coupled to the spatial integral.

Terms 1,2 and 2,1 are complementary, resulting in matrix transposes of one another. The same applies for the remaining pairs 1,3 and 3,1 along with 2,3 and 3,2 . Their construction follows principles shown previously, and will be omitted for brevity. Similar principles apply to terms on the right hand side of Eq. 3.16, which ultimately collapses to a source vector.

Many values in the global matrix, for example basis function parameters can be calculated in parallel using GPU kernel, then mapped to their final destination in memory also using a SIMD parallelization approach which will be described.

### 3.2.5 Novel Algorithms for Sparse Matrix Assembly and Kronecker product

Noting that CFEM global matrix assembly is the most time consuming step which is repeated for each energy group, and the locations of non-zeros remain unchanged over all energy groups, this motivates the development of novel memory mapping algorithms tailored to the SIMD architecture of the GPU, a high level overview illustrated in Figure 3.5.


Figure 3.5: Algorithm schematic for (a) precalculating direct memory mapping to for global spatial FEM matrix in CSR format. Starting from the T-array of an unstructured tetrahedral mesh, (i) Enumerate all permutations ( $i, j$ ) of basis function and weighting function, generating an array of vectors (A): weighting function (row) in global matrix, (B): basis function (column) in global matrix, (C): memory index for weighting function in source repository, (D): memory index for basis function in source repository, (E): unique address in contiguous memory assuming final dense matrix. (ii) Sort by key of column E, such that overlapping nodes are listed adjacent in sequence. (iii) Generate coloring vector where contributions to the same location in the global matrix are enumerated with increasing index. (iv) Sort by key of the color vector such that $\mathrm{F}^{\prime}$ and associated vectors represent contiguous nonoverlapping sets which can be launched simultaneously. (v) Extract the row pointer and column vector data structures for CSR by performing prefix-sum on the first color segment of columns $\mathrm{A}^{\prime \prime}$ and $\mathrm{B}^{\prime \prime}$ respectively. Generate value-pointer corresponding to destination mapping in contiguous memory of the sparse global
matrix. (vi) Columns $\mathrm{C}^{\prime \prime}$ and $\mathrm{D}^{\prime \prime}$ correspond to the memory source locations of the weighting function and basis function respectively used to fetch element specific attributes from repositories during assembly. (b) precalculating space-angle kronecker product and vacuum boundary condition mappings, starting with the spatial CSR data structures which are modified by (vii) kronecker product with angular matrix either in the diagonal form for terms 1 and 2 , or dense form for term 3, (viii) removal of degrees of freedom corresponding to vacuum boundary conditions to generate (ix) memory mapping for final space-angle CSR data structure

The number of unique spatial contributions to the CFEM global matrix considers all permutations of $i$ and $j$ in every tetrahedral element, totaling $16 \cdot N_{\text {spaElem }}$. However, it is possible for several elements to intersect and share the same node, which means it has a multiplicity greater than 1. Implemented on GPU, this can result in a race-condition where multiple threads attempt to populate the same node location in memory concurrently. Therefore, a GraphColoring approach is used to sort the elements into non-overlapping sets which sequentially populate the global matrix at runtime.

The second stage in Figure 3.5 concerns the Kronecker tensor product which couples the entire angular domain to each spatial node. Nesting of diagonal and dense angular matrices (see Eq. 3.22) each alter the CSR structure in a predictable manner, thus can be mapped for efficient deployment at runtime. Finally, vacuum boundary conditions applied to a global space-angle domain can be strictly enforced by removing their corresponding memory mappings. Since the LSFEM formulation generates a system matrix which is symmetric by design, further memory savings are realized by mapping only the upper triangular half.

The operating abstraction for GPU kernels through Nvidia's Compute Unified Device Architecture (CUDA) is to establish a calculation grid adapted to the characteristic dimensions of the problem, consisting of simple threads all executing the same instructions though parameterized by unique data elements addressed according to its position within the grid. Principles such as memory access coalescing, explicit management of cache hierarchy, and structuring of algorithms to make best use of contextual thread index within the calculation grid are used to guide the design efficient SIMD implementations on GPU.

Implementation details for the GPU architecture are beyond the scope of detailed discussion, however the schematic of operation is summarized in Figure 3.6.


Figure 3.6: Overall schematic of LS-CFEM GPU framework.

### 3.2.6 Setup for Initial Validation

A heterogeneous slab phantom with dimensions illustrated in Figure 3.2a was used to validate the prototype LS-CFEM against the previously published Discrete Ordinates Fortran code of StAubin et al $(2015)^{8}$ using DFEM in space. The phantom contained slabs of water $\left(1.00 \mathrm{~g} / \mathrm{cm}^{3}\right)$, bone $\left(1.92 \mathrm{~g} / \mathrm{cm}^{3}\right.$ ), and a low density medium (lung $0.26 \mathrm{~g} / \mathrm{cm}^{3}$ or air $0.0012 \mathrm{~g} / \mathrm{cm}^{3}$ ), irradiated by a polyenergetic 6 MV point source $^{8}$ at $100 \mathrm{~cm} \operatorname{SSD}$ for a $2 \times 2 \mathrm{~cm}^{2}$ surface field size. Multigroup discretization of energy used 16 photon and 40 electron intervals, while $\mathrm{S}_{6}$ angular quadratures produced 72 discrete directions. Unstructured tetrahedral meshes of various refinement levels were generated using COMSOL Multiphysics ${ }^{9}$, ranging from approximately

18,000 elements to 250,000 elements, with greater element density allocated near boundaries and beam edges.

Matrix assembly and the entire dose calculation was implemented in CUDA-C on a single Nvidia Titan-X GPU was compared in runtime against an algorithmically equivalent serial implementation in MATLAB ${ }^{10}$ running on an Intel i7-6700K CPU.

### 3.3 Results and Discussion

### 3.3.1 Runtime of Matrix Assembly and Fluence Calculation

Preliminary assessment of matrix assembly runtimes offered an order of magnitude indicator of algorithm performance on typical meshes as seen in Table 3.1:

Table 3.1: Comparison of runtime to perform spatial matrix assembly on first 16 energy groups ${ }^{11}$

| Platform | \# of mesh elements $\longrightarrow$ | $\mathbf{8 1 4 2}$ | $\mathbf{3 0 9 5 0}$ |
| :--- | :--- | :---: | :---: |
| CPU (core i7-6700K) | Total Assembly Time | $176,000 \mathrm{~ms}$ | $556,000 \mathrm{~ms}$ |
| GPU (GeForce TITAN-X) | Generation of memory <br> map based on sparsity <br> pattern of mesh | 125 ms | 452 ms |
|  | Apply mapping to 16 <br> energy groups | 93 ms | 358 ms |
|  | Total Assembly Time | 218 ms | 810 ms |

Evident in this subroutine is 2 orders of magnitude speedup when implemented on GPU. For a moderately sized problem of approximately 18,000 elements, calculating the fluence of 16 photon groups took 46s on GPU, down from 9 hours 22 minutes on CPU. The entire dose calculation including electrons took 3 minutes 42 s on GPU, down from 25 hours 40 minutes on CPU. Ultimately the GPU architecture provided the only feasible way to obtain reasonable runtimes for a global CFEM formulation of the LBTE, delivering 2 orders of magnitude speedup by using a novel SIMD approach for sparse matrix assembly of each energy group, along with highly parallel conjugate gradient solver built on BLAS primitives.

### 3.3.2 Dosimetric Accuracy of LS-CFEM Approach

Figures 3.7 and 3.8 compare the total electron fluence calculated by the new LS-CFEM formulation relative to reference DFEM for a heterogeneous slab phantom containing lung.


Figure 3.7: Total electron fluence on central plane for (a) reference DFEM calculation, (b) LS-CFEM calculation, (c) \% difference.


Figure 3.8: Central axis electron fluence comparison between benchmark DFEM code and new LS-CFEM formulation, with \% difference plotted on secondary axis.

In this case with lung $\left(0.26 \mathrm{~g} / \mathrm{cm}^{3}\right)$ as the intervening low density medium, the LSFEM code demonstrates good agreement with reference calculations, such that differences are constrained to within $6 \%$ along the central axis. Larger differences in the penumbra (Figure 3.7c) arise because shared nodes in CFEM does not allow for as abrupt of transitions from high to low fluence, especially evident with meshing at a relatively coarse 25,047 tetrahedral elements. The
overall result is promising as it demonstrates the ability to arrive at the same solution as St -Aubin et $a^{8}{ }^{8}$ through a completely different formulation and implementation.

The more challenging case arises when lung is substituted with air $\left(0.0012 \mathrm{~g} / \mathrm{cm}^{3}\right)$, representing 3 orders of magnitude drop in density relative to the neighboring slabs.


Figure 3.9: Central axis electron fluence with intervening slab of air, showing LSCFEM at various mesh refinement with reference DFEM calculation.

As observed in Figure 3.9, the LS-CFEM solution exhibits reasonable agreement in proximal layers of water and bone. However upon reaching the air slab, CFEM is unable to adapt to the transport properties of this new medium, exhibiting major deviations up to $40 \%$, and thereafter establishing erroneous buildup characteristics in the distal water layer. By enforcing continuity at global nodes, CFEM is unable to resolve the sharp changes in fluence at locations of material discontinuities. This persists despite successive mesh refinement near the boundaries, evident in the air region of Figure 3.9. Increasing the number of mesh elements (even by an order of magnitude and concentrated around these material boundaries), had little effect in bringing the LS-CFEM solution closer to the true electron fluence in air. This inaccuracy when transitioning to low density media can be problematic for modeling the electron return effect introduced by perpendicular magnetic fields, which causes sharp lateral deflection of electron fluence in air. Moreover, increasing the inherent problem complexity an order of magnitude through mesh refinement negates the speedup gained through a parallelized GPU implementation.

Ultimately a more robust framework is needed to accommodate the spatial variation of heterogeneities encountered in radiotherapy. Such capability is inherent to discontinuous finite elements (DFEM) in space which do not share nodes between neighboring elements, thus fully dedicated to modeling the material in each element accurately.


Figure 3.10: Central axis electron fluence with intervening slab of air, comparing LS-DFEM and reference DFEM calculation.

Using a DFEM approach in space, the calculated electron fluence achieved far better agreement with the benchmark code (also DFEM) in the challenging case of a low density air slab, as shown in Figure 3.10, despite using only 17,576 elements. The tradeoff with DFEM is not being able to assemble a global matrix encompassing the entire domain. Nevertheless, achieving accurate results with an order of magnitude fewer elements than CFEM provides confidence that DFEM forms the appropriate foundation magnetic fields for MRIgRT.

Much of the useful potential of LSFEM was realized in conjunction with continuous finite elements to formulate a large sparse global SPD matrix efficiently assembled and solved on GPU. In transitioning to DFEM, much of the explicit parallelism is lost, such that the drawbacks of a second order LSFEM formulation outweigh its benefits compared to a first order Galerkin approach. The self-adjoint property of LSFEM requires application of the operator to not only the basis functions but also the weighting functions, resulting in $N^{2}$ inner product terms
(compared to $N$ for Galerkin). Had magnetic fields been introduced, LS-DFEM would require 16 terms for the left hand side matrix, and 4 terms in the right hand source vector. The computational penalty of needing to assemble 4 times the number of terms on relatively small subsets of the domain not benefitting parallelization renders LSFEM impractical in conjunction with DFEM. Moreover the tight-coupling formalism between space and angle is very memory intensive. Had angular finite elements been used instead of DO, memory usage would increase 12 orders of magnitude, no longer feasible to deploy on standard workstation hardware.

The transition of DFEM as dictated by physics requirements is hypothesized as best suited to a first-order Galerkin source-iteration framework, though with great potential for algorithmic improvement, as will be explored in upcoming chapters.

### 3.4 Conclusions

The LS-CFEM formulation enabled exploration of an approach which maximized explicit parallelization, for which novel algorithms were developed on GPU for sparse matrix assembly and Kronecker product mappings, achieving a large speedup through SIMD parallelization. This novel formalism converges on the correct solution for less demanding cases involving lung, however challenging conditions at the transition between tissue and air would benefit from a more robust DFEM framework.

This study illustrates the importance of establishing an appropriate mathematical framework at the outset, which accommodates the physics requirements for a given scope of problems. In radiotherapy, where the heterogeneous distribution of materials can change by orders of magnitude in density between neighboring anatomical regions, DFEM provides robust accuracy using an order of magnitude fewer elements.

Nevertheless, novel algorithmic building blocks were developed on GPU which can be deployed to problem contexts suitably modeled using continuous FEM.

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# Chapter 4 Framework for Angular Upwind Stabilization and Harmonious Space-Angle Interplay 

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R. Yang, O. Zelyak, B.G. Fallone, and J. St-Aubin, "A novel upwind stabilized discontinuous finite element angular framework for deterministic dose calculations in magnetic fields, " Phys. Med. Biol. 63(3), 035018 (2018). DOI: 10.1088/1361-6560/aaa2b1.

### 4.1 Purpose and Hypothesis

Attempts to maximize explicit parallelization by formulating the entire space-angle domain into a global finite element matrix system required the use of continuous finite elements, where nodes were shared between neighboring elements. The limitation of such approach was evident in modeling the sharp transition between bone and air, where nodes straddling the interface must assume average properties between materials having vastly different transport kinetics. Even with an excessive degree of spatial mesh refinement, this approach failed to capture the true solution in the manner a discontinuous approach could. Despite highly efficient parallelization of global matrix assembly and iterative conjugate gradients on GPU, any inherent speedup is largely lost by the need for an unreasonably high number of spatial elements to model material transitions.

Discontinuous finite elements (DFEM) were shown to be more suitable for applications to radiotherapy, by providing each element its unique set of nodes (not shared with any other elements), enabling accurate resolution of abrupt transitions between materials using far fewer degrees of freedom. As seen in Figure 3.9, a problem for which 250,000 continuous finite elements was unable to approach the correct solution was accurately modeled using only 18,000 discontinuous elements (Figure 3.10). However a major tradeoff of DFEM is the introduction of serial dependencies due to the requirement that boundary conditions are applied to each element individually based on elements that were previously solved. Specifically, a procedure of upwind stabilization is needed for the first order Galerkin DFEM approach, where the streaming operator is evaluated over the range of directions subtended by each angular element, and spatial elements are solved in batches which share upstream dependencies.


Figure 4.1: Conceptual illustration of error incurred with (a) Continuous FEM, where nodes are shared between neighboring elements, introducing difficulties in resolving material transitions. (b) Discontinuous FEM, where nodes belong exclusively to each element, offering improved approximation of material discontinuities, however introducing serial dependencies in needing to propagate elemental boundary conditions.

Proof of concept work by St-Aubin et al (2016) ${ }^{1}$ has shown a first order discontinuous spaceangle Galerkin framework is capable of highly accurate dose calculations in magnetic fields. However, the calculation required excessive angular degrees of freedom to minimize errors due to cyclic directed graphs in the space-angle interplay. Specifically, the choice of unstructured tetrahedral elements in space allows for faces having arbitrary oblique orientations (encoded by normal vector $\hat{n}$ ) such that over the range of directions $\hat{\Omega}_{\alpha}$ spanned by an angular element there can arise both $\hat{\Omega} \cdot \hat{n}<0$ (in which case fluence is treated as a known incoming boundary condition), as well as $\hat{\Omega} \cdot \hat{n}>0$ (in which case fluence is treated as outgoing, to be solved). To minimize the probability and impact of these dual conditions arising (which created instabilities in the solution), the angular mesh needed to be refined to 520 elements ${ }^{1}$. It was hypothesized that this was an order of magnitude beyond the number needed to model the inherent anisotropy in photon beam radiotherapy. Since each angular element introduces a nested 'transport sweep' solution encompassing the entire spatial domain, a reformulation of space-angle interplay to significantly reduce the angular element count would have the greatest impact on reducing computational complexity towards feasible patient calculations. As an alternative to aggressive angular mesh refinement, the acyclic components of the sweep graph could be broken using a Riemann decomposition. However, this method was shown to be very computationally intensive ${ }^{2}$ when applied to every unstructured spatial element in the domain, therefore a different approach was investigated in this work.

By adopting different space-angle discretizations and developing new solution techniques, several objectives were accomplished:
(i) Conventions for space-angle interplay were established to eliminate ambiguity concerning inflow / outflow face designations of spatial elements during the transport sweep, eliminating the need for excessive angular mesh refinement as an error mitigation measure. The number of angular elements and resultant transport sweeps per source iteration were reduced an order of magnitude, while still accurately modeling the inherent anisotropy of the problem.
(ii) Angular finite elements conforming to the sphere's surface were implemented as a more natural representation of the angular domain enabling the minimum possible 8 elements (one per quadrant) to be deployed. Moreover we investigate higher order angular basis functions to accommodate greater anisotropy without increasing the number of angular elements.
(iii) Techniques for angular upwind stabilization of the magnetic field term for curvilinear angular elements on the sphere's surface were developed, involving piecewise partitioning of path integrals along curved element edges into uninterrupted segments of incoming and outgoing flux, where incoming components are updated iteratively from neighboring elements.
(iv) Correctness of the resulting mathematical framework and its implementation was verified by order of convergence tests using the Method of Manufactured Solution (MMS) ${ }^{3,4}$. Additionally this yielded insight on the nature of angular $h$ and $p$ refinement, as well as the effect of magnetic fields.
(v) A rotational coordinate transformation formalism was developed to efficiently simulate magnetic fields at oblique orientations by rotating the angular mesh on the sphere, without needing to re-grid the underlying spatial geometry.
(vi) Dosimetric accuracy of the framework was validated against Monte Carlo calculations in GEANT4 for several challenging radiotherapy cases in the presence of magnetic fields.

### 4.2 Methods

The Discontinuous Galerkin system of equations will be introduced in its full mathematical form, including expressions for upwind stabilization of advection in space and angle. Discretization conventions will be introduced in the context of establishing a space-angle sweep solver, followed by details on the calculation of integrals in the full upwind system of equations.

### 4.2.1 Stabilization of Advection in Galerkin System of Equations

Applying the first-order space-angle multi-group Galerkin method with source iteration, there arise terms indicated in Eq. 4.1 which contain first derivatives, corresponding to the physical process of advection: in space due to streaming, in angle due to the magnetic field operator,

$$
\begin{gather*}
\sum_{i=1}^{I} \sum_{p=1}^{p} \psi_{g, i, p}^{(t+1)} \int_{\Omega_{\alpha}} d \hat{\Omega} \gamma_{p}(\hat{\Omega}) \gamma_{q}(\hat{\Omega}) \underbrace{\int_{V^{e}} d V \hat{\Omega} \cdot \vec{\nabla}\left(\lambda_{\mathrm{i}}(\vec{r})\right) \lambda_{\mathrm{j}}(\vec{r})}_{\text {spatial advection }},  \tag{4.1a}\\
\kappa_{g} \sum_{i=1}^{I} \sum_{p=1}^{p} \psi_{g, i, p}^{(t+1)} \underbrace{\int_{\Omega_{\alpha}} d \hat{\Omega} \vec{\tau}(\vec{B}, \hat{\Omega}) \cdot \vec{\nabla}_{\Omega}\left(\gamma_{p}(\hat{\Omega})\right) \gamma_{q}(\hat{\Omega})}_{\text {angular advection }} \int_{V^{e}} d V \lambda_{\mathrm{i}}(\vec{r}) \lambda_{\mathrm{j}}(\vec{r}), \tag{4.1b}
\end{gather*}
$$

where symbols have been defined in Chapter 2.

Solving equations containing advection using a first order Galerkin scheme is problematic because the first derivative applied to any basis function causes it to reside in a different function space than the weighting functions. This violates the fundamental premise by which the Galerkin technique arrives at the best approximation.

An illustrative example in Jiang (1998) ${ }^{5}$ shows the impact of basis and weighting functions not belonging to the same space. First order partial differential equations using the Galerkin method can be problematic in the absence of modifications.

Consider the 1D case of pure advection:

$$
\begin{equation*}
u^{\prime}(x)=f(x) . \tag{4.2}
\end{equation*}
$$

A specific example over the domain $\Omega: x \in[0,1]$ being:

$$
\begin{equation*}
u^{\prime}(x)=2 \pi \cos (\pi x) \tag{4.3}
\end{equation*}
$$

with the boundary condition:

$$
\begin{equation*}
u(0)=0 . \tag{4.4}
\end{equation*}
$$

By inspection, the exact solution is simply:

$$
\begin{equation*}
u_{\text {exact }}(x)=2 \sin (\pi x) . \tag{4.5}
\end{equation*}
$$

FEM begins with a set of basis functions, in this case the space of mutually orthogonal sine functions satisfying the boundary condition Eq. 4.4,

$$
\begin{equation*}
\{\sin (\pi x), \sin (2 \pi x), \sin (3 \pi x), . . .\} . \tag{4.6}
\end{equation*}
$$

Weighting functions in the Galerkin method are chosen as identical to the set of basis functions, spanning a subspace where the approximation resides (as depicted in Figure 2.13). The formal criteria to establish optimal coefficients for each functional degree of freedom is given by:

$$
\begin{equation*}
\int_{\Omega} R(x) v(x) d x=0 . \tag{4.7}
\end{equation*}
$$

Analogous to how the dot product is used for vectors, the inner product (Eq. 4.7) determines how much each weighting function component $v(x)$ is present in the residual $R(x)$, and adjusts coefficients such that any shared components are minimized. For such projection operation to be mathematically valid, the residual and weighting functions have components in the same function space, an underlying requirement of Galerkin's method.

However, applying the first derivative to any basis function yields a cosine function no longer belonging to the set of Eq. 4.6. If the operator produces an expression belonging to a different function space than the weighting functions, there will be no longer be shared components for the projection to be mathematically valid.

To see the consequences arising from pure advection, Eq. 4.3 is substituted into the criterion for Galerkin's method, Eq. 4.7, yielding:

$$
\begin{gather*}
\int_{0}^{1}\left(\tilde{u}^{\prime}(x)-2 \pi \cos (\pi x)\right) v(x) d x=0,  \tag{4.8}\\
\int_{0}^{1} \tilde{u}^{\prime}(x) v(x) d x=2 \pi \int_{0}^{1} \cos (\pi x) v(x) d x . \tag{4.9}
\end{gather*}
$$

Specifically, let the trial function be $\tilde{u}(x)=a_{1} \sin (\pi x)$, which yields the exact solution when $a_{1}=2$. According to the Galerkin method, the weighting function is prescribed $v(x)=\sin (\pi x)$, substituted along with $\tilde{u}^{\prime}(x)=a_{1} \pi \cos (\pi x)$ into Eq. 4.9,

$$
\begin{equation*}
a_{1} \pi \int_{0}^{1} \cos (\pi x) \sin (\pi x) d x=2 \pi \int_{0}^{1} \cos (\pi x) \sin (\pi x) d x \tag{4.10}
\end{equation*}
$$

Since $\sin (\pi x)$ and $\cos (\pi x)$ are orthogonal over $\Omega$, the integrals collapse to 0 , yielding

$$
\begin{equation*}
a_{1} \cdot 0=0 . \tag{4.11}
\end{equation*}
$$

Evidently $a_{1}$ could not be determined for pure advection using the Galerkin method. Moreover, any value of $a_{1}$ satisfies Eq. 4.11, an indicator that the error in the advection component is unbounded ${ }^{5}$. This was observed empirically with the LBTE, a system containing terms other than advection, where the unmodified Galerkin method despite yielding numerical coefficients, produced solutions with spurious oscillations and failure to converge, indicative of unbounded error in the advection component.

An alternative perspective presented in Jiang (1998) ${ }^{5}$ is to recognize the matrix formulation of the Galerkin method as being equivalent to a central-finite-difference numerical scheme, where odd-even decoupling leads to oscillatory solutions, shown through Fourier analysis to be unconditionally unstable, regardless of mesh refinement. A well-known resolution to recover stability of Finite Differences is to employ a backwards-difference scheme where the solution from nodes upstream of the direction of propagation are used to update the current node being solved. The resulting scheme is unconditionally stable. The analogous concept is implemented as upwind stabilization of the discontinuous Galerkin finite element method, which will be discussed for space and angle.

### 4.2.2 Upwind Stabilization in Space

The divergence theorem is applied to the spatial advection component (Eq. 4.1a) which introduces a set of surface integrals parameterized by $\hat{\Omega} \cdot \hat{n}_{k}$, where $\hat{\Omega}$ is the direction of fluence propagation under consideration and $\hat{n}_{k}$ is the outward-directed unit-normal to the spatial element face $k$ under consideration. Eq. 4.1a becomes:

$$
\begin{align*}
& \sum_{k=1}^{K} \sum_{i=1}^{I} \sum_{p=1}^{P} \psi_{g, i, p, k}^{(t+1)} \int_{\Omega_{\alpha}} d \hat{\Omega} \gamma_{p}(\hat{\Omega}) \gamma_{q}(\hat{\Omega}) \hat{\Omega} \cdot \hat{n}_{k} \int_{S_{k}} d S \lambda_{i}(\vec{r}) \lambda_{j}(\vec{r}),  \tag{4.12a}\\
& -\sum_{i=1}^{I} \sum_{p=1}^{P} \psi_{g, i, p}^{(t+1)} \int_{\Omega_{\alpha}} d \hat{\Omega} \gamma_{p}(\hat{\Omega}) \gamma_{q}(\hat{\Omega}) \hat{\Omega} \cdot \int_{V^{d}} d V \lambda_{i}(\vec{r}) \vec{\nabla}\left(\lambda_{j}(\vec{r})\right) . \tag{4.12b}
\end{align*}
$$

The surface integrals of Eq. 4.12a provide a mechanism to communicate spatial boundary conditions for the element, and treated according to the sign of $\hat{\Omega} \cdot \hat{n}_{k}$. Specifically,

$$
\psi_{g, i, p, k}^{(t+1)}=\left\{\begin{array}{ccc}
\psi_{g, i, p}^{i n c_{s}(t+1)} & \hat{\Omega} \cdot \hat{n}_{k}<0 \quad \text { (upwind facing boundary) }  \tag{4.13}\\
\psi_{g, i, p}^{(t+1)} & \hat{\Omega} \cdot \hat{n}_{k}>0 & \text { (downwind facing boundary) }
\end{array},\right.
$$

where $\psi_{g, i, p}^{i n c_{s}(t+1)}$ indicates nodes of known incoming fluence from a neighboring element in space which was either solved earlier during Source Iteration $(t+1)$ or is a vacuum boundary condition when situated at the edge of the spatial domain.
An example of these conventions applied to hexahedral elements is depicted in Figure 4.2, below


Figure 4.2: Face designations for a hexahedral element in the direction $\hat{\Omega}$ shown.
(a) Blue denotes the upwind facing boundaries where $\hat{\Omega} \cdot \hat{n}_{k}<0$, (b) Green denotes downwind facing boundaries where $\hat{\Omega} \cdot \hat{n}_{k}>0$.

By convention, upwind contributions are displaced to the right hand side of the elemental equations, to act as a source term. Since $\psi_{g, i, p}^{i n c_{s}(t+1)}$ represents known values of the solution from upstream elements in space, Eq. 4.12a should no longer contribute to the elemental matrix for upwind faces. Specifically, the partitioning of Eq. 4.12a will follow:

$$
\begin{align*}
& L H S: \underbrace{\sum_{i=1}^{I} \sum_{p=1}^{P} \sum_{k_{\text {downwind }}} \psi_{g, i, p}^{(t+1)} \int_{\Omega_{\alpha}} d \hat{\Omega} \gamma_{p}(\hat{\Omega}) \gamma_{q}(\hat{\Omega}) \hat{\Omega}_{q} \cdot \hat{n}_{k} \int_{S_{k}} d S_{i}(\vec{r}) \lambda_{j}(\vec{r})}_{\text {downwind spatial (surface integral) contribution, coupled to nodes of solution vector (to be solved) }} \\
& R H S:-\underbrace{\sum_{i=1}^{I} \sum_{p=1}^{P} \sum_{k_{\text {upwind }}} \psi_{g, i, p}^{i n c_{s},(t+1)} \int_{\Omega_{\alpha}} d \hat{\Omega} \gamma_{p}(\hat{\Omega}) \gamma_{q}(\hat{\Omega}) \hat{\Omega}_{q} \cdot \hat{n}_{k} \int_{S_{k}} d S_{i}(\vec{r}) \lambda_{j}(\vec{r})}_{\text {upwind spatial (surface integral) contribution, coupled to solved nodes of upstream element in space }} . \tag{4.14}
\end{align*}
$$

Consistent with the nomenclature of upwind stabilization, it is upwind boundaries that are placed on the right hand side, supplied with known solution values. Details in developing a transport sweep solver in space will be covered in §4.2.4.

### 4.2.3 Angular Upwind Stabilization on the Unit-Sphere

A unique consequence of magnetic fields is to introduce advection in angle, treated analogously with the Divergence theorem as shown in Eq. 4.15, introducing a set of path integrals which communicate boundary conditions in angle. These are treated based on the whether the magnetic field sweep vector $\vec{\tau}(\vec{B}, \hat{\Omega})$ is seen as flowing into or out of the angular element, using the sign of $\vec{\tau}(\vec{B}, \hat{\Omega}) \cdot \hat{n}_{k^{\prime}}(\hat{\Omega})$.

$$
\begin{align*}
& \kappa_{g} \sum_{k^{\prime}=1}^{K^{\prime}} \sum_{i=1}^{I} \sum_{p=1}^{P} \psi_{g, i, p, k^{\prime}}^{(t+1)} \oint_{\Gamma_{k^{\prime}}} d \Gamma_{p}(\hat{\Omega}) \gamma_{q}(\hat{\Omega}) \vec{\tau}(\vec{B}, \hat{\Omega}) \cdot \hat{n}_{k^{\prime}}(\hat{\Omega}) \int_{V^{e}} d V \lambda_{\mathrm{i}}(\vec{r}) \lambda_{\mathrm{j}}(\vec{r}),  \tag{4.15a}\\
& \quad-\kappa_{g} \sum_{i=1}^{I} \sum_{p=1}^{P} \psi_{g, i, p}^{(t+1)} \int_{\Omega_{\alpha}} d \hat{\Omega} \gamma_{p}(\hat{\Omega}) \vec{\tau}(\vec{B}, \hat{\Omega}) \cdot \vec{\nabla}_{\Omega}\left(\gamma_{q}(\hat{\Omega})\right) \int_{V^{e}} d V \lambda_{\mathrm{i}}(\vec{r}) \lambda_{\mathrm{j}}(\vec{r}), \tag{4.15b}
\end{align*}
$$

where

$$
\psi_{g, i, p, k^{\prime}}^{(t+1)}=\left\{\begin{array}{cc}
\psi_{g, i, p}^{i n c_{a}(t+1)} & \vec{\tau}(\vec{B}, \hat{\Omega}) \cdot \hat{n}_{k^{\prime}}(\hat{\Omega})<0 \quad \text { (upwind facing boundary) }  \tag{4.16}\\
\psi_{g, i, p}^{(t+1)} & \vec{\tau}(\vec{B}, \hat{\Omega}) \cdot \hat{n}_{k^{\prime}}(\hat{\Omega})>0 \quad \text { (downwind facing boundary). }
\end{array}\right.
$$

Specifically, $\hat{n}_{k^{\prime}}(\hat{\Omega})$ is the outward-directed unit-normal tangential to the surface of the sphere, which varies with angular ordinate $\hat{\Omega}$ along the curved edge $k^{\prime}$ of a given angular element, formally defined as:

$$
\begin{equation*}
\hat{n}_{k^{\prime}}(\hat{\Omega})=\frac{d \vec{l}(\hat{\Omega}) \times \hat{r}}{|d \vec{l}(\hat{\Omega}) \times \hat{r}|}, \tag{4.17}
\end{equation*}
$$

where $d \vec{l}(\hat{\Omega})$ is a differential path segment along an edge, directed such that a clockwise path is traced about the perimeter of the angular element, and $\hat{r}$ is the unit outward radial vector.

For correct implementation of upwind stabilization, it is crucial that edges where $\vec{\tau}(\vec{B}, \hat{\Omega}) \cdot \hat{n}_{k^{\prime}}(\hat{\Omega})<0$ use incoming flux which has been solved previously in angle. Moreover, along any given edge, the sign of $\vec{\tau}(\vec{B}, \hat{\Omega}) \cdot \hat{n}_{k^{\prime}}(\hat{\Omega})$ can change, causing it to contain both upwind and downwind contributions. This is unsurprising since (i) the orientation of $\hat{n}_{k^{\prime}}$ varies along the curvature of each edge, and (ii) the orientation of sweep vector $\vec{\tau}$ in general varies over the angular domain. An appropriate treatment pre-computes all inflection points of $\vec{\tau}(\vec{B}, \hat{\Omega}) \cdot \hat{n}_{k^{\prime}}(\hat{\Omega})$ then partitions each edge into piecewise segments of upwind and downwind contributions as shown in Figure 4.3a.


Figure 4.3: Upwind (blue) and downwind (red) edge designations relative to the magnetic field sweep vector $\vec{\tau}$ for a curved element on the unit-sphere. (a) two of the edges contain both upwind and downwind contributions; (b) along representative edge $k^{\prime}=1$, segment AC faces downwind, while CB faces upwind.

Integration along edge $k^{\prime}=1$, as shown in Figure 4.3b, is split as:

$$
\begin{equation*}
\int_{A}^{B} d \Gamma \gamma_{p}(\hat{\Omega}) \gamma_{q}(\hat{\Omega}) \vec{\tau}(\vec{B}, \hat{\Omega}) \cdot \hat{n}_{1}(\hat{\Omega})=\int_{A}^{C} d \Gamma \gamma_{p}(\hat{\Omega}) \gamma_{q}(\hat{\Omega}) \vec{\tau}(\vec{B}, \hat{\Omega}) \cdot \hat{n}_{1}(\hat{\Omega})+\int_{C}^{B} d \Gamma \gamma_{p}(\hat{\Omega}) \gamma_{q}(\hat{\Omega}) \vec{\tau}(\vec{B}, \hat{\Omega}) \cdot \hat{n}_{1}(\hat{\Omega}), \tag{4.18}
\end{equation*}
$$

where the upwind segment from C to B is coupled to $\psi_{g, i, p}^{\mathrm{inc}(t+1)}$, representing nodes of known incoming fluence from an adjacent angular element, thus displaced to the right hand side of the elemental system of equations to act as a source term.

Using more general notation, partitioning of Eq. 4.15a becomes:

$$
\begin{align*}
& L H S: \underbrace{\kappa_{g} \sum_{i=1}^{I} \sum_{p=1}^{P} \sum_{k_{\text {dounwwid }}} \psi_{g, i, p}^{(t+1)} \int_{\Gamma_{k}} d \Gamma \gamma_{p}(\hat{\Omega}) \gamma_{q}(\hat{\Omega}) \vec{\tau}(\vec{B}, \hat{\Omega}) \cdot \hat{n}_{k^{\prime}}(\hat{\Omega}) \int_{V^{e}} d V \lambda_{i}(\vec{r}) \lambda_{j}(\vec{r})}_{\text {downwind angular (path integral) contribution, coupled to nodes of solution vector (to be solved) }} \\
& R H S:-\underbrace{\kappa_{g} \sum_{i=1}^{I} \sum_{p=1}^{P} \sum_{k_{\text {lpwwind }}} \psi_{g, i, p}^{i n c_{a}(t+1)} \int_{\widetilde{\Gamma}_{k^{\prime}}} d \Gamma \gamma_{p}(\hat{\Omega}) \gamma_{q}(\hat{\Omega}) \vec{\tau}(\vec{B}, \hat{\Omega}) \cdot \hat{n}_{k^{\prime}}(\hat{\Omega}) \int_{V^{e}} d V \lambda_{i}(\vec{r}) \lambda_{j}(\vec{r})}_{\text {upwind angular (path integral) contribution, coupled to solved nodes of upstream element in angle }}, \tag{4.19}
\end{align*}
$$

where $\delta \Gamma_{k^{\prime}}$ indicates partial contributions of segments along an edge.

### 4.2.4 Sweep Solver for Upwind Stabilized Elemental Equations

Incorporating terms responsible for upwind stabilization of advection in both space and angle, the elemental system of equations becomes:

$$
\underbrace{\sum_{i=1}^{I} \sum_{p=1}^{P} \sum_{k_{k_{\text {mammad }}}} \psi_{g, i, p}^{(t+1)} \int_{\Omega_{\alpha}} d \hat{\Omega} \gamma_{p}(\hat{\Omega}) \gamma_{q}(\hat{\Omega}) \hat{\Omega} \cdot \hat{n}_{k} \int_{S_{S_{k}}} d S \lambda_{i}(\vec{r}) \lambda_{j}(\vec{r})}
$$

downwind spatial (surface integral) contribution, coupled to nodes of solution vector (to be solved)

$$
-\sum_{i=1}^{I} \sum_{p=1}^{P} \psi_{g, i, p}^{(t+1)} \int_{\Omega_{\alpha}} d \hat{\Omega} \gamma_{p}(\hat{\Omega}) \gamma_{q}(\hat{\Omega}) \hat{\Omega} \cdot \int_{V^{e}} d V \lambda_{i}(\vec{r}) \vec{\nabla}\left(\lambda_{j}(\vec{r})\right)
$$

$$
+\underbrace{\kappa_{g} \sum_{i=1}^{I} \sum_{p=1}^{P} \sum_{k_{\text {doownind }}} \psi_{g, i, p}^{(t+1)} \int_{\delta \Gamma_{k^{\prime}}} d \Gamma \gamma_{p}(\hat{\Omega}) \gamma_{q}(\hat{\Omega}) \vec{\tau}(\vec{B}, \hat{\Omega}) \cdot \hat{n}_{k^{\prime}}(\hat{\Omega}) \int_{V^{e}} d V \lambda_{i}(\vec{r}) \lambda_{j}(\vec{r})}_{\text {downwind angular (path integral) contribution, coupled to nodes of solution vector (to be solved) }}
$$

$$
-\kappa_{g} \sum_{i=1}^{I} \sum_{p=1}^{P} \psi_{g, i, p}^{(t+1)} \int_{\Omega_{\alpha}} d \hat{\Omega} \gamma_{p}(\hat{\Omega}) \vec{\tau}(\vec{B}, \hat{\Omega}) \cdot \vec{\nabla}_{\Omega}\left(\gamma_{q}(\hat{\Omega})\right) \int_{V^{e}} d V \lambda_{i}(\vec{r}) \lambda_{j}(\vec{r})
$$

$$
\begin{equation*}
+\sigma_{T}\left(e l_{s}\right) \sum_{i=1}^{I} \sum_{p=1}^{P} \psi_{g, i, p}^{(t+1)} \int_{\Omega_{\alpha}} d \hat{\Omega}_{p}(\hat{\Omega}) \gamma_{q}(\hat{\Omega}) \int_{V^{e}} d V \lambda_{i}(\vec{r}) \lambda_{j}(\vec{r}) \tag{4.20}
\end{equation*}
$$

$$
=\sum_{g^{\prime}=1}^{g} \sum_{l=0}^{L} \sum_{m=-l}^{l} \sum_{i=1}^{I}\left(\phi_{F S D S, g^{\prime}, l, m, i}+\phi_{g^{\prime}, l m, i}\right) \sigma_{s, g^{\prime} \rightarrow g, l}\left(e l_{s}\right) \int_{\Omega_{\alpha}} d \hat{\Omega} Y_{l, m}(\hat{\Omega}) \gamma_{q}(\hat{\Omega}) \int_{V^{e}} d V \lambda_{i}(\vec{r}) \lambda_{j}(\vec{r})
$$

$$
+\sum_{l=0}^{L} \sum_{m=-l}^{l} \sum_{i=1}^{I} \phi_{g, l, m, i}^{(t)} \sigma_{s, g \rightarrow g, l}\left(e l_{s}\right) \int_{\Omega_{\alpha}} d \hat{\Omega} Y_{l, m}(\hat{\Omega}) \gamma_{q}(\hat{\Omega}) \int_{V^{e}} d V \lambda_{i}(\vec{r}) \lambda_{j}(\vec{r})
$$

$$
-\underbrace{\sum_{i=1}^{I} \sum_{p=1}^{P} \sum_{k_{p p \text { puid }}} \psi_{g, i, p}^{i n c_{s},(t+1)} \int_{\Omega_{\alpha}} d \hat{\Omega} \gamma_{p}(\hat{\Omega}) \gamma_{q}(\hat{\Omega}) \hat{\Omega} \cdot \hat{n}_{k} \int_{S_{k}} d S \lambda_{i}(\vec{r}) \lambda_{j}(\vec{r})}_{\text {upwind spatial (surface integral) contribution, coupled to solved nodes of upstream element in space }}
$$

$$
-\underbrace{\kappa_{g} \sum_{i=1}^{I} \sum_{p=1}^{P} \sum_{k_{\text {uppind }}^{\prime}} \psi_{g, i, p}^{i n c_{a}(t+1)} \int_{\sigma \Gamma_{k^{\prime}}} d \Gamma \gamma_{p}(\hat{\Omega}) \gamma_{q}(\hat{\Omega}) \vec{\tau}(\vec{B}, \hat{\Omega}) \cdot \hat{n}_{k^{\prime}}(\hat{\Omega}) \int_{V^{e}} d V \lambda_{i}(\vec{r}) \lambda_{j}(\vec{r})}_{\text {upwind angular (path integral) contribution, coupled to solved nodes of upstream element in angle }},
$$

with elemental boundary conditions in space (Eq. 4.13) and angle (4.16) introduced through upwind stabilization, requiring known solutions to be transferred from nodes of neighboring elements upstream. These serial dependencies forbid the entire domain from being processed concurrently. Instead, by mapping interconnections between the elements, and grouping those which share the same set of upstream dependencies, the architecture of a Sweep Solver arises. The concept is illustrated in Figure 4.4 below.


Figure 4.4: (a) Sweep vector orientation $\vec{v}_{s w}$ relative to elements of a 2D domain, (b) Sweep groups (i,ii,iii,iv) whose constituent elements can be solved concurrently.

In the direction of propagation (parameterized by sweep vector $\vec{v}_{s w}$ ) of Figure 4.4, element $\{1\}$ can be solved based on external boundary conditions. Its nodes provide upwind fluence needed to stabilize elements $\{2$ and 6$\}$ which can be solved concurrently as a 'sweep group.' Their solutions in turn feed into $\{3$ and 5$\}$, and finally $\{4\}$. Elements within each sweep group can be solved in parallel, thus avoiding the monotonic looping structure in Schematic 2.1 (§2.3.4).

Equation 4.20 involves upwind stabilized advection in both space and angle, with sweep solvers nested in a way to allow the solution to be updated by Source Iteration. Specifically an iterative update to inscatter requires solving the entire angular domain in order to generate updated spherical harmonic coefficients, defined globally over all angles. However, at interior nodes of the geometry, arriving at the solution for a given angle necessitates sweeping through all upstream elements in space in order to reach it. Therefore, a nested solution architecture arises where an angular sweep iterates over elements on the unit sphere, and for the range of directions encompassed by a given element in angle, a nested spatial transport sweep steps through elements of the 3D spatial geometry.

### 4.2.5 Space-Angle interplay ensuring Acyclic Directed Sweep Graphs

Correct enforcement of upwind stabilization boundary conditions is essential for solution stability. By adopting conventions of a structured Cartesian grid of spatial elements in conjunction with angular elements not crossing octant boundaries on the unit-sphere, it is possible to align the octant boundaries of the angular mesh with the cardinal planes of the spatial grid, such that each spatial element face $k$ (characterized by its normal vector $\hat{n}_{k}$ ) is
unambiguously categorized as upwind $\hat{\Omega}_{\alpha} \cdot \hat{n}_{k}<0$ or downwind $\hat{\Omega}_{\alpha} \cdot \hat{n}_{k}>0$ over the entire range of angles $\hat{\Omega}_{\alpha}$ encompassed by a given angular element $e l_{a}$ (i.e. the sign of $\hat{\Omega}_{\alpha} \cdot \hat{n}_{k}$ will not change for each face over the entire octant, as illustrated in Figure 4.5). This discretization convention results in an acyclic directed sweep graph.


Figure 4.5: With conventions of angular octant boundaries aligned to spatial cardinal planes (a) Upwind faces in blue, (b) Downwind faces in green, for an octant (highlighted in purple) encompassing angles under consideration.

In the previous work of St-Aubin et al (2016) ${ }^{1}$, the faces of unstructured tetrahedral spatial elements were oriented randomly such that over a single angular element, the designation of a face as upwind or downwind can change, as illustrated in Figure 4.6.


Figure 4.6: Ambiguous face designations for unstructured spatial tetrahedral element over large angular element $\hat{\Omega}_{\alpha}$. (a) Over subdomain $\hat{\Omega}_{\alpha(A)}$ : face 1 is downwind, face 2 is upwind. (b) Over subdomain $\hat{\Omega}_{\alpha(B)}$ : face 1 is upwind, face 2 is downwind.

Such ambiguity in the dependence between spatial elements can lead to stability problems, which the previous work ${ }^{1}$ attempted to mitigate by aggressive refinement of the angular mesh to a point where each element on the unit-sphere spans a small enough range of angles to minimize the probability that any given spatial element face on an unstructured grid contains both incoming and outgoing contributions. The result is an angular mesh containing 520 angular elements, far more than hypothesized are needed to model the inherent anisotropy in external beam radiotherapy, and contributes a major source of computational complexity.

However, by adopting the conventions of Figure 4.5, an unambiguous face designation and spatial solution ordering can be attained, such that angular mesh density can be dictated by the inherent anisotropy of the problem. As will be seen for oblique magnetic field and beam orientations, preserving an alignment between the spatial grid and octant boundaries is the single most important property for an efficient solution.

### 4.2.6 Discretization of Space

To achieve the desired space-angle interplay as outlined in $\S 4.25$, spatial discretization is established on a structured Cartesian grid of hexahedral voxel elements, each uniquely parameterized by its centroid $\left(x_{0}, y_{0}, z_{0}\right)$ and edge dimension $L$.

(c)


Figure 4.7: (a) Spatial domain of hexahedral elements on structured Cartesian grid, (b) Local node numbering convention, (c) Local face numbering convention.

Linear Lagrange basis functions take the form:

$$
\begin{equation*}
\lambda_{i}(\vec{r})=\frac{1}{8}\left(1 \pm \frac{x-x_{0}}{L / 2}\right)\left(1 \pm \frac{y-y_{0}}{L / 2}\right)\left(1 \pm \frac{z-z_{0}}{L / 2}\right)=\frac{1}{8}\left(\frac{2}{L}\right)^{3}\left(\frac{L}{2} \pm\left(x-x_{0}\right)\right)\left(\frac{L}{2} \pm\left(y-y_{0}\right)\right)\left(\frac{L}{2} \pm\left(z-z_{0}\right)\right) . \tag{4.21}
\end{equation*}
$$

Since limits of integration involving these basis functions always span $\pm L / 2$ about its centroid, Eq. 4.21 can be simplified by setting $x_{0}=y_{0}=z_{0}=0$ without loss of generality:

$$
\begin{equation*}
\lambda_{i}(\vec{r})=\frac{1}{L^{3}}\left(\frac{L}{2} \pm x\right)\left(\frac{L}{2} \pm y\right)\left(\frac{L}{2} \pm z\right),(x, y, x) \in \pm \frac{L}{2} . \tag{4.22}
\end{equation*}
$$

The resulting linear basis functions are illustrated in Figure 4.8, according to the node numbering conventions of Figure 4.7b.


Figure 4.8: Illustration of linear Lagrange spatial basis functions centered at each corner of a hexahedral element. (a) $\lambda_{1}(\vec{r})$, (b) $\lambda_{2}(\vec{r})$, (c) $\lambda_{3}(\vec{r})$, (d) $\lambda_{4}(\vec{r})$, (e) $\lambda_{5}(\vec{r})$, (f) $\lambda_{6}(\vec{r})$, (g) $\lambda_{7}(\vec{r})$, (h) $\lambda_{8}(\vec{r})$. Color-scale used to indicate value.

Since elements are defined on a common Cartesian grid, they all share the same orientation, and for a given mesh refinement the same dimension $L$. This regularity of structure along with the simple form of Eq. 4.22 enables spatial integrals of Eq. 4.20 to be pre-calculated analytically and applied over the entire spatial domain. Shown in Figure 4.8 are basis functions corresponding to each of the 8 corners, differing only in the sign convention applied to Eq. 4.22 based on the corner's position $x_{i} y_{i}, z_{i}$. Coupling between $\lambda_{i}(\vec{r})$ and $\lambda_{j}(\vec{r})$ can be characterized by the number of sign mismatches, resulting in the elemental integrals summarized in Table 4.1.

Table 4.1: Summary of Analytic Integrals for Spatial Elements

| Expression | 0 sign mismatches | 1 sign mismatch | 2 sign mismatches | 3 sign mismatches |
| :---: | :---: | :---: | :---: | :---: |
| $\int_{V^{e}} d V \lambda_{i}(\vec{r}) \lambda_{j}(\vec{r})$ | $\frac{L^{3}}{27}$ | $\frac{1}{2} \cdot \frac{L^{3}}{27}$ | $\frac{1}{4} \cdot \frac{L^{3}}{27}$ | $\frac{1}{8} \cdot \frac{L^{3}}{27}$ |
| $\int_{S_{k}} d S \lambda_{i}(\vec{r}) \lambda_{j}(\vec{r})$ | $\frac{L^{2}}{9}$ | $\frac{1}{2} \cdot \frac{L^{2}}{9}$ | $\frac{1}{8} \cdot \frac{L^{2}}{9}$ |  |

0 sign mismatches corresponds to $i=j$ on the main diagonal, where a node couples to itself.
1 sign mismatch arises when nodes are coupled along the same edge.
2 sign mismatches arise for nodes at opposite corners of the same face.
3 sign mismatches arise for nodes at opposite corners of the spatial element.

Surface integrals for each of the 6 faces populate their own $8 \times 8$ matrix, with only 4 of the rows and 4 of the columns containing non-zeros, corresponding to nodes of a given face.

An efficient spatially adaptive hexahedral mesh generator was developed from scratch, offering flexibility to set the spatial grid to several discrete refinement levels based on region. Usually the finest grid is reserved for regions within the beam and penumbra, then growing by successive factors of 2 in neighboring regions. The restriction that hexahedral edge dimension can only differ by a factor of 2 between adjacent regions enables the systematic treatment of upwind stabilization between refinement levels, characterized by fluence transfer to or from 4 smaller elements forming equal quadrants on the face of an adjacent larger element.

### 4.2.7 Angular Discretization on the Unit-Sphere

The surface of the unit-sphere offers a natural habitat to parameterize the angular domain, allowing for greater flexibility than the previous angular DFEM implementation ${ }^{1}$ which consisted of triangles on a flattened $\varphi-\theta$ space. Elements on the sphere enable exploration of the minimum 8 angular elements, corresponding to the octants, each having a unique spatial sweep ordering. Moreover, the entire angular mesh can be rotated collectively about any axis while constrained to the surface of the sphere, providing an efficient way to preserve space-angle
mesh alignment (§4.2.5) at oblique magnetic field orientations without re-gridding the underlying geometry.

Angular basis functions are initially defined in terms of canonical coordinates as $\gamma\left(\eta_{1}, \eta_{2}\right)$, with $0 \leq \eta_{1} \leq 1$ and $0 \leq \eta_{2} \leq 1$. The three linear basis functions spanning the canonical triangle can be expressed as,

$$
\begin{align*}
& \gamma_{1}=1-\eta_{1}-\eta_{2} \\
& \gamma_{2}=\eta_{1}  \tag{4.23}\\
& \gamma_{3}=\eta_{2} .
\end{align*}
$$

Higher order polynomial basis functions can be constructed in terms of this linear set ${ }^{6}$, as illustrated in Figure 4.9. Linear, quadratic, and cubic polynomial orders are investigated, having 3,6 , and 10 nodal degrees of freedom per angular element, while obeying the properties of Lagrange basis functions as established in Eq. 2.62(a,b).


Figure 4.9: Location of nodes and functional variation of angular Lagrange basis functions in canonical coordinates for (a) linear order, (b) quadratic order.

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 ${ }^{7,8}$.


Figure 4.10: Schematic depicting the transformation of an angular element from (a) canonical coordinate system, to (b) flat surface of octahedron, to (c) curved surface of the unit sphere.

The angular mesh is initially defined on the flat faces of an octahedron with vertices at $\pm 1$ along the cardinal axes (Figure 4.10b), the most elementary case being a single angular element per octant ( 8 elements total). Each face can undergo systematic refinement by recursively bisecting the edges of triangles on the octahedron, producing angular meshes with 32, 128, 512, 2048, and 8192 elements used in this work.

The canonical element is mapped onto each triangle of the octahedron using Eq. 4.24:

$$
\vec{T}=\left[\begin{array}{c}
x  \tag{4.24}\\
y \\
z
\end{array}\right]=\left[\begin{array}{c}
X_{1} \\
Y_{1} \\
Z_{1}
\end{array}\right]+\left[\begin{array}{cc}
X_{2}-X_{1} & X_{3}-X_{1} \\
Y_{2}-Y_{1} & Y_{3}-Y_{1} \\
Z_{2}-Z_{1} & Z_{3}-Z_{1}
\end{array}\right] \cdot\left[\begin{array}{c}
\eta_{1} \\
\eta_{2}
\end{array}\right] .
$$

A given element is uniquely defined by the coordinates of its corner vertices $\left(X_{1}, Y_{1}, Z_{1}\right)$, $\left(X_{2}, Y_{2}, Z_{2}\right),\left(X_{3}, Y_{3}, Z_{3}\right)$ as shown in Figure 4.10b. Next, elements on the octahedron are projected onto the curved surface of the unit-sphere (Figure 4.10c), such that all points are constrained to the radial coordinate $\hat{r}=1$.

$$
\hat{\Omega}=\left[\begin{array}{c}
\Omega_{x}  \tag{4.25}\\
\Omega_{y} \\
\Omega_{z}
\end{array}\right]=\frac{\vec{T}}{|\vec{T}|}=\frac{\left[\begin{array}{c}
\left(X_{1}+\eta_{1} \cdot\left(X_{2}-X_{1}\right)+\eta_{2} \cdot\left(X_{3}-X_{1}\right)\right) \\
\left(Y_{1}+\eta_{1} \cdot\left(Y_{2}-Y_{1}\right)+\eta_{2} \cdot\left(Y_{3}-Y_{1}\right)\right) \\
\left(Z_{1}+\eta_{1} \cdot\left(Z_{2}-Z_{1}\right)+\eta_{2} \cdot\left(Z_{3}-Z_{1}\right)\right)
\end{array}\right]}{\sqrt{\left(X_{1}+\eta_{1} \cdot\left(X_{2}-X_{1}\right)+\eta_{2} \cdot\left(X_{3}-X_{1}\right)\right)^{2}}}=\left[\begin{array}{c}
\sin (\theta) \cos (\varphi) \\
\sin (\theta) \sin (\varphi) \\
\cos (\theta)
\end{array}\right]
$$

Transformations through Eqs. 4.24 and 4.25 map the polynomial basis functions from canonical coordinates $\gamma\left(\eta_{1}, \eta_{2}\right)$ to the angular domain $\gamma(\hat{\Omega})$ as shown in Figure 4.10.

The first four angular mesh refinements on unit-sphere are shown in Figure 4.11.


Figure 4.11: Systematic angular mesh refinement on the unit-sphere while respecting octant boundaries, depicting (a) 8 elements, (b) 32 elements, (c) 128 elements, (d) 512 elements.

When integrating over the angular domain $\int_{\Omega_{\alpha}} d \hat{\Omega}$ with respect to basis functions in canonical coordinates $\left(\eta_{1}, \eta_{2}\right)$, a Jacobian $|J|_{\dot{\eta} \rightarrow \hat{\Omega}}$ is needed to preserve area in the Cartesian space $R^{3}$ where elements have been mapped onto the surface of the unit-sphere. Specifically,

$$
\begin{equation*}
\int_{\Omega_{\alpha}} d \hat{\Omega}=\int_{\Omega_{\alpha}} r \sin (\theta) d \varphi \cdot r d \theta \stackrel{r=1}{=} \int_{\Omega_{\alpha}} \sin \theta d \varphi d \theta=\int_{\Omega_{\alpha}} \sin \theta\left|\frac{d \vec{\alpha}}{d \vec{\eta}}\right| d \eta_{1} d \eta_{2} \tag{4.26}
\end{equation*}
$$

where $\left|\frac{d \vec{\alpha}}{d \vec{\eta}}\right|$ transforms $d \eta_{1} d \eta_{2}$ to $d \varphi d \theta$, defined as:

$$
\left|\frac{d \vec{\alpha}}{d \vec{\eta}}\right|=\left|\begin{array}{cc}
\frac{\partial \varphi}{\partial \eta_{1}} & \frac{\partial \varphi}{\partial \eta_{2}}  \tag{4.27}\\
\frac{\partial \theta}{\partial \eta_{1}} & \frac{\partial \theta}{\partial \eta_{2}}
\end{array}\right|=\frac{\partial \varphi}{\partial \eta_{1}} \frac{\partial \theta}{\partial \eta_{2}}-\frac{\partial \varphi}{\partial \eta_{2}} \frac{\partial \theta}{\partial \eta_{1}}
$$

Using Eq. 4.25, $\varphi$ and $\theta$ can be expressed in terms of canonical coordinates as:

$$
\begin{gather*}
\varphi=\tan ^{-1}\left(\frac{\Omega_{y}}{\Omega_{x}}\right)=\tan ^{-1}\left(\frac{\left(Y_{1}+\eta_{1} \cdot\left(Y_{2}-Y_{1}\right)+\eta_{2} \cdot\left(Y_{3}-Y_{1}\right)\right)}{\left(X_{1}+\eta_{1} \cdot\left(X_{2}-X_{1}\right)+\eta_{2} \cdot\left(X_{3}-X_{1}\right)\right)}\right),  \tag{4.28a}\\
\theta=\cos ^{-1}\left(\Omega_{z}\right)=\cos ^{-1}\left(\frac{\left(Z_{1}+\eta_{1} \cdot\left(Z_{2}-Z_{1}\right)+\eta_{2} \cdot\left(Z_{3}-Z_{1}\right)\right)}{\left.\sqrt{\left(X_{1}+\eta_{1} \cdot\left(X_{2}-X_{1}\right)+\eta_{2} \cdot\left(X_{3}-X_{1}\right)\right)^{2}+\left(Y_{1}+\eta_{1} \cdot\left(Y_{2}-Y_{1}\right)+\eta_{2} \cdot\left(Y_{3}-Y_{1}\right)\right)^{2}+\left(Z_{1}+\eta_{1} \cdot\left(Z_{2}-Z_{1}\right)+\eta_{2} \cdot\left(Z_{3}-Z_{1}\right)\right)^{2}}\right) .}\right. \tag{4.28b}
\end{gather*}
$$

The Jacobian is calculated symbolically for each angular element, by substituting its unique corner coordinates $\left(X_{1}, Y_{1}, Z_{1}\right),\left(X_{2}, Y_{2}, Z_{2}\right),\left(X_{3}, Y_{3}, Z_{3}\right)$.

Whereas spatial basis integrals could be calculated analytically, several challenges in the angular domain necessitate numerical integration, mainly attributed to irregular bounds of integration and highly nonlinear form of the Jacobian. Integrals are approximated numerically by Gaussian Quadratures (§2.4), where evaluating the integrand at $N$ points provides exact integration to polynomial order $2 N-1$, specifically:

$$
\begin{equation*}
\int_{\Omega_{\alpha}} d \vec{\eta}|J|_{\dot{\eta} \rightarrow \hat{\Omega}} \gamma\left(\eta_{1}, \eta_{2}\right) \approx A_{e} \sum_{n=1}^{n G Q} w_{n}|J|_{\hat{\eta}_{n} \rightarrow \hat{\Omega}_{n}} \gamma\left(\eta_{1_{n}}, \eta_{2_{n}}\right), \tag{4.29}
\end{equation*}
$$

where $A_{e}$ denotes the area of a triangular element in canonical coordinates. Angular integrals are listed in Table 4.2 below, along with their respective treatments:

Table 4.2: Angular FEM Integrals and their Implementation

| Expression | Implementation |
| :---: | :---: |
| $\int_{\Omega_{\alpha}} d \hat{\Omega} \gamma_{p}(\hat{\Omega}) \gamma_{q}(\hat{\Omega})$ | $A_{e} \sum_{n=1}^{n G Q} w_{n}\|J\|_{\vec{\eta}_{n} \rightarrow \hat{\Omega}_{n}} \gamma_{p}\left(\eta_{1_{n}}, \eta_{2_{n}}\right) \gamma_{q}\left(\eta_{1_{n}}, \eta_{2_{n}}\right)$ |
| $\int_{\Omega_{\alpha}} d \hat{\Omega} \gamma_{p}(\hat{\Omega}) \gamma_{q}(\hat{\Omega}) \hat{\Omega}$ | $A_{e} \sum_{n=1}^{n G Q} w_{n}\|J\|_{\hat{\eta}_{n} \rightarrow \hat{\Omega}_{n}} \gamma_{p}\left(\eta_{1_{n}}, \eta_{2_{n}}\right) \gamma_{q}\left(\eta_{1_{n}}, \eta_{2_{n}}\right) \hat{\Omega}\left(\eta_{1_{n}}, \eta_{2_{n}}\right)$ |
| $\int_{\Omega_{\alpha}} d \hat{\Omega} \gamma_{p}(\hat{\Omega}) \vec{\tau}(\vec{B}, \hat{\Omega}) \cdot \overrightarrow{\nabla_{\Omega}}\left(\gamma_{q}(\hat{\Omega})\right)$ | Magnetic field surface integral (§4.2.9) |
| $\int_{\Gamma_{k^{\prime}}} d \Gamma \gamma_{p}(\hat{\Omega}) \gamma_{q}(\hat{\Omega}) \vec{\tau}(\vec{B}, \hat{\Omega}) \cdot \hat{n}_{k^{\prime}}(\hat{\Omega})$ | Magnetic field edge integral $(\S 4.2 .9)$ |
| $\int_{\Omega_{\alpha}} d \hat{\Omega} Y_{l, m}(\hat{\Omega}) \gamma_{q}(\hat{\Omega})$ | $A_{e} \sum_{n=1}^{n G Q} w_{n}\|J\|_{\vec{\eta}_{n} \rightarrow \hat{\Omega}_{n}} \gamma_{q}\left(\eta_{1_{n}}, \eta_{2_{n}}\right) Y_{l, m}\left(\hat{\Omega}\left(\eta_{1_{n}}, \eta_{2_{n}}\right)\right)$ |

Angular FEM surface integrals are performed using an 88-point numerical quadrature with order 20 accuracy $^{9}$, found to be sufficient for regions up to the size of an octant. Line integrals are performed using a 64 -point Gaussian quadrature (order 127 accurate) ${ }^{10}$.

### 4.2.8 Rotational Formalism for Oblique $B_{0}$ Configurations

For external beam radiotherapy, we establish the patient coordinate frame $\mathbb{S}=(x, y, z)$ as the static Cartesian grid to which image voxels are aligned during treatment planning, and whose cardinal planes divide the unit-sphere into octants (Figure 4.12a). These form the octant boundaries which angular mesh elements must respect in order to retain an unambiguous spatial sweep ordering, as established in §4.2.5.

Advection in the angular domain is characterized by the vector field $\vec{\tau}(\vec{B}, \hat{\Omega})$ which produces complex patterns, as shown in Figure 4.12a such that an acyclic sweep ordering is difficult (and sometimes impossible) to establish in angle. One way to constrain angular advection to be well defined along $\pm \hat{\varphi}$ is to set $\vec{B}=\left\{0,0, B_{z}\right\}$ such that the magnetic field is restricted to the $z$-axis in the coordinate system where calculations are performed ${ }^{1}$ :

$$
\begin{equation*}
\vec{\tau}(\hat{\Omega})=B_{z} \sin (\theta) \hat{\varphi} \tag{4.30}
\end{equation*}
$$

Having elements on the unit-sphere introduces new flexibility for the entire angular mesh to be rotated. For radiotherapy systems such as the Alberta Linac-MR ${ }^{11,12}$ where $\vec{B}_{0}$ rotates with gantry angle $\chi$, a calculation coordinate frame $\mathbb{S}_{r}=\left(x, y_{r}, z_{r}\right)$ 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 4.12b). This recovers the simple azimuthal sweep ordering in $\mathbb{S}_{r}$, where:

$$
\begin{equation*}
\vec{\tau}\left(\hat{\Omega}_{r}\right)=B_{z_{r}} \sin \left(\theta_{r}\right) \hat{\varphi}_{r} \tag{4.31}
\end{equation*}
$$



Figure 4.12: (a) Patient coordinate frame $\mathbb{S}$, with planes dividing octant boundaries shown. On the left is the angular domain, with sweep vector $\overrightarrow{\boldsymbol{\tau}}$ shown for an oblique magnetic field. For each element, blue designates upwind, while red designates downwind. On the right is the corresponding Cartesian spatial grid aligned to the octant boundaries. (b) Calculation coordinate frame $\mathbb{S}_{r}$ overlaid with planes of the patient coordinate frame. On the left is the angular domain in $\mathbb{S}_{r}$ with sweep vector $\overrightarrow{\boldsymbol{\tau}}$ shown for an oblique magnetic field. On the right is the corresponding Cartesian spatial grid, aligned with the octant boundaries of the patient frame of reference.

As shown in Figure 4.12 b, the transformation to $\mathbb{S}_{r}$ is 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. Another invariant under rotation are the spatial integrals in Table 4.1, which can be reused at all gantry angles. However, the inflection points of $\vec{\tau}\left(\hat{\Omega}_{r}\right) \cdot \hat{n}_{k^{\prime}}\left(\hat{\Omega}_{r}\right)$ and the resulting integrals of Eq. 4.19 need to be reevaluated, along with redefining sweep ordering on the unit-sphere for each
magnetic field direction. As the number of angular elements can be made quite low, this is not a computationally intensive calculation.

### 4.2.9 Treatment of Magnetic Field Terms

With the magnetic field established along $z$, the angular sweep vector become:

$$
\begin{equation*}
\vec{\tau}(\vec{B}, \hat{\Omega}) \cdot \vec{\nabla}_{\Omega}=\left(\tau_{\varphi} \hat{\boldsymbol{\varphi}}+{\underset{\nu}{\alpha_{0}}}_{\substack{\text { for } \\ B_{z}}} \hat{\boldsymbol{\theta}}\right) \cdot\left(\frac{1}{\sqrt{1-\mu^{2}}} \frac{\partial}{\partial \varphi} \hat{\boldsymbol{\varphi}}+\frac{\partial}{\partial \theta} \hat{\boldsymbol{\theta}}\right)=B_{z} \frac{\partial}{\partial \varphi}=B_{z}\left(\frac{\partial \eta_{1}}{\partial \varphi} \cdot \frac{\partial}{\partial \eta_{1}}+\frac{\partial \eta_{2}}{\partial \varphi} \cdot \frac{\partial}{\partial \eta_{2}}\right), \tag{4.32}
\end{equation*}
$$

where the chain rule has been used to express the azimuthal derivative in terms of canonical coordinates of the angular basis functions. To calculate $\frac{\partial \eta_{1}}{\partial \varphi}$ and $\frac{\partial \eta_{2}}{\partial \varphi}$ requires $\eta_{1}(\varphi)$ and $\eta_{2}(\varphi)$, which are obtained for each angular element using the inverse mappings of Eqs. 4.24 and 4.25. Consider the stages outlined in Eq. 4.33:

$$
\begin{equation*}
\vec{\eta} \stackrel{(i)}{\longleftrightarrow} \vec{T} \stackrel{(i i)}{\longleftrightarrow} \hat{\Omega} . \tag{4.33}
\end{equation*}
$$

In stage (i) the forward mapping from conical coordinates $\vec{\eta}$ to points on an octahedron face $\vec{T}$ within a triangle with corners $T_{1}=\left(X_{1}, Y_{1}, Z_{1}\right), T_{2}=\left(X_{2}, Y_{2}, Z_{2}\right), T_{3}=\left(X_{3}, Y_{3}, Z_{3}\right)$ is:

$$
\vec{T}=\vec{T}_{1}+[M] \vec{\eta}, \text { where }[M]=\left[\begin{array}{c|c}
X_{2}-X_{1} & X_{3}-X_{1}  \tag{4.34}\\
Y_{2}-Y_{1} & Y_{3}-Y_{1} \\
Z_{2}-Z_{1} & Z_{3}-Z_{1}
\end{array}\right]_{3 \times 2}
$$

For the inverse mapping $\vec{\eta} \leftarrow \vec{T}$, the Moore-Penrose pseudoinverse is defined and unique ${ }^{13}$, yielding for each angular element,

$$
\begin{equation*}
[\operatorname{piM}]_{2 \times 3}=\operatorname{pinv}(M)=\left(M^{T} M\right)^{-1} M^{T} . \tag{4.35}
\end{equation*}
$$

Although the transformation appears to reduce 3 degrees of freedom to 2 degrees of freedom, the forward mapping by construction is constrained to a plane and thus the 2 independent degrees of freedom are spanned by $\left(\eta_{1}, \eta_{2}\right)$. Likewise, the transformation to curved geometry in stage (ii) is
constrained to the surface of the unit-sphere, spanned by $(\varphi, \theta)$. Taking the inverse of Eq. 4.25 involves a scaling of the components from the sphere's surface to the octahedron face by:

$$
\left[\begin{array}{c}
T_{x}  \tag{4.36}\\
T_{y} \\
T_{z}
\end{array}\right]=\frac{\overrightarrow{T_{1}} \cdot \hat{n}}{\hat{\Omega} \cdot \hat{n}}\left[\begin{array}{c}
\sin (\theta) \cos (\varphi) \\
\sin (\theta) \sin (\varphi) \\
\cos (\theta)
\end{array}\right],
$$

where $\hat{n}$ designates the outward unit normal of the octahedron face, such that:

$$
\begin{equation*}
\hat{n}=\frac{\vec{n}}{|\vec{n}|}, \text { where } \vec{n}=\left(\vec{T}_{2}-\vec{T}_{1}\right) \times\left(\vec{T}_{3}-\vec{T}_{1}\right) . \tag{4.37}
\end{equation*}
$$

Combining the inverse mappings of stage (i) and (ii) yields:

$$
\vec{\eta}=\left[\begin{array}{l}
\eta_{1}  \tag{4.38}\\
\eta_{2}
\end{array}\right]=[\text { piM }]_{2 x 3}\left(\vec{T}-\vec{T}_{1}\right)=\left[\begin{array}{lll}
\text { piM } M_{1,1} & \text { piM } M_{1,2} & \text { piM } M_{1,3} \\
\text { piM }_{2,1} & \text { piM } & 2,2
\end{array} \text { piM } 2,3\right]\left(\frac{\overrightarrow{T_{1}} \cdot \hat{n}}{\hat{\Omega} \cdot \hat{n}}\left[\begin{array}{c}
\sin (\theta) \cos (\varphi) \\
\sin (\theta) \sin (\varphi) \\
\cos (\theta)
\end{array}\right]-\left[\begin{array}{c}
T_{1 x} \\
T_{1 y} \\
T_{1 z}
\end{array}\right]\right) \text {. }
$$

From Eq. 4.38, $\frac{\partial \eta_{1}}{\partial \varphi}$ and $\frac{\partial \eta_{2}}{\partial \varphi}$ are calculated.
The derivatives of basis functions in canonical coordinates, $\frac{\partial \gamma_{q}}{\partial \eta_{1}}$ and $\frac{\partial \gamma_{q}}{\partial \eta_{2}}$ are straightforward to calculate and remain invariant regardless how the angular elements are rotated on the sphere's surface.

The magnetic field surface integral can be approximated at Gaussian quadrature points as:

$$
\begin{align*}
& \int_{\Omega_{\alpha}} d \hat{\Omega} \gamma_{p}(\hat{\Omega}) \vec{\tau}(\vec{B}, \hat{\Omega}) \cdot \vec{\nabla}_{\Omega}\left(\gamma_{q}(\hat{\Omega})\right) \\
& \left.\approx B_{z} A_{e} \sum_{n=1}^{n G Q} w_{n}|J|\right|_{\eta_{n} \rightarrow \hat{\Omega}_{n}} \gamma_{p}\left(\eta_{1 n}, \eta_{2 n}\right)\left(\frac{\partial \gamma_{q}}{\partial \eta_{1}}\left(\eta_{1 n}, \eta_{2 n}\right) \cdot \frac{\partial \eta_{1}}{\partial \varphi}\left(\varphi_{n}, \theta_{n}\right)+\frac{\partial \gamma_{q}}{\partial \eta_{2}}\left(\eta_{1 n}, \eta_{2 n}\right) \cdot \frac{\partial \eta_{2}}{\partial \varphi}\left(\varphi_{n}, \theta_{n}\right)\right) . \tag{4.39}
\end{align*}
$$

With regards to path integration constrained on the surface of the unit-sphere,

$$
\begin{equation*}
d \vec{l}=d \theta \hat{\boldsymbol{\theta}}+\sin (\theta) d \varphi \hat{\boldsymbol{\varphi}} . \tag{4.40}
\end{equation*}
$$

Substituting this differential path length into Eq. 4.17 yields:

$$
\begin{equation*}
\hat{n}_{k^{\prime}}(\varphi, \theta)=\frac{(-d \theta \hat{\boldsymbol{\varphi}}+\sin (\theta) d \varphi \hat{\boldsymbol{\theta}})}{\sqrt{(d \theta)^{2}+\sin ^{2}(\theta)(d \varphi)^{2}}} . \tag{4.41}
\end{equation*}
$$

With the magnetic field along $z$, it can be shown:

$$
\begin{equation*}
\vec{\tau}(\varphi, \theta) \cdot \hat{n}_{k^{\prime}}(\varphi, \theta)=\frac{-B_{z} \sin \theta(d \theta)}{\sqrt{(d \theta)^{2}+\sin ^{2}(\theta)(d \varphi)^{2}}} . \tag{4.42}
\end{equation*}
$$

Substituting $\vec{\tau} \cdot \hat{n}_{k^{\prime}}$ and $d l$ into the line integral,

$$
\begin{equation*}
\int_{\sigma_{k}} \gamma_{p}(\vec{\eta}) \gamma_{q}(\vec{\eta}) \underbrace{\frac{-B_{z} \sin \theta(d \theta)}{\sqrt{(d \theta)^{2}+\sin ^{2}(\theta)(d \varphi)^{2}}}}_{\vec{\eta} \cdot \overrightarrow{r_{k}}} \underbrace{\sqrt{(d \theta)^{2}+\sin ^{2}(\theta)(d \varphi)^{2}}}_{d l}=-B_{z} \int_{\sigma_{k}} \sin \theta \gamma_{p}(\vec{\eta}) \gamma_{q}(\vec{\eta})(d \theta) . \tag{4.43}
\end{equation*}
$$

Since Gaussian quadrature is defined in canonical coordinates $\left(\eta_{1}, \eta_{2}\right)$, the differential step $d \theta$ needs to be parameterized by taking the total derivative:

$$
\begin{equation*}
d \theta=\frac{\partial \theta}{\partial \eta_{1}} d \eta_{1}+\frac{\partial \theta}{\partial \eta_{2}} d \eta_{2} \tag{4.44}
\end{equation*}
$$

which contains terms of the Jacobian $|J|_{\vec{\eta} \rightarrow \hat{\Omega}}$. Finally path integration is implemented as:

$$
\begin{align*}
& \int_{\sigma_{K_{k}}} d \Gamma \gamma_{p}(\hat{\Omega}) \gamma_{q}(\hat{\Omega}) \vec{\tau}(\vec{B}, \hat{\Omega}) \cdot \hat{n}_{k^{\prime}}(\hat{\Omega}) \\
& \approx-B_{z}^{n} \sum_{n=1}^{n G Q} w_{n} \sin \left(\theta_{n}\right) \gamma_{p}\left(\eta_{1 n}, \eta_{2 n}\right) \gamma_{q}\left(\eta_{1 n}, \eta_{2 n}\right)\left(\frac{\partial \theta}{\partial \eta_{1}}\left(\eta_{1 n}, \eta_{2 n}\right) d \eta_{1 n}+\frac{\partial \theta}{\partial \eta_{2}}\left(\eta_{1 n}, \eta_{2 n}\right) d \eta_{2 n}\right) . \tag{4.45}
\end{align*}
$$

Only basis function pairings $(p, q)$ which are nonzero along a given edge $k^{\prime}$ contribute to the integral. Furthermore, piecewise classification of upwind / downwind designation determines deployment on the left of right hand of the system of equations.

### 4.2.10 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 ${ }^{3}$. Formally, this observed order-of-accuracy under mesh refinement ( $h$-refinement) can be compared with well-established theoretical values for the Finite Element Method ${ }^{14}$.

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, which in this case is chosen to be a spatially uniform but directionally anisotropic of the form:

$$
\begin{equation*}
\Psi_{a}(\hat{\Omega})=P_{m s} \cdot \exp \left(\frac{\omega_{x} \Omega_{x}{ }^{2}+\omega_{y} \Omega_{y}{ }^{2}+\omega_{z}\left(\Omega_{z}-0.9\right)^{2}}{4 v^{2}}\right) \tag{4.46}
\end{equation*}
$$

where $\hat{\Omega}=\left(\Omega_{x}, \Omega_{y}, \Omega_{z}\right)$ is the angular ordinate.

Although MMS does not require a physically realistic solution ${ }^{3,15}$, the form of Eq. 4.46 and the choice of parameters $\left\{P_{m s}=\frac{1}{3.2 \cdot 10^{6} \mathrm{~cm}^{2}}, \omega_{x}=1, \omega_{y}=2, \omega_{z}=1, v=1 / 4\right\}$ was used to produce an angular fluence distribution resembling the electron fluence solution for the highest energy group ( 6 MeV ) of the LBTE based on previous numerical radiotherapy calculations. The angular fluence of Eq. 4.46 is substituted into the monoenergetic multigroup LBTE (Eq. 2.37) to yield the corresponding source function:

$$
\begin{equation*}
S_{a}(\hat{\Omega})=\sigma \Psi_{a}(\hat{\Omega})+\kappa B_{z} \frac{\partial}{\partial \varphi} \Psi_{a}(\hat{\Omega})-\int d \hat{\Omega}^{\prime} \sigma^{s}\left(\hat{\Omega}^{\prime} \cdot \hat{\Omega}\right) \Psi_{a}\left(\hat{\Omega}^{\prime}\right) \tag{4.47}
\end{equation*}
$$

where the energy group index $g$ has been suppressed without loss of generality. The macroscopic differential scattering cross section $\sigma^{s}\left(\hat{\Omega}^{\prime} \cdot \hat{\Omega}\right)$ is approximated in the form of the HenyeyGreenstein model ${ }^{16}$ as:

$$
\begin{equation*}
\sigma^{s}\left(\hat{\Omega}^{\prime} \cdot \hat{\Omega}\right)=\frac{\sigma}{2} \frac{1-\zeta^{2}}{\left(1-2 \zeta \mu+\zeta^{2}\right)^{3 / 2}} \tag{4.48}
\end{equation*}
$$

where $\mu=\hat{\Omega}^{\prime} \cdot \hat{\Omega}=\cos \left(\theta^{\prime}\right)$, and the anisotropy parameter is set at $\zeta=0.5$. The scattering integral in Eq. 4.47 with the cross section of Eq. 4.48 is evaluated numerically using a level
symmetric $\mathrm{S}_{64}$ quadrature set comprising 8192 points, with $\sigma^{s}\left(\hat{\Omega}^{\prime} \cdot \hat{\Omega}\right)$ expanded in Legendre polynomial moments $\sigma_{l}^{s}$, where the maximum Legendre expansion order of $L=8$ was chosen.

A numerical implementation of the mathematical framework was prototyped in MATLAB ${ }^{17}$. Unaccelerated Source Iteration (SI) was used to converge on the numerical solution of the angular fluence, with the termination condition presented by Adams to avoid false convergence which can occur when the iteration count is very large ${ }^{18}$,

$$
\begin{equation*}
\frac{\left\|\Phi_{l, m}^{t-1}-\Phi_{l, m}^{t-2}\right\|_{2}}{\left\lvert\, 1-\frac{\left\|\Phi_{l, m}^{t}-\Phi_{l, m}^{t-1}\right\|_{2}}{\left\|\Phi_{l, m}^{t-1}-\Phi_{l, m}^{t-2}\right\|_{2}}\right.} \leq 10^{-5} . \tag{4.49}
\end{equation*}
$$

The error between the code's numerical solution $\Psi_{n}(\hat{\Omega})$ and the reference $\Psi_{a}(\hat{\Omega})$ is quantified using the $L 2$ norm over angle,

$$
\begin{equation*}
\varepsilon=\left\|\Psi_{n}-\Psi_{a}\right\|_{2}=\sqrt{\int d \hat{\Omega}\left(\Psi_{n}(\hat{\Omega})-\Psi_{a}(\hat{\Omega})\right)^{2}} \tag{4.50}
\end{equation*}
$$

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

$$
\begin{equation*}
m=-\frac{\log _{10}(\varepsilon)}{\log _{10}(1 / h)} \tag{4.51}
\end{equation*}
$$

MMS was performed for linear, quadratic, and cubic basis functions in angle, for material cross sections with magnitudes of $\sigma=10^{-3}, 10^{0}, 10^{3} \mathrm{~cm}^{-1}$, 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 $10^{-3} \mathrm{~cm}^{-1}$ while materials such as water and bone can have cross section magnitudes of $10^{3} \mathrm{~cm}^{-1}$ 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 $\kappa B_{z}=10 \mathrm{~cm}^{-1}$ which was chosen as an extreme case representative of a 20 T magnetic field.

### 4.2.11 Dosimetric Validation Setup

Accuracy of the deterministic framework was validated against the Monte Carlo package GEANT4 ${ }^{19,20}$ over a range of angular discretization parameters for a dosimetrically challenging scenario containing high density bone $\left(1.92 \mathrm{~g} / \mathrm{cm}^{3}\right)$ immediately followed by low density air $\left(0.0012 \mathrm{~g} / \mathrm{cm}^{3}\right)$ in the presence of a strong 1.5 T magnetic field. This setup was implemented for a test geometry of a $10 \times 10 \times 10 \mathrm{~cm}^{3}$ heterogeneous phantom comprising slabs of water, bone, and air, irradiated by a polyenergetic 6 MV point source ${ }^{21}$ at 100 cm SSD for a $2 \times 2 \mathrm{~cm}^{2}$ 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 $37^{\circ}$ clockwise in the $y-z$ plane. By choosing a non-cardinal angle, we test the performance of this framework in the most general case. Lastly, investigations were performed on a $30 \times 30 \times 30 \mathrm{~cm}^{3}$ phantom with a $10 \times 10 \mathrm{~cm}^{2}$ field size.

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 angular 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 were generated using the CEPXS software ${ }^{22}$ with a maximum Legendre expansion order of $L=5$. These parameters were shown in previous works ${ }^{1,21}$ 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 $10 \times 10 \times 10 \mathrm{~cm}^{3}$ test phantom used a Cartesian hexahedral grid with a minimum element size of $1.25 \times 1.25 \times 1.25 \mathrm{~mm}^{3}$ within the beam and penumbra, which grew by successive factors of 2 in edge dimension to $10 \times 10 \times 10 \mathrm{~mm}^{3}$ for the largest elements outside of the beam, for a total of 52,800 spatial elements. The larger $30 \times 30 \times 30 \mathrm{~cm}^{3}$ phantom used a minimum element size of $2.5 \times 2.5 \times 2.5 \mathrm{~mm}^{3}$ within the beam and penumbra, growing to a maximum of $10 \times 10 \times 10 \mathrm{~mm}^{3}$ outside the beam, for a total of 410,040 spatial elements. Notably, each discontinuous spatial finite element has 8 spatial degrees of freedom, corresponding to dose at the corners, whereas the same sized voxel in Monte Carlo has one dose value ascribed to its centroid.

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 ${ }^{23}$ and EEDL ${ }^{24}$ respectively), providing equivalent material cross sections as generated by CEPXS ${ }^{22}$. For the $10 \times 10 \times 10 \mathrm{~cm}^{3}$ phantom, 5 billion histories were run with dose scored on a $1.25 \times 1.25 \times 1.25 \mathrm{~mm}^{3}$ voxel grid. For the $30 \times 30 \times 30 \mathrm{~cm}^{3}$ phantom, 20 billion histories were run with dose scored on a $2.5 \times 2.5 \times 2.5 \mathrm{~mm}^{3}$ voxel grid. The path length cutoff for production of secondary particles in GEANT4 was set to $10 \mu \mathrm{~m}$. Both the deterministic and Monte Carlo calculations were normalized to dose per particle fluence of primary photons ( $\mathrm{Gy} \mathrm{cm}^{2}$ ).

Central axis depth dose and lateral profiles were compared for a variety of angular mesh refinement levels and angular basis function orders. For representative cases, a 3D gamma analysis ${ }^{25}$ was performed using a $2 \% / 2 \mathrm{~mm}$ as well as a $1 \% / 1 \mathrm{~mm}$ global dose maximum Van Dyk gamma criterion ${ }^{26}$, 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.

### 4.3 Results and Discussion

### 4.3.1 Framework Verification by MMS

Plotted in Figure 4.13 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, and this is presented as a solid baseline in each grouping of Figure 4.13. 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.


Figure 4.13: Order of convergence plots of the $L 2$ norm of the error with increasing mesh refinement. Convergence plots for the largest cross section ( $\sigma=10^{3} \mathrm{~cm}^{-1}$ ) are not shown here as they overlap with the $\kappa B_{z}=0$ case.

In each case, adding magnetic fields ( $\kappa B_{z}=10 \mathrm{~cm}^{-1}$ ) caused the error in the numerical solution to increase, the effect becoming progressively greater in materials with lower magnitude cross sections (i.e. $\sigma=10^{-3} \mathrm{~cm}^{-1}$ ). 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 Eq. 2.37) 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 (Eq. 4.51) in Figure 4.13, we extract the observed order of accuracy in the asymptotic limit of mesh refinement (Table 4.3).

Table 4.3: Calculated Order of Accuracy from MMS

| Basis function order | $\boldsymbol{\kappa}_{\boldsymbol{Z}}=\mathbf{0} \mathbf{c m}^{\mathbf{- 1}}$ | $\boldsymbol{\kappa} \boldsymbol{B}_{\mathbf{z}}=\mathbf{1 0} \mathbf{c m}^{\mathbf{- 1}}$ |  |  |
| :---: | :---: | :---: | :---: | :---: |
|  |  | $\boldsymbol{\sigma}=\mathbf{1 0}^{\mathbf{3}} \mathbf{c m}^{\mathbf{- 1}}$ | $\boldsymbol{\sigma}=\mathbf{1 0}^{\mathbf{0}} \mathbf{c m}^{\mathbf{- 1}}$ | $\boldsymbol{\sigma}=\mathbf{1 0}^{\mathbf{- 3}} \mathbf{c m}^{\mathbf{- 1}}$ |
| Linear $(p=1)$ | 1.99 | 1.94 | 1.99 | 1.89 |
| Quadratic $(p=2)$ | 2.98 | 2.93 | 3.05 | 3.05 |
| Cubic $(p=3)$ | 3.97 | 3.89 | 4.08 | 4.16 |

Order-of-accuracy is the most comprehensive and difficult verification criterion, encompassing all aspects of the code's mathematical methods and programming implementation ${ }^{3}$. 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 ${ }^{14}$.
From Table 4.3, it can be seen that even in strong magnetic fields with 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.

### 4.3.2 Impact of Angular Refinement on Dosimetric Accuracy

To assess the practical implications of angular discretization parameters in challenging dosimetric scenarios, the accuracy of our code was 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 (each occupying an octant), each characterizing a transport sweep ordering. Figure 4.14 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 4.14a shows the effect of angular mesh refinement ( $h$-refinement) for linear basis functions, and Figure 4.14b shows the effect of higher order basis functions ( $p$-refinement) for the minimum eight angular elements.


Figure 4.14: Depth dose and percent difference against reference Monte Carlo in a $10 \times 10 \times 10 \mathrm{~cm}^{3}$ 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.

As expected, increasing the number of angular elements leads to improved agreement with Monte Carlo, especially in the air and distal regions (Figure 4.14a), 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 4.14b). It was observed each angular $h$-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. In 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 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 that 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.

### 4.3.3 Validation against Monte Carlo

Further comparisons to Monte Carlo employed 32 quadratic elements in angle, hypothesized to be adequate for challenging radiotherapy cases.


Figure 4.15: 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 4.16: 2D coronal slice images for (a) Monte Carlo, (b) DFEM with 32 elements and quadratic basis functions, (c) gamma map at $2 \% / 2 \mathrm{~mm}$ criterion for $2 \times 2$ $\mathrm{cm}^{2}$ beam in 1.5 T parallel field.

The test case spanning Figures 4.15 and 4.16 was particularly challenging due to the small field size and configuration of inhomogeneities. Nevertheless, over $99.96 \%$ of points analyzed passed the $2 \% / 2 \mathrm{~mm}$ criterion while $96.22 \%$ passed the $1 \% / 1 \mathrm{~mm}$ criterion. A larger $10 \times 10 \mathrm{~cm}^{2}$ standard radiotherapy field size is tested on a larger phantom geometry also in the presence of a 1.5 T parallel magnetic field as shown in Figures 4.17-4.18.


Figure 4.17: Comparing the deterministic calculations using 32 angular elements with quadratic basis functions with Monte Carlo calculations for a large phantom in the presence of a 1.5 T parallel magnetic field, (a) depth dose, (b) cross-beam profiles taken halfway through the depth of each layer.


Figure 4.18: 2D coronal slice images for (a) Monte Carlo, (b) DFEM with 32 elements and quadratic basis functions, (c) gamma map at $2 \% / 2 \mathrm{~mm}$ criterion for $10 \times 10 \mathrm{~cm}^{2}$ beam in 1.5 T parallel magnetic field.

In this case, $99.97 \%(96.56 \%)$ of qualifying points passed a $2 \% / 2 \mathrm{~mm}(1 \% / 1 \mathrm{~mm})$ gamma criterion. The agreement achieved with 32 angular elements and quadratic basis functions is comparable to previously published results ${ }^{1}$ which utilized 520 linear elements on a flattened
angular domain. This represents a 12 -fold improvement of efficiency in the context of the current framework, made possible by an acyclic directed space-angle sweep graph along with higher order basis functions.

### 4.3.4 Simulation of Oblique Magnetic Field Orientations

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 4.19 presents the depth dose and profiles, while the 2D slice comparison is shown in Figure 4.20.


Figure 4.19: Comparing the deterministic solution using 32 angular elements with quadratic basis functions against reference Monte Carlo for a 1.5 T magnetic field oriented $\chi=37^{\circ}$ from the $z$-axis, (a) depth dose, (b) cross-beam profiles taken halfway through the depth of each layer.


Figure 4.20: 2D coronal slice images for a) Monte Carlo, b) DFEM with 32 elements and quadratic basis functions, c) gamma map at $2 \% / 2 \mathrm{~mm}$ criterion for $10 \times 10 \mathrm{~cm}^{2}$ beam in 1.5 T field oriented $37^{\circ}$ from the z -axis.

Gamma analysis for the rotated magnetic field calculation had over $99.42 \%$ ( $95.45 \%$ ) of points analyzed pass the $2 \% / 2 \mathrm{~mm}(1 \% / 1 \mathrm{~mm})$ 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, and requires minimal computational complexity to simulate oblique magnetic fields. The flattened angular domain used previously ${ }^{1}$ does not allow for a simple rotation of its angular elements due to the Cartesian nature of the flattened angular space. In this newly developed formalism (§4.2.8), the spatial meshing, element connectivities, and the transport sweep ordering remain unchanged for every orientation of magnetic field.

### 4.4 Conclusions

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 downwind contribution, and iteratively updating upwind 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 were 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.

Dosimetric results were validated against the Monte Carlo code GEANT4 for computationally challenging scenarios involving air and bone, in a strong 1.5 T magnetic field. With spatial elements on a Cartesian grid, and angular elements respecting octant boundaries on the unit sphere, an unambiguous transport 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 $2 \% / 2 \mathrm{~mm}(1 \% / 1 \mathrm{~mm})$ criterion for every case tested. Finally, a computationally efficient method to simulate oblique angles of magnetic field was
presented which does not require spatial re-meshing. These developments form important building blocks towards a fast, clinically feasible deterministic dose calculation in magnetic fields.

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# Chapter 5 Robust Framework for Energy-Adaptive Forward-Peaked Angular Meshing 

A version of this chapter has been published as a journal article:
R. Yang, D.M. Santos, B.G. Fallone, and J. St-Aubin, "Feasibility of energy adaptive angular meshing for perpendicular and parallel magnetic fields in a grid based Boltzmann solver, " Biomed. Phys. Eng. Express 6(2), 025006 (2020). DOI:10.1088/2057-1976/ab6e15.

### 5.1 Purpose and Hypothesis

The number of angular elements in a DFEM solution represents an overarching metric of computational complexity which governs the number of spatial transport sweeps required for each source iteration within an energy group. Having established conventions to ensure an acyclic directed sweep graph both in space and angle, the number of angular elements required is ultimately dictated by the need to model the intrinsic anisotropy in photon and electron fluence solutions for megavoltage radiotherapy. No longer needing 520 angular elements to mitigate upwind stabilization errors associated with unstructured tetrahedral elements in space, it was found 32 quadratic elements in angle was the minimum required to retain dosimetric accuracy across a range of challenging scenarios ${ }^{1}$. However, this was for a static isotropic mesh deployed across all energies. There is potential for significant further reduction by adapting to the energy dependent variation of fluence anisotropy. In particular, photon and electron scattering are known to be highly forward peaked at megavoltage energies.

The addition of magnetic fields complicates any adaptive angular meshing strategy. This work develops algorithmic underpinnings which enable forward-peaked adaptive angular meshing to be compatible with the angular advection of magnetic fields by communicating fluence between hemispheres having different elemental and basis function refinement. These new algorithms were developed to retain an acyclic space-angle sweep graph for oblique beam orientations. By elucidating the energy dependent anisotropy of electrons in parallel and perpendicular magnetic fields, appropriate adaptive meshing schemes were developed which greatly reduce numerical degrees of freedom and associated iterative calculations while preserving high dosimetric
accuracy as validated against the Monte Carlo research code GEANT4. Reduced problem complexity confers benefit independent of hardware platform or software implementation language, as novel algorithmic building blocks are applied to future MRIgRT frameworks.

### 5.2 Methods

### 5.2.1 Independent Meshing of Hemispheres and Transfer of Fluence

In anticipation of distinct solution anisotropy, different in the forward and back-scattering directions, we implement the flexibility to independently parameterize each hemisphere, both in the number of angular elements ( $h$-refinement) and the polynomial order of angular basis functions ( $p$-refinement). These conventions open the possibility of a forward-peaked angular mesh having greater refinement in the direction of the beam, as illustrated in Figure 5.1 for a beam in the -z direction, where $\theta$ is defined as the polar angle in the global coordinate system.


Figure 5.1: Schematic illustrating (a) $h$-refinement, responsible for the number of angular elements, (b) p-refinement, responsible for the polynomial order of basis function, and (c) flexibility to independently parameterize hemispheres with different $h$ and $p$ refinement, enabling a forward-peaked angular mesh, shown for a beam in the $-z$ direction. Conventions for the polar and azimuthal angles in the global coordinate system are shown alongside.

The inclusion of magnetic fields complicates any adaptive meshing strategy as the advection operator in angle requires fluence to be communicated between curvilinear elements on the sphere. Different meshing schemes in forward and backscattering hemispheres requires special
consideration in the context of angular DFEM to preserve upwind stabilization as well as an acyclic directed sweep graph both in space and angle.

Angular advection is characterized by the vector field $\vec{\tau}(\vec{B}, \hat{\Omega})$, which for arbitrary magnetic field configurations can lead to cyclic dependencies in the angular sweep graph. It has been shown that orienting the magnetic field along $z$ results in a purely azimuthal flow of $\vec{\tau}$, which can be realized for arbitrary magnetic field orientations through a coordinate transformation ${ }^{2}$ :

$$
\begin{equation*}
\vec{\tau}\left(\hat{\Omega}_{r}\right)=B_{z_{r}} \sin \left(\theta_{r}\right) \hat{\varphi}_{r} \tag{5.1}
\end{equation*}
$$

where the magnetic field is aligned to $z_{r}$ in the coordinate system where calculations are performed. By allowing the angular mesh to be rotated on the sphere's surface (§4.2.8) curvilinear edges may intersect this azimuthal flow at an arbitrary orientation, thus the need arises to transfer fluence between hemispheres having different $h$ and/or $p$ refinement.


Figure 5.2: An azimuthal magnetic field sweep vector $\vec{\tau}(\vec{B}, \hat{\Omega})$ (arrows) crosses the edge $A B$ between element $\{U\}$ in the upper hemisphere, and elements $\{L 1, L 2\}$ in the lower hemisphere.

As illustrated in Figure 5.2, the vector flow is seen to exit element $U$ of the upper hemisphere into element L1 of the lower hemisphere between points A and F, while the flow exits element L1 into element $U$ from $F$ to $M$. The vector flow from element $L 2$ enters element $U$ from $M$ to $B$. The integral along edge AB must be partitioned accordingly, with each piecewise segment coupled to the correct nodes for accurate upwind stabilization of the magnetic field operator. With respect to the upper hemisphere at source iteration $(t)$, this flow is captured by the equation:

$$
\begin{align*}
& \sum_{p} \psi_{p}^{U(t)} \int_{A}^{B} d l \gamma_{p}^{U}(\hat{\Omega}) \gamma_{q}^{U}(\hat{\Omega}) \vec{\tau}(\vec{B}, \hat{\Omega}) \cdot \hat{n}_{A B}^{U}(\hat{\Omega})= \\
& \sum_{p} \psi_{p}^{U(t)} \int_{A}^{F} d l \gamma_{p}^{U}(\hat{\Omega}) \gamma_{q}^{U}(\hat{\Omega}) \vec{\tau}(\vec{B}, \hat{\Omega}) \cdot \hat{n}_{A B}^{U}(\hat{\Omega})+\sum_{p} \psi_{p}^{U(t)} \int_{F}^{B} d l \gamma_{p}^{U}(\hat{\Omega}) \gamma_{q}^{U}(\hat{\Omega}) \vec{\tau}(\vec{B}, \hat{\Omega}) \cdot \hat{n}_{A B}^{U}(\hat{\Omega}) . \tag{5.2}
\end{align*}
$$

A segment is classified as downwind if $\vec{\tau}(\vec{B}, \hat{\Omega}) \cdot \hat{n}_{\text {edge segement }}^{\text {ang }}$ element $(\hat{\Omega})>0$, such as the outflow from element U along the boundary from A to F, given by the first term on the right hand size of Eq. 5.2. A segment is upwind if $\vec{\tau}(\vec{B}, \hat{\Omega}) \cdot \hat{n}_{\text {edge }}^{\text {angemement }}$ element $(\hat{\Omega})<0$, such as the inflow into element U along the boundary from F to B . This boundary is given by the second term on the right hand size of Eq. 5.2, which must be further partitioned and coupled to nodes solved in the previous iteration ( $t-1$ ) of the neighboring elements L1 and L2 as:

$$
\begin{align*}
& \sum_{p} \psi_{p}^{U(t)} \int_{F}^{B} d l \gamma_{p}^{U}(\hat{\Omega}) \gamma_{q}^{U}(\hat{\Omega}) \vec{\tau}(\vec{B}, \hat{\Omega}) \cdot \hat{n}_{A B}^{U}(\hat{\Omega})= \\
& \sum_{p} \psi_{p}^{L 1(t-1)} \int_{F}^{M} d l \gamma_{p}^{L 1}(\hat{\Omega}) \gamma_{q}^{U}(\hat{\Omega}) \vec{\tau}(\vec{B}, \hat{\Omega}) \cdot \hat{n}_{A B}^{U}(\hat{\Omega})  \tag{5.3}\\
& +\sum_{p} \psi_{p}^{L 2(t-1)} \int_{M}^{B} d l \gamma_{p}^{L 2}(\hat{\Omega}) \gamma_{q}^{U}(\hat{\Omega}) \vec{\tau}(\vec{B}, \hat{\Omega}) \cdot \hat{n}_{A B}^{U}(\hat{\Omega}) .
\end{align*}
$$

The edge normal in Eqs. 5.2-5.3 is formally defined as pointing outward from the edge of the receiving element while being tangent to the surface of the sphere,

$$
\begin{equation*}
\hat{n}_{\text {edge_ segment }}^{\text {ang element }}(\hat{\Omega})=\frac{d \vec{l} \times \hat{r}}{|d \vec{l} \times \hat{r}|}, \tag{5.4}
\end{equation*}
$$

where $d \vec{l}$ is the differential edge vector and $\hat{r}$ is the radial unit vector. The generality of this formalism enables coupling between elements having different $h$ and $p$ refinement over applicable edge regions. For a given angular mesh, these integrals can be pre-computed and coupled to each spatial elemental matrix through the Kronecker tensor product.

### 5.2.2 Cardinal Forward Peaked Mesh Orientations for Oblique Beams and Fields

The purpose of a forward-peaked mesh is to preferentially refine the angular resolution in the hemisphere containing greater solution anisotropy and/or contribution to scalar dose (usually the beam direction) while reducing unneeded degrees of freedom elsewhere. In the context of radiotherapy, where the beam can be directed at arbitrary angles, the refined hemisphere should ideally be aligned along the beam axis. However, arbitrary orientations of the angular mesh do not generally preserve alignment between its octant boundaries and planes of the underlying spatial Cartesian grid, the condition required for an acyclic directed spatial sweep graph, as shown in Chapter 4.

One option as depicted in Figure 5.3 is to redefine a spatial grid aligned to the arbitrary octant orientation of an oblique forward-peaked mesh. However, this would involve not only adjusting the boundaries of the spatial domain to accommodate the original geometry, but also resampling the underlying CT voxels at each oblique orientation, introducing angle specific partial volume errors near material boundaries which can be problematic when combining multiple beams.


Figure 5.3: Convention for (a) aligning apex of forward-peaked angular mesh towards oblique beam direction, and (b) required spatial regridding, where the original geometry is shown using solid lines, and new calculation grid shown using dotted lines, oriented to align with octant boundaries of the angular mesh.

Instead, a convention is established to restrict the orientation of forward-peaked angular meshes to cardinal angles, where its octant boundaries are fully aligned to the planes of the underlying Cartesian grid. Since angular mesh refinement is defined over an entire hemisphere, radiation
beam directions within $\pm 45^{\circ}$ of a cardinal orientation will still be directed within the refined hemisphere. Any gantry rotation of coplanar beam deliveries can be classified as within $\pm 45^{\circ}$ of the nearest cardinal forward peaked orientation (Figure 5.4a). For example, gantry angles between $315^{\circ}$ and $45^{\circ}$ would use the angular mesh configuration I in Figure 5.4a. Through this convention an acyclic directed spatial sweep graph is preserved without regridding the underlying geometry.


Figure 5.4: (a) Cardinal forward-peaked mesh orientations and their designated range of gantry angles, (b) representative coordinate transform of angular mesh and spatial voxels for parallel magnetic field from native coordinate system $\mathbb{S}$ to calculation coordinate system $\mathbb{S}_{\mathbf{r}}$.

For Linac-MR systems where the magnetic field orientation stays parallel to the beam central axis at each gantry angle $\left(\operatorname{Magnet} \tau_{\chi}\right.$ AuroraRT) ${ }^{3}$, reorientation of the magnetic field (shared with the beam axis) to point along $z_{r}$ in the calculation coordinate frame (Eq. 5.1) is accomplished through a coordinate transformation that rotates elements on the unit-sphere together with the spatial voxels (Figure 5.4b).

For systems which configure the magnetic field perpendicular to the radiation beam (Elekta Unity $^{4}$, Viewray MRIdian ${ }^{5}$ ), the forward-peaked meshes can use the convention shown in Figure 5.4 a , with the magnetic field initially in the $-x$ coordinate axis of $\mathbb{S}$, where an out-of-plane rotation of the angular mesh is performed about the $y$-axis such that the $B_{z_{r}}$ is obtained in $\mathbb{S}_{\mathrm{r}}$ as shown in Figure 5.5.


Figure 5.5: Transformation from native coordinate system $\mathbb{S}$ to calculation coordinate system $\mathbb{S}_{\mathbf{r}}$ for oblique beam angles in the presence of a perpendicular magnetic field directed towards $-x$.

### 5.2.3 Development and Validation of Energy Adaptive Schemes

Techniques in §5.2.1 and §5.2.2 enable the investigation of adaptive angular meshing schemes in the presence of magnetic fields, tailored to the observed anisotropy over each energy interval. A consistent reference frame is established with the beam oriented in the $-z$ direction, such that forward-scatter is modeled by the lower hemisphere ( $\pi / 2 \leq \theta \leq \pi$ ), and back-scatter modeled by the upper hemisphere $(0 \leq \theta<\pi / 2)$, where $\theta$ has been defined in Figure 5.1c. This enables systematic investigation and comparisons without loss of generality.

Starting with an isotropic mesh of 16 quadratic elements per hemisphere ( $h=1, p=1$ ) deployed across all energy intervals, validated to achieve high accuracy in dosimetrically challenging scenarios ${ }^{1}$, angular mesh coarsening was applied to a given hemisphere when the observed anisotropy over an energy interval exhibits the following conditions:
i) angular fluence in the hemisphere under consideration contributes an order of magnitude less than the opposing hemisphere to the overall fluence,
ii) angular fluence is nearly isotropic such that it does not vary significantly with polar angle $\theta$.

The accuracy of the resulting adaptive angular meshing schemes are validated against GEANT4 Monte Carlo calculations in the presence of clinical Linac-MR system configurations of 0.5 T parallel (AuroraRT) and 1.5 T perpendicular (Elekta Unity).

The first set of validation studies used slab geometry phantoms containing water ( $1.00 \mathrm{~g} / \mathrm{cm}^{3}$ ), cortical bone $\left(1.92 \mathrm{~g} / \mathrm{cm}^{3}\right)$, air $\left(0.0012 \mathrm{~g} / \mathrm{cm}^{3}\right)$ and $/$ or low density lung $\left(0.1 \mathrm{~g} / \mathrm{cm}^{3}\right)$. The phantoms were irradiated by a 6 MV polyenergetic point source spectrum ${ }^{6}$ at 100 cm source to surface distance (SSD). Robustness of cardinal forward-peaked meshing for oblique beam angles is validated on an anthropomorphic lung phantom (Figure 5.6). Three treatment beams were prescribed at 100 cm source to axis distance (SAD) with incident angles of $37^{\circ}, 90^{\circ}$, and $135^{\circ}$, each intersecting the refined hemisphere of their respective cardinal mesh (§5.2.2).

For deterministic calculations using our prototype GBBS, the finest grid size was allocated to regions of the beam ( $2.5 \times 2.5 \times 2.5 \mathrm{~mm}^{3}$ spatial elements) plus a 12 mm margin for the beam penumbra. Elsewhere, spatial elements were permitted to grow by factors of 2 to a maximum of $10 \times 10 \times 10 \mathrm{~mm}^{3}$. Raytracing was performed to node points within the beam using a first-scatter-distributed-source (FSDS) model.


Figure 5.6: Axial slice through an anthropomorphic phantom showing material geometries and the configuration of the three radiation beams.

Identical test geometries were replicated for GEANT4 Monte Carlo reference calculations ${ }^{7}$, using the physics list G4EmStandardPhysics_option3 with the production cutoff of secondary particles set to $8.75 \mu \mathrm{~m}$ providing fine resolution for deflection by magnetic fields. Dose is scored on a uniform $2.5 \times 2.5 \times 2.5 \mathrm{~mm}^{3}$ isotropic voxel grid. Each beam was simulated with
approximately 3 billion primary particle histories, for an approximate uncertainty within the beam of less than $0.1 \%$.

Both deterministic GBBS and Monte Carlo calculations were normalized to dose per fluence $\left(\mathrm{Gy} \cdot \mathrm{cm}^{2}\right)$ at isocenter and the resulting dose distributions were compared using 3D gamma analysis ${ }^{8}$ based on the global Van-Dyk criterion ${ }^{9}$ with a minimum dose threshold of $10 \%$ of the maximum dose ( $\mathrm{D}_{\max }$ ).

### 5.3 Results

### 5.3.1 Variation of Angular Fluence Anisotropy as a function of Energy and Magnetic Field Configuration



Figure 5.7: 3D polar plots showing converged angular fluence solution for photons (a-d) and electrons with no magnetic field (e-h) for a beam in the $-z$ direction in water at representative energies.

In the absence of magnetic fields, angular fluence of both photons (Figure 5.7a-d) and electrons (e-h) evolve from highly forward-peaked to nearly isotropic as energy decreases. Specifically, for photons $>250 \mathrm{keV}$ and electrons $>500 \mathrm{keV}$, the forward hemisphere contributes 1-2 orders of magnitude more to the total fluence while varying anisotropically by 1-2 orders of magnitude between $\theta=\pi / 2$ and $\theta=\pi$. At lower energies, the angular fluence becomes almost equally distributed between the hemispheres, exhibiting significantly less variation with $\theta$.


Figure 5.8: Calculated electron angular fluence in air, at 6 MeV for (a) no magnetic field, (b) 0.5 T parallel magnetic field, and (c) 1.5 T perpendicular magnetic field.

MRIgRT introduces a strong magnetic field having the potential to alter electron fluence distributions, especially in low density media. The behavior of electrons being confined to helical trajectories by a 0.5 T parallel magnetic field manifests in an electron phase-space distribution nearly identical to the case of no magnetic field, as shown in Figure 5.8b. The presence of a perpendicular magnetic field deflects electrons towards $\pi / 2$ in a manner consistent with the Lorentz force such that lower and upper hemispheres receive nearly equal contributions as shown in Figure 5.8c. These effects are most pronounced at high energies in low density media. As energy decreases, angular fluence becomes nearly isotropic regardless of magnetic field orientation.

### 5.3.2 Application of Forward-Peaked Adaptive Angular Meshing

Applying the principles for angular mesh adaptation (§5.2.3) to energy dependent anisotropy observed (§5.3.1), forward-peaked adaptive angular meshing schemes were developed for photons (Table 5.1) and electrons in a parallel magnetic field (Table 5.2). The notation for mesh parameterization indicates the number of angular elements allocated to the hemisphere (16 for $h=1 ; 4$ for $h=0$ ), followed by the angular basis function order (Linear for $p=0$; Quadratic for $p=1) . \mathrm{N}_{\mathrm{g}}$ indicates the number of multigroup intervals in each energy range.

Table 5.1: Forward-Peaked Adaptive Meshing Scheme applied to Photon Calculations

| Energy Range | $\mathbf{N}_{\mathbf{g}}$ | hemisphere |  |
| :---: | :---: | :---: | :---: |
|  |  | forward-scatter | back-scatter |
| 386 keV to 6 MeV | 14 | 16-Quadratic | 4-Linear |
| 172 keV to 386 keV | 4 | 16-Quadratic | 4- Quadratic |
| 10 keV to 172 keV | 6 | 4- Quadratic | 4- Quadratic |

Table 5.2: Forward-Peaked Adaptive Meshing Scheme applied to Electron Calculations in Parallel Magnetic Field

| Energy Range | $\mathbf{N}_{\mathbf{g}}$ | hemisphere |  |
| :---: | :---: | :---: | :---: |
|  |  | forward-scatter | back-scatter |
| 1.81 MeV to 6 MeV | 4 | 16- Quadratic | 4-Linear |
| 493 keV to 1.81 MeV | 4 | 16- Quadratic | 4- Quadratic |
| 10 keV to 493 keV | 12 | 4- Quadratic | 4- Quadratic |

Starting with a $10 \times 10 \mathrm{~cm}^{2}$ field on a heterogeneous slab phantom containing air in the presence of a 0.5 T parallel magnetic field, applying forward-peaked adaptive meshing for photons and electrons retained high accuracy, with $98.6 \%$ of points passing a stringent $1 \% / 1 \mathrm{~mm}$ gamma criterion, and $100 \%$ of points passing the $2 \% / 2 \mathrm{~mm}$ criterion (Figure 5.9).


Figure 5.9: Comparing deterministic forward-peaked adaptive solution against Monte Carlo in the presence of a 0.5 T parallel magnetic field, on a $30 \times 30 \times 30 \mathrm{~cm}^{3}$ heterogeneous slab phantom containing air: (a) depth dose, (b) crossplane beam profiles, and (c) gamma map for $1 \% / 1 \mathrm{~mm}$ criterion.

Likewise, a smaller $4 \times 4 \mathrm{~cm}^{2}$ field size incident on a phantom containing low density lung $\left(0.1 \mathrm{~g} / \mathrm{cm}^{3}\right)$, retained $98.8 \%$ of points passing a $1 \% / 1 \mathrm{~mm}$ gamma criterion, and $100 \%$ of points passing a $2 \% / 2 \mathrm{~mm}$ criterion (Figure 5.10).


Figure 5.10: Comparing deterministic forward-peaked adaptive solution against Monte Carlo in the presence of a 0.5 T parallel magnetic field on a $20 \times 20 \times 20 \mathrm{~cm}^{3}$ heterogeneous slab phantom containing low density lung $\left(0.1 \mathrm{~g} / \mathrm{cm}^{3}\right)$ : (a) depth dose, (b) crossplane beam profiles, and (c) gamma map for $1 \% / 1 \mathrm{~mm}$ criterion.

While achieving comparable accuracy to our previously benchmarked solution using a uniform $h=1, p=1$ refinement ( 32 quadratic elements across all energy intervals), forward-peaked adaptive meshing reduced the number of elements solved by 360 over the photon calculation and 384 over the electron calculation, where each element is associated with up to 50 transport sweeps across the entire spatial domain during Source Iteration (SI).

In the presence of perpendicular magnetic fields, applying forward-peaked adaptive meshing to electrons results in an under-dose compared to Monte Carlo throughout the region of low density lung (Figure 5.11). In this case, only $76.1 \%$ of qualifying points pass a $1 \% / 1 \mathrm{~mm}$ gamma criterion. However, reasonable agreement was achieved at $2 \% / 2 \mathrm{~mm}$ and $3 \% / 3 \mathrm{~mm}$ gamma criteria with $92.8 \%$ and $99.4 \%$ passing rates respectively.


Figure 5.11: Comparing deterministic forward-peaked adaptive solution against Monte Carlo in the presence of a 1.5 T perpendicular magnetic field, on a $20 \times 20 \times 20 \mathrm{~cm}^{3}$ heterogeneous slab phantom containing low density lung ( 0.1 $\mathrm{g} / \mathrm{cm}^{3}$ ): (a) comparison of depth dose, (b) crossplane beam profiles, and (c) gamma map for $1 \% / 1 \mathrm{~mm}$ criterion.

### 5.3.3 Application of Isotropic Adaptive Angular Meshing

In the presence of perpendicular magnetic fields, a forward-peaked adaptive meshing strategy sacrifices accuracy for a very stringent $1 \% / 1 \mathrm{~mm}$ gamma criterion as evidenced in the dosimetric result of Figure 5.11, due to altered electron anisotropy in low density media (Figure 5.8c). To regain accuracy at the $1 \% / 1 \mathrm{~mm}$ level, an isotropic adaptive meshing scheme was proposed for electrons in perpendicular magnetic fields by identifying the energy range where both hemispheres are highly anisotropic and contribute nearly equally to the total fluence (Table 5.3).

Table 5.3: Isotropic Adaptive Meshing Scheme applied to Electron Calculations in
Perpendicular Magnetic Field

| Energy Range | $\mathbf{N}_{\mathbf{g}}$ | hemisphere |  |
| :---: | :---: | :---: | :---: |
|  |  | forward-scatter | back-scatter |
| 683 keV to 6 MeV | 7 | 16-Quadratic | 16-Quadratic |
| 10 keV to 683 keV | 13 | 4-Quadratic | 4-Quadratic |

Applying the isotropic scheme recovers accuracy in low density lung (Figure 5.12), such that $97.4 \%$ of points passed a $1 \% / 1 \mathrm{~mm}$ gamma criterion, and $100 \%$ of points passed at $2 \% / 2 \mathrm{~mm}$. Compared to the uniform $h=1, p=1$ refinement of our previous work, the number of elements for the isotropic adaptive mesh was reduced by 312 over the electron calculation. Photon calculations unaffected by magnetic fields retained the forward-peaked meshing.


Figure 5.12: Comparing deterministic GBBS isotropic adaptive solution against Monte Carlo in the presence of 1.5 T perpendicular magnetic field on a $20 \times 20 \times 20 \mathrm{~cm}^{3}$ heterogeneous slab phantom containing low density lung: (a) depth dose, (b) crossplane beam profiles, and (c) gamma map for $1 \% / 1 \mathrm{~mm}$ criterion.

### 5.3.4 Application of Cardinal Forward-Peaked Meshes for Oblique Beams

Magnetic field calculations for the more general case of multiple oblique beams irradiating an anthropomorphic phantom require the cardinal forward-peaked formalism developed in §5.2.2. Using a forward-peaked adaptive mesh for both photons and electrons, Figure 5.13 compares the isodose contours and dose profiles where a 0.5 T magnetic field is parallel to each beam, associated to its nearest forward-peaked mesh. Overall, $97.9 \%$ of qualifying points passed a stringent $1 \% / 1 \mathrm{~mm}$ gamma criterion while $99.8 \%$ pass at $2 \% / 2 \mathrm{~mm}$. Even when a beam deviates $45^{\circ}$ from the apex of the forward hemisphere, accuracy is retained by using the appropriate cardinal mesh orientation.


Figure 5.13: Comparison between Monte Carlo and deterministic GBBS (forwardpeaked adaptive meshing scheme for electrons) on a multi-field plan for an anthropomorphic phantom in the presence of a 0.5 T magnetic field parallel to each beam, showing (a) isodose contours, (b) profile along $y$-axis through the isocenter.

Using a forward-peaked adaptive mesh in the presence of a perpendicular 1.5 T magnetic field, gamma pass rates achieved $79.8 \%, 98.5 \%$, and $99.7 \%$ at $1 \% / 1 \mathrm{~mm}, 2 \% / 2 \mathrm{~mm}$, and $3 \% / 3 \mathrm{~mm}$ respectively. Although the pass rates were substantially decreased at the $1 \% / 1 \mathrm{~mm}$ level, very high pass rates were achieved at the $2 \% / 2 \mathrm{~mm}$, and $3 \% / 3 \mathrm{~mm}$ level showing that a forward peaked mesh could still have utility for perpendicular magnetic fields.

Using the isotropic adaptive meshing scheme achieved pass rates of $97.3 \%$ at a $1 \% / 1 \mathrm{~mm}$ gamma criterion while $99.6 \%$ and $99.8 \%$ passed at $2 \% / 2 \mathrm{~mm} 3 \% / 3 \mathrm{~mm}$ respectively (Figure 5.14). Photons retained a forward-peaked cardinal adaptive mesh for these calculations.


Figure 5.14: Comparing deterministic GBBS (using isotropic adaptive meshing scheme for electrons) against Monte Carlo and on a multi-field plan of an anthropomorphic phantom in the presence of a 1.5 T magnetic field perpendicular to each beam, showing (a) isodose contours, (b) profile along y-axis through the isocenter.

### 5.4 Discussion

### 5.4.1 Utility of Meshing Schemes and Techniques Developed

Compared to classical Discrete Ordinates, DFEM in angle offers flexibility to independently mesh forward and backscattering hemispheres with different $h$ and $p$ order while maintaining an unconditionally stable solution in magnetic fields ${ }^{10}$, with significantly reduced ray-effect artifacts. However, the inclusion of magnetic fields within a deterministic framework complicates any adaptive meshing strategy. Specifically, angular advection introduced by the magnetic field operator needs to be communicated between curvilinear elements on the unitsphere following a vector field $\vec{\tau}(\vec{B}, \hat{\Omega})$, required to form an acyclic directed sweep graph in angle. For arbitrary magnetic fields this requires angular mesh elements to be rotated to obtain an azimuthal sweep ordering such that fluence may need to cross between hemispheres. Moreover, the requirement for an acyclic directed spatial sweep graph requires alignment between octant boundaries and faces of the spatial grid, preferably through a convention that does not require
regridding the underlying geometry. These issues pertaining to magnetic fields are addressed through the development of techniques to orchestrate angular advection between angular hemispheres having different mesh parameterization, and establishing cardinal forward-peaked mesh orientations such that any beam angle can be modeled using a forward-peaked formalism while preserving an acyclic spatial sweep graph without resampling the underlying geometry.

Principles for adaptive mesh coarsening in §5.2.3 establish guidelines to efficiently reduce computational degrees of freedom in accordance with the observed anisotropy in §5.3.1. Often, backscatter contributes negligibly to total fluence at high energies, allowing aggressive reduction to the minimum of $h=0$ and $p=0$ for the backscattering hemisphere at the highest energy intervals, while retaining $h=1$ and $p=1$ to model the high anisotropy in the hemisphere directed towards the beam (Row 1 of Tables 5.1 and 5.2). The exception arises with perpendicular magnetic fields which perturb electron fluence laterally, such that a high degree of anisotropy and equal contributions of both hemispheres to the total fluence must be resolved, hence $h=1$ and $p=1$ for both forward and backscatter at higher energies (Row 1 in Table 5.3). As energy decreases, the overarching shift to fluence becoming more isotropic allowed reduction to $h=0$ and $p=1$ for both hemispheres, which contributed nearly equally to total fluence. Compared to a static angular discretization using $h=1$ and $p=1$ (32 quadratic elements), a forward-peaked adaptive meshing scheme was developed suitable for parallel magnetic fields, with $>97 \%$ of points consistently passing a $1 \% / 1 \mathrm{~mm}$ gamma criterion while reducing the number of angular elements solved by $52.8 \%$. Applied to perpendicular magnetic fields, accuracy was affected in low density regions, but still achieved good pass rates at $2 \% / 2 \mathrm{~mm}$ and $3 \% / 3 \mathrm{~mm}$ gamma criteria. However, for the highest levels of accuracy, an isotropic adaptive scheme was developed for perpendicular magnetic fields with $>97 \%$ of points passing gamma $1 \% / 1 \mathrm{~mm}$ while reducing the number of angular elements solved by $47.7 \%$. Energy adaptive angular meshing confers tangible benefit independent of hardware platform or software implementation, by reducing the number of elements solved while retaining high accuracy, as enabled by techniques to be compatible with magnetic fields and oblique beams.

### 5.5 Conclusions

Algorithmic techniques and conventions developed in this work enabled forward-peaked angular meshing in the presence of angular advection of magnetic fields for a deterministic solution to the Linear Boltzmann Transport Equation. Based on the observed energy dependent anisotropy, forward-peaked and isotropic adaptive meshing schemes were developed. Using these respective schemes, both parallel and perpendicular magnetic fields retained close agreement with the GEant4 Monte Carlo calculations with $>97 \%$ passing rates at a stringent $1 \% / 1 \mathrm{~mm}$ gamma criterion while reducing the number of angular elements solved by $52.8 \%$ and $47.7 \%$ respectively. The angular meshing infrastructure and novel techniques for magnetic fields enabled significant reduction in overarching computational degrees of freedom, and contributes a key building block towards efficient deterministic dose calculation for MRI-guided radiotherapy.

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# Chapter 6 Efficient Framework for Transport Sweep and Patient Material Parameterization 

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R. Yang, D.M. Santos, B.G. Fallone, and J. St-Aubin, "A Novel Transport Sweep Architecture for Efficient Deterministic Patient Dose Calculations in MRI-guided Radiotherapy," Phys. Med.

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### 6.1 Purpose and Hypothesis

By far the most computationally intensive primitive in a space-angle DFEM solution to the LBTE with magnetic fields is the spatial transport sweep. Over the range of angles subtended by each angular element, this involves solving coupled elemental matrix systems (Figure 2.14) over the entire spatial domain (usually tens or hundreds of thousands of elements) in a sequence which respects spatial upwind dependencies (as illustrated in Figure 4.6). This process is repeated for every angular element to obtain an update to source iteration, which in the case of strong magnetic fields can take more than 50 iterations to converge. Source iteration is restarted for each multigroup energy.

Considering the fundamental and deeply nested way in which the spatial transport sweep plays a role in the solution process, developing an efficient architecture to orchestrate the transport sweep is hypothesized to have the greatest overall impact on solution efficiency, and thus feasibility of a space-angle DFEM grid based Boltzmann solver (GBBS) with magnetic fields for clinical MRIgRT applications.

An efficient operating paradigm is presented based on batched matrix-matrix multiplication on a limited set of discrete material densities specified by $k$-means clustering. Dose distributions calculated in the presence of clinical magnetic field configurations using the proposed transport sweep formalism are benchmarked against GEANT4 Monte Carlo calculations for a selection of anatomical sites including lung, liver, and brain.

Even with discrete material densities used in the transport sweep scatter calculations, accuracy is maintained by optimizing the material density assignments using $k$-means clustering, and by performing the primary photon fluence calculations (ray-tracing) using the underlying continuous density of the computed tomography (CT) image. In the presence of 0.5 T parallel and 1.5 T perpendicular magnetic fields, this approach demonstrates high levels of accuracy with gamma $2 \% / 2 \mathrm{~mm}(1 \% / 1 \mathrm{~mm})$ passing rates exceeding $99 \%(94 \%)$ across a range of anatomical sites compared to GEANT4 Monte Carlo dose calculations which used continuous densities.

This deterministic GBBS approach maintains unconditional stability, minimizes ray-effect artifacts, and benefits from no statistical uncertainty. Runtime on a non-parallelized Matlab implementation averaged 10 minutes per beam averaging 80,000 spatial elements, paving the way for future development based on this algorithmically efficient paradigm.

### 6.2 Methods

### 6.2.1 Transport Sweep by Batched Matrix-Matrix Multiplication

Having introduced a fully upwind stabilized space-angle DFEM elemental system of equations (Eq. 4.20), Schematic 2.1 is revised to incorporate the resultant sweep-solver architecture:
(a) For $g=1, . ., N_{g} \%$ outer loop over Multigroup energies
(b) While $\delta_{\text {resid }}^{t+1}>e p s \quad \%$ perform Source Iteration to update solution for index $t+1$
(c) For $S G_{\text {Ang }}=1, . ., N_{S G_{\text {Ang }}} \%$ iterate over angular sweep groups
(d) For $\operatorname{angElem}=\operatorname{angIdxGbl}\left(1, . ., N_{\operatorname{angElem}\left(S G_{\text {ang }}\right)}\right) \%$ iterate over angular elements of angular sweep group
(e) For $S G_{S p a}=1, . ., N_{S G_{S p a}(\text { angElem })} \%$ iterate over spatial sweep groups in direction of current angular element
(f) For $\operatorname{spaElem}=\operatorname{spaIdxGbl}\left(1, . ., N_{\left.\text {spaElem(SG } S_{\text {Spa }}\right)}\right) \%$ iterate over spatial elements belonging to spatial sweep group (g) Assemble elemental matrix $[A]_{g, e l_{s, a}}$ and elemental source $\vec{b}_{g, e l_{s, a}}^{(t)}$ (h) Solve the system and update corresponding entry in $\left[\vec{\psi}_{g}^{t}\right]_{g b l}$ for current $e l_{s}, e l_{a}$

Update $\left[\vec{\phi}_{g}^{t}\right]_{g b l}$ using $\left[\vec{\psi}_{g}^{t}\right]_{g b l}$, and evaluate $\delta_{\text {resid }}^{t}$ over the entire domain.
If $\delta_{\text {resid }}^{t} \leq e p s$, integrate $\left[\vec{\psi}_{g}^{t}\right]_{g b l}$ over angle, and store in $\left[\psi_{g, \text { converged }}\right]_{g b l}$
Obtain dose per fluence: $[D]_{g b l}=\sum_{g=1}^{G}\left[\sigma_{E D} / \rho\right]_{g b l} * *\left[\psi_{g, \text { converged }}\right]_{g b l}$

Schematic 6.1: Outline of numerical source-iteration sweep-solver scheme to converge on space-angle DFEM solution to angular fluence.

Steps (e-h) constitute the spatial transport sweep, where the most literal approach involves looping at runtime over each volume element in a spatial sweep group, to assemble and solve the respective space-angle elemental system of equations one at a time using direct methods (LU factorization), or iteratively (Gauss-Seidel or Jacobi). Such an approach would be extremely computationally intensive, though partially necessitated by the need to accommodate unique basis functions for each unstructured tetrahedral element.

Given the inherent regularity of discretization conventions developed in Chapter 4, many of the spatial and angular integrals can be pre-calculated and applied to larger subsets of the domain. Specifically, a Cartesian grid of hexahedral voxels aligned to octant boundaries of an angular mesh on the unit-sphere, results in the space-angle matrix $[A]_{g, e l_{s, a}}$ being identical when sweeping in the direction of a given angular element, apart from the material assigned to each voxel, and its edge dimension. Typically only 3 to 4 discrete voxel dimensions exist for a given geometry, permitted to vary by factors of 2 (for example $2.5 \mathrm{~mm}, 5 \mathrm{~mm}, 10 \mathrm{~mm}$ ). For simplicity, though without loss of generality, we assume all voxels to have the same dimension, and focus on parameterization of material, which has a greater potential variability.

A material is formally specified by its atomic composition and mass density. For the transport sweep matrix $[A]_{g, e l_{s, a}}$, the only variability between voxels is the total removal cross section $\sigma_{T, g}\left(e l_{s}\right)$. Likewise, assembly of the right hand side is only affected by the differential cross section term $\sigma_{s, g \rightarrow g, l}\left(e l_{s}\right)$. Solving on a phantom comprising a small number of discrete materials (in the extreme case composed uniformly of water), this elucidates redundancies in looping over each spatial element one at a time. For example, when solving in a phantom of pure water, every system matrix in Schematic 6.1(f) is identical, therefore so is its inverse $[A]_{g, l_{s, a}}^{-1}$.

Considering the solution for one element can be written as pre-multiplying the right hand side vector by the inverse of the transport matrix:

$$
\begin{equation*}
\psi_{i}=\boldsymbol{A}^{-1} b_{i}, \tag{6.1}
\end{equation*}
$$

the solution over multiple elements given the same transport sweep can be generalized as matrixmatrix multiplication:

$$
\begin{equation*}
\left[\vec{\psi}_{1}, \vec{\psi}_{2}, . ., \vec{\psi}_{N_{\text {bact }}}\right]=\boldsymbol{A}^{-1}\left[\vec{b}_{1}, \vec{b}_{2}, \ldots, \vec{b}_{N_{\text {bacth }}}\right], \tag{6.2}
\end{equation*}
$$

where $N_{\text {batch }}$ is the number of voxels in a sweep group having the same voxel dimensions and material composition. Complexity is therefore reduced from solving $N_{\text {batch }}$ systems of linear equations, to performing a single matrix-matrix multiplication, the latter being an efficient BLAS operation, vectorized on all modern microprocessors ${ }^{1}$.

Moreover, a limited number of matrix inverses can be rapidly pre-computed before runtime, and stored, given sufficiently constrained discrete parameterizations over (i) energy groups, (ii) voxel sizes, (iii) angular elements, and (iv) materials (composition and mass density). Typical parameters during early development on slab phantoms involved 52 energy groups, 3 voxel refinements, 32 angular element, and 4 materials (water, air, bone, lung). This resulted in just under 20,000 unique elemental matrices which were collectively assembled and pre-inverted in less than 5 seconds prior to runtime.

### 6.2.2 Conditioning and Stability of Transport-Sweep Matrix Inversion

An important consideration when working with matrix inverses is the condition number,

$$
\begin{equation*}
\kappa(\boldsymbol{A})=\|\boldsymbol{A}\| \cdot\left\|\boldsymbol{A}^{-1}\right\|, \tag{6.3}
\end{equation*}
$$

which estimates the upper bounds of numerical error incurred during its inversion ${ }^{2}$, with the implication that:

$$
\begin{equation*}
\frac{\left\|(A+\Delta \boldsymbol{A})^{-1}-\boldsymbol{A}^{-1}\right\|}{\left\|\boldsymbol{A}^{-1}\right\|} \leq \kappa(\boldsymbol{A}) \frac{\|\Delta \boldsymbol{A}\|}{\|\boldsymbol{A}\|} . \tag{6.4}
\end{equation*}
$$

A condition number of 1 is ideal, but never realized for real problems. Over the range of materials (air to cortical bone), angular discretizations (4-linear to 16-quadratic elements per hemisphere), energy intervals ( 10 keV to 6 MeV ), and magnetic field configurations ( 0.5 T parallel or 1.5 T perpendicular) investigated in this work, the highest condition number observed
for a transport sweep matrix was 868 . The lowest was 55 , while most condition numbers ranged between 200 and 500 .

Assuming every matrix element is subject to roundoff error on the order of machine precision $e p s \approx 2.2 \cdot 10^{-16}$,

$$
\begin{equation*}
\|\Delta \boldsymbol{A}\| \approx \sqrt{\left(e p s \cdot A_{11}\right)^{2}+\left(e p s \cdot A_{12}\right)^{2}+. .+\left(e p s \cdot A_{N N}\right)^{2}}=\sqrt{N^{2} \cdot e p s^{2} \cdot\left(A_{11}{ }^{2}+A_{12}{ }^{2}+. .+A_{N N}{ }^{2}\right)}=N \cdot e p s \cdot\|\boldsymbol{A}\|, \tag{6.5}
\end{equation*}
$$

where the transport sweep matrix has dimension $N=48$. Therefore, the estimated upper-bound relative error of the matrix inverse for the worst-case conditioning is approximately $9.25 \cdot 10^{-12}$, or 1 part in 100 billion. Overall, conditioning was not a limiting factor to numerical precision in our problem, and all transport sweep matrices were inverted without issue. Having far greater impact on $\|\Delta \boldsymbol{A}\|$ and overall accuracy of the solution is how a set of discrete bulk densities is chosen to model the underlying continuum of materials.

Independent of discretization errors in modeling the physics, or numerical errors in matrix inversion, Source Iteration with DFEM in angle has been shown to be unconditionally stable ${ }^{3}$. Factors detrimental to the rate of convergence, including increased magnetic field strength and low density media, were uncorrelated with condition number. The classical interpretation that $\kappa(\boldsymbol{A}) \approx 10^{c}$ results in a maximum loss of $c$ digits of precision ${ }^{4}$ relative to machine $e p s \approx 2.2 \cdot 10^{-16}$, would not impact the convergence of Source Iteration, which required a relative precision of $10^{-4}$ in its stop-criterion.

### 6.2.3 Hierarchical Batched Assembly of Source Vectors

Likewise, the principle of batched matrix multiplication can be used to orchestrate assembly of the source vector in a far more efficient manner than calculating $\vec{b}_{g, e l_{s, a}}^{(t)}$ at the inner-most level of the transport sweep, as implied in step $(\mathrm{g})$ of Schematic 6.1.

Revisiting terms comprising the right hand side of the elemental DFEM equations (Eq. 6.6) reveals a hierarchy of dependencies, around which calculations can be efficiently structured at distinct levels of granularity:

$$
\begin{align*}
& \underbrace{\sum_{g^{\prime}=1}^{g} \sum_{l=0}^{L} \sum_{m=-l}^{l} \sum_{i=1}^{I}\left(\phi_{F S S S, g^{\prime}, l, m, i}+\phi_{g^{\prime}, l m, i}\right) \sigma_{s, g^{\prime} \rightarrow g, l}\left(e l_{s}\right) \int_{\Omega_{\alpha}} d \hat{\Omega} Y_{l, m}(\hat{\Omega}) \gamma_{q}(\hat{\Omega}) \int_{V^{e}} d V \lambda_{i}(\vec{r}) \lambda_{j}(\vec{r})}_{\text {raytraing and downscater componenst, remaining unchanged during surce ieration }} \\
& +\underbrace{\sum_{l=0}^{L} \sum_{m=-l}^{l} \sum_{i=1}^{I} \phi_{g, l, m, i}^{(t)} \sigma_{s, g \rightarrow g, l}\left(e l_{s}\right) \int_{\Omega_{\Omega_{d}}} d \hat{\Omega} Y_{l, m}(\hat{\Omega}) \gamma_{q}(\hat{\Omega}) \int_{V^{e}} d V \lambda_{i}(\vec{r}) \lambda_{j}(\vec{r})}_{\text {incenter component }} \\
& \text { inscatter component, unchanged during transport sweep } \tag{6.6}
\end{align*}
$$

For example, raytracing and downscatter components (first term in Eq. 6.6) can be calculated once over the entire domain at the start of each energy group, remaining unchanged during source iteration. Inscatter contributions (second term in Eq. 6.6) can also be updated for the entire domain every source iteration, instead of during the transport sweep. Upwind boundaries in space and angle (terms 3 and 4 of Eq. 6.6) are the only contributions which need to be operated at the finest level of granularity, per sweep group, to ensure coupling from dependent elements. The revised solution flow becomes:
(a) For $g=1, . ., N_{g} \%$ outer loop over Multigroup energies
(a.1.i) Generate static source repository for downscatter and raytracing over entire domain, batched per material: For matIdx $=1, .$. , Nmat generate:

$$
\boldsymbol{S}_{D S, F S D S, g}^{\text {mattdx }}=\sum_{g^{\prime}=1}^{g} \sum_{l=0}^{L} \sum_{m=-l}^{l} \sum_{i=1}^{I}\left(\phi_{i, l m, g^{\prime}}^{\text {converged,mattdx }}+\phi_{i, m m, g^{\prime}}^{F S D s_{s}} \text { surce,matldx }\right) \lambda_{i}(\vec{r}) \sigma_{S, l, g^{\prime} \rightarrow g}\left(e l_{s}\right) Y_{l m}(\hat{\Omega})
$$

(b) While $\delta_{\text {resid }}^{t}>e p s$ \% source iteration (index $t$ )
(b.1.i) Calculate contribution from source iteration:
$\boldsymbol{S}_{S I, g}^{m a t I d x, t}=\sum_{l=0}^{L} \sum_{m=-l}^{l} \sum_{i=1}^{I} \phi_{i, l m, g}^{m a t d x, t} \lambda_{i}(\vec{r}) \sigma_{S, l, g \rightarrow g}\left(e l_{s}\right) Y_{l m}(\hat{\Omega})$
$\left(\right.$ Where $\phi_{i, m, g}^{\text {matldx }, t}(\vec{r})=\sum_{e l_{a}=1}^{\text {NangElem }} \sum_{p=1}^{P} \int d \hat{\Omega}_{e l l_{a}} \psi_{i, p, g}^{\text {matd }, t-1} \gamma_{p}(\hat{\Omega}) Y_{l m}(\hat{\Omega})$ )

Form global repository $\boldsymbol{S}_{\Sigma, g}^{m a t I d x, t}=\boldsymbol{S}_{D S, F S D S, g}^{m a t I d x}+\boldsymbol{S}_{S I, g}^{m a t I d x, t}$ (total right hand side contribution excluding upwind nodes of transport sweep)
(c) For $S G_{\text {Ang }}=1, . ., N_{S G_{A n g}} \%$ iterate over angular sweep groups
(d) For $e l_{a}=\operatorname{angIdx} \operatorname{Gbl}\left(1, . ., N_{\operatorname{angElem}\left(S G_{\text {Ang }}\right)}\right) \%$ iterate over elements of angular sweep group
(e) For $S G_{S p a}=1, . ., N_{S G_{S p a}\left(e l_{a}\right)} \%$ iterate over spatial sweep groups in direction of angular element (e.1.i) Gather \& operate on upwind fluence contributions in space (and angle if magnetic field present) for all members in a sweep group as a batched process
(f) For matIdx $=1, . .$, Nmat
(f.1.i) Fetch relevant addresses of right-hand-side vectors in $\boldsymbol{S}_{\Sigma, g}^{\text {matddx,t }}$ containing raytracing, downscatter, and inscatter; append by upwind space-angle flux contributions into a matrix of concatenated column vectors $\left[\vec{b}_{1}, \vec{b}_{2}, . ., \vec{b}_{N_{\text {batch }}}\right]$ (f.1.ii) Perform matrix-matrix multiplication over the batch

$$
\left[\vec{\psi}_{1}, \vec{\psi}_{2}, . ., \vec{\psi}_{N_{\text {batch }}}\right]=\boldsymbol{A}^{-1}\left[\vec{b}_{1}, \vec{b}_{2}, . ., \vec{b}_{N_{\text {batch }}}\right] \text {, updating respective entries in }\left[\vec{\psi}_{g}^{t}\right]_{g b l}
$$

(b.0.i) Update $\left[\vec{\phi}_{g}^{t}\right]_{g b l}$ using $\left[\vec{\psi}_{g}^{t}\right]_{g b l}$, and evaluate $\delta_{r e s i d}^{t}$ over the entire domain

If $\delta_{\text {resid }}^{t} \leq e p s$, integrate $\left[\vec{\psi}_{g}^{t}\right]_{g b l}$ over angle, and store in $\left[\psi_{g, \text { converged }}\right]_{g b l}$
(a.0.i) Obtain dose per fluence: $[D]_{g b l}=\sum_{g=1}^{G}\left[\sigma_{E D} / \rho\right]_{g b l} *\left[\psi_{g, \text { converged }}\right]_{g b l}$

Schematic 6.2: Revised solution flow for efficient source vector assembly and transport sweep.

### 6.2.4 $k$-means Parameterized Discrete Density Assignment from CT Data

A discrete material is formally defined by its atomic composition and mass density, from which the total cross section $\sigma_{T}$, and differential scattering cross section $\sigma_{s}$ can be specified. To assign a material to each spatial element from the patient CT scans, a calibration curve is generated between measured Hounsfield Units and known mass density (Figure 6.1). Once a density value is obtained from the calibration curve, material composition of an element is classified based on the density ranges in Table 6.1.


Figure 6.1: HU to mass density calibration curve.

Table 6.1: Density limits parameterized to each material composition

| Material <br> Composition |  | Density $\left(\mathbf{g} / \mathbf{c m}^{\mathbf{3}}\right)$ |  |  |
| :---: | :---: | :---: | :---: | :---: |
|  | $\mathbf{Z}_{\text {eff }}$ | $\mathbf{m i n}$ | $\max$ | range |
| Air | 7.66 | 0.00 | 0.005 | 0.005 |
| Lung | 7.75 | 0.005 | 0.65 | 0.645 |
| Adipose | 6.47 | 0.65 | 0.95 | 0.30 |
| Muscle | 7.72 | 0.95 | 1.10 | 0.15 |
| Cartilage | 8.16 | 1.10 | 1.25 | 0.15 |
| Bone | 13.18 | 1.25 | 3.00 | 1.75 |

The exact demarcation between materials in Table 1 does not have a significant impact on cross section values, which vary primarily as a function of mass density as opposed to atomic composition (Figure 6.2). This is evident for both the macroscopic total cross section (Figure $6.2 \mathrm{a}, \mathrm{b}$ ) and restricted stopping power in the CSD operator (Figure 6.2c,d). Both scale in proportion with mass density, which is responsible for the three orders of magnitude span between air and bone (Figure $6.2 \mathrm{a}, \mathrm{c}$ ). When normalized to the same density $1 \mathrm{~g} / \mathrm{cm}^{3}$, the maximum variation between different compositions is less than $5 \%$ for the total cross section (Figure 6.2b), and less than $8 \%$ for the restricted stopping power (Figure 6.2d).


Figure 6.2: Macroscopic total cross section as a function of energy for physiological materials, (a) at typical mass density within patient, (b) normalized to mass density at $1 \mathrm{~g} / \mathrm{cm}^{3}$. Restricted stopping power, (c) at typical mass density within patient, (d) normalized to mass density at $1 \mathrm{~g} / \mathrm{cm}^{3}$.

To investigate the impact of selecting a limited number of material densities in our deterministic calculation, different conventions to parameterize discrete density subintervals were dosimetrically benchmarked on patient cases against Monte Carlo calculations parameterized using a continuous density. Specifically, each CT scan was re-gridded onto a $2.5 \times 2.5 \times 2.5 \mathrm{~mm}^{3}$ calculation grid, where the underlying HU within each grid element was sampled at 0.5 mm resolution, averaged, and rounded to the nearest 5 HU to account for partial volume uncertainties and noise in the CT scan. This provided an effective mass-density resolution of $\pm 0.005 \mathrm{~g} / \mathrm{cm}^{3}$, hereafter referred to as continuous for all practical purposes.

For a given histogram of mass densities, the task of optimally allocating $k$ subintervals can be cast as a 1D $k$-means clustering problem ${ }^{5}$, where the density of each spatial element $x_{i}$ gets
associated with the nearest discrete density centroid $c_{k}$ based on the minimum squared Euclidean distance. By iteratively adjusting the placement of the $k$ centroids, total within-cluster sum-of-squares (WCSS) in Eq. 6.7 is minimized over all clusters:

$$
\begin{equation*}
W C S S=\sum_{k=1}^{N_{k}} \sum_{i=1}^{N_{i(k)}}\left(x_{i}-c_{k}\right)^{2} . \tag{6.7}
\end{equation*}
$$

The number of material density intervals $N_{k}$ must be specified a priori. Tradeoffs between reducing the number of clusters while maximizing the dosimetric accuracy are investigated to determine the appropriate conventions for a range of patient CT scans. As shown in Figure 6.2, cross section values scale in proportion to mass density, and are less sensitive to atomic composition, for which the density demarcations in Table 6.1 serve to parameterize the material based on its central density determined by $k$-means. In general, $k$-means considers the entire density distribution, not constrained by atomic composition boundaries, empowering flexibility to mediate the most efficient placement of centroids. Often this manifests in (i) narrow clusters containing a large number of elements, such that none deviate too far from it central density, and (ii) clusters encompassing a wide range of densities containing relatively few elements. Given limited degrees of freedom, the overall dosimetric impact of bulk density assignment is minimized through $k$-means.

In anticipation of regions where dose is more sensitive to accurate parameterization of density, such as lung and adipose, provisions for constrained $k$-means can enforce more clusters to be allocated to specific density ranges, for example lung and adipose, which are lower density, and span a larger range.

### 6.2.5 Hybrid Approach to Treatment of Primaries and Scatter

The deterministic calculation utilizes a hybrid approach, where continuous density parameterization is used to ray-trace the primary fluence, while discrete bulk densities are used for the iterative in-scatter calculations. This separation in the treatment of primaries and scatter enables the deterministic framework to preserve as much of the underlying physics properties for the one-time raytracing of primary fluence, while in-scatter calculations, requiring the
computationally intensive transport sweep, can proceed efficiently by approximating with bulk material densities allowing batched matrix-matrix multiplication (§6.2.1).

### 6.2.6 Validation on Patient Cases

As part of an institutional review board (IRB) approved study, anonymized CT scans were exported from the Eclipse radiotherapy planning system at the Cross Cancer Institute for anatomical sites of lung, liver, and brain. Specifically chosen were patients having lower density lung (mean lung density $\bar{\rho}_{\text {lung }}=0.118 \mathrm{~g} / \mathrm{cm}^{3}$ ) and higher density lung ( $\bar{\rho}_{\text {lung }}=0.246 \mathrm{~g} / \mathrm{cm}^{3}$ ) to validate the robustness of the deterministic approach. For each patient, three oblique beams (between $2.8 \times 2.8 \mathrm{~cm}^{2}$ and $4.0 \times 4.0 \mathrm{~cm}^{2}$ ) were prescribed to intersect plan isocenter at 100 cm SAD and cover the target.

Monte Carlo calculations in GEANT4 ${ }^{6}$ are parameterized with continuous densities as described in §6.2.4, and launched with approximately 3 billion histories per beam, for a statistical uncertainty of $<0.1 \%$. The physics list G4EmStandardPhysics_option3 was chosen with a secondary production cutoff set at $8.75 \mu \mathrm{~m}$.

Bulk materials for the deterministic calculation were parameterized following the $k$-means conventions in $\S 6.2 .4$. The spatial elements were defined with a resolution of $2.5 \times 2.5 \times 2.5 \mathrm{~mm}^{3}$ in the beam and extending 12 mm beyond the field size. Elsewhere, spatial elements were permitted to grow by factors of two up to $10 \times 10 \times 10 \mathrm{~mm}^{3}$ to minimize spatial degrees of freedom in the transport sweep.

Angular meshing utilized a forward-peaked or isotropic energy-adaptive strategy based on magnetic field configuration ${ }^{7}$. The multigroup energy discretization consisted of 24 photon and 20 electron groups, using $\mathrm{CEPXS}^{8}$ to generate macroscopic interaction cross sections for each material composition normalized to $1 \mathrm{~g} / \mathrm{cm}^{3}$ and scaled at runtime to the mass density parameterized to the spatial element.

Dose distributions generated by the two formalisms were compared by 3D gamma analysis ${ }^{9}$ using Monte Carlo voxel centroids as a reference grid, for points exceeding $10 \%$ of the maximum dose and evaluated at a $1 \% / 1 \mathrm{~mm}$ and $2 \% / 2 \mathrm{~mm}$ criterion using the global Van-Dyk
criterion ${ }^{10}$. Each DFEM spatial element, with eight degrees of freedom, was interpolated onto a 0.1 mm search grid in the gamma calculations. For each dose calculation, magnetic field configurations of 0.5 T parallel and 1.5 T perpendicular were investigated, corresponding to clinical systems of the Magnet $\tau_{\chi}$ AuroraRT ${ }^{11}$ and Elekta Unity ${ }^{12}$ MRI-linacs. Calculations were performed on a prototype non-parallelized implementation in MATLAB ${ }^{13}$, with runtimes determined on an Intel i7-6700K workstation.

### 6.3 Results

### 6.3.1 k-means Parameterizations of Density Distributions

Material density distributions for three anatomical sites are shown in Figure 6.4. Since the material density distributions have the largest impact on dose within the primary radiation field, the application of $k$-means focused on optimizing the density selections for elements contained within the beam and penumbra as defined by the primary ray-trace photon radiation field plus a 12 mm margin.

It was found for anatomical sites containing significant proportions of lung, additional discrete density intervals were required to accurately model dose. This is due to the longer particle path lengths in low density media increasing the effect of the magnetic fields. Assigning a single bulk density for the entire range $\left(0.05-0.65 \mathrm{~g} / \mathrm{cm}^{3}\right)$ yielded poor gamma passing rates relative to Monte Carlo parameterized with continuous density (Figure 6.3a). Increasing to four uniform sub-intervals reduced dose discrepancies leading to improved gamma (Figure 6.3b) since each spatial element is assigned a discrete density much closer to its true value. Furthermore, introducing $k$-means offers the flexibility to adapt the centroids and widths of these four intervals tailored to the underlying density distribution. This resulted in even greater accuracy (Figure 6.3 c ) with the same computational complexity. Across different lung patients and beam configurations, four discrete $k$-means densities in the range $\left(0.05-0.65 \mathrm{~g} / \mathrm{cm}^{3}\right)$ as shown in Table 6.2 was found to be sufficient achieve very high accuracy, while reducing computational complexity and runtimes.


Figure 6.3: Distribution of $1 \% / 1 \mathrm{~mm}$ gamma results for elements in the lung region using different lung density subinterval schemes. (a) single bulk density for all lung, (b) four uniformly spaced subintervals, (c) four subintervals specified by $k$-means.

For anatomical sites of brain and liver, where the vast majority of spatial elements are clustered near $1 \mathrm{~g} / \mathrm{cm}^{3}$ (Figure $6.4 \mathrm{c}, \mathrm{d}$ ), the entire density range ( $0.05-3 \mathrm{~g} / \mathrm{cm}^{3}$ ) was parameterized using four $k$-means densities (Table 6.3), found to be sufficient to achieve good accuracy against the continuous density Monte Carlo calculation. A large number of elements will be assigned to a narrow cluster close to $1 \mathrm{~g} / \mathrm{cm}^{3}$, while other ranges comprising a lesser proportion of total elements in the beam are parameterized into clusters encompassing a wider spread of densities, because these have less relative contribution to the total error.

A patient is classified as including lung if over $25 \%$ of elements fall within the range $(0.05-$ $0.65 \mathrm{~g} / \mathrm{cm}^{3}$ ), to determine if conventions are applied according to Table 6.2 or Table 6.3. $k$-means is run 50 times with random initialization. The converged centroids are averaged over the 50 runs to provide high quality seeds to a final run to discretize the material distribution. In this way, the centroids stabilize to the same values for the same patient each time, in keeping with a deterministic formalism. The total runtime for all executions of $k$-means on a typical patient is less than 1 second.

Table 6.2: $k$-means conventions for anatomical sites including lung

| Composition | Density $\left(\mathrm{g} / \mathbf{c m}^{\mathbf{3}}\right)$ |  | $\mathbf{N}_{\mathrm{k}}$ |
| :---: | :---: | :---: | :---: |
|  | $\min$ | $\max$ |  |
| Air | 0.00 | 0.005 | 1 |
| Lung | 0.005 | 0.65 | 4 |
| Adipose | 0.65 | 0.95 | 2 |
| Muscle | 0.95 | 1.10 | 2 |
| Cartilage | 1.10 | 1.25 |  |
| Bone | 1.25 | 3.00 | 1 |

Table 6.3: $k$-means conventions for anatomical sites excluding lung (e.g. brain, liver)

| Composition | Density $\left(\mathbf{g} / \mathbf{c m}^{\mathbf{3}}\right)$ |  | $\mathbf{N}_{\mathrm{k}}$ |
| :---: | :---: | :---: | :---: |
|  | $\mathbf{m i n}$ | $\mathbf{m a x}$ |  |
| Air | 0.00 | 0.005 | 1 |
| Lung | 0.005 | 0.65 |  |
| Adipose | 0.65 | 0.95 | 4 |
| Muscle | 0.95 | 1.10 |  |
| Cartilage | 1.10 | 1.25 |  |
| Bone | 1.25 | 3.00 |  |

Figure 6.4 shows examples of density discretization following the conventions of Tables 6.2 and 6.3. By applying $k$-means in a patient-specific manner, the center and width of discrete density bins is adjusted to accommodate anatomical differences for example between patients having higher and lower lung densities (Figure 6.4a,b).


Figure 6.4: k-means discretization applied to density distributions at anatomical sites of (a) high density lung $\bar{\rho}_{\text {lung }}=0.246 \mathrm{~g} / \mathrm{cm}^{3}$, (b) low density lung $\bar{\rho}_{\text {lung }}=0.118 \mathrm{~g} / \mathrm{cm}^{3}$, (c) brain, and (d) liver.

### 6.3.2 Dosimetric Validation of Patient Cases against Monte Carlo

The Deterministic GBBS and GEANT4 Monte Carlo calculated dose distributions are compared in the presence of both 0.5 T parallel and 1.5 T perpendicular magnetic field configurations for three anatomical sites: lung (Figures 6.5-6.7), brain (Figures 6.8-6.9), and liver (Figures 6.106.11). All Monte Carlo voxels were parameterized with continuous mass density (to nearest 5 HU ), representing the full underlying CT data, while deterministic GBBS calculations employed a hybrid approach (§6.2.5) using continuous CT density raytracing with $k$-means to parameterize discrete density intervals (Tables 6.2 and 6.3) for scatter calculations. Average runtime per beam, average spatial elements per beam, and overall gamma are summarized in Table 6.4.


Figure 6.5: Lung Patient 1. Isodose contours comparing deterministic GBBS against GEANT4 Monte Carlo dose calculations for a three-beam lung treatment plan ( $\bar{\rho}_{\text {lung }}=0.246 \mathrm{~g} / \mathrm{cm}^{3}$ ) for axial, coronal, and sagittal slices through isocenter, as well as a dose profile along the $y$-axis through isocenter, in the presence of (a) $\mathrm{B}_{0}=0.5 \mathrm{~T}$ parallel, (b) $\mathrm{B}_{0}=1.5 \mathrm{~T}$ perpendicular.


Figure 6.6: Lung Patient 2. Isodose contours comparing deterministic GBBS against GEANT4 Monte Carlo dose calculations for a three-beam lung treatment plan ( $\left.\bar{\rho}_{\text {lung }}=0.188 \mathrm{~g} / \mathrm{cm}^{3}\right)$ for axial, coronal, and sagittal slices through isocenter, as well as a dose profile along the y -axis through isocenter, in the presence of (a) $\mathrm{B}_{0}=0.5 \mathrm{~T}$ parallel, (b) $\mathrm{B}_{0}=1.5 \mathrm{~T}$ perpendicular.


Figure 6.7: Lung Patient 3. Isodose contours comparing deterministic GBBS against GEANT4 Monte Carlo dose calculations for a three-beam lung treatment plan ( $\bar{\rho}_{\text {lung }}=0.118 \mathrm{~g} / \mathrm{cm}^{3}$ ) for axial, coronal, and sagittal slices through isocenter, as well as a dose profile along the $y$-axis through isocenter, in the presence of (a) $\mathrm{B}_{0}=0.5 \mathrm{~T}$ parallel, (b) $\mathrm{B}_{0}=1.5 \mathrm{~T}$ perpendicular.


Figure 6.8: Brain Patient 1. Isodose contours comparing deterministic GBBS against GEANT4 Monte Carlo calculations for a three-beam brain treatment plan, showing axial, coronal, and sagittal slices through isocenter, as well as a dose profile along the y-axis through isocenter, in the presence of (a) $\mathrm{B}_{0}=0.5 \mathrm{~T}$ parallel, (b) $\mathrm{B}_{0}=1.5 \mathrm{~T}$ perpendicular.


Figure 6.9: Brain Patient 2. Isodose contours comparing deterministic GBBS against GEANT4 Monte Carlo dose calculations for a three-beam brain treatment plan for axial, coronal, and sagittal slices through isocenter, as well as a dose profile along the y-axis through isocenter, in the presence of (a) $\mathrm{B}_{0}=0.5 \mathrm{~T}$ parallel, (b) $\mathrm{B}_{0}=1.5 \mathrm{~T}$ perpendicular.


Figure 6.10: Liver Patient 1. Isodose contours comparing deterministic GBBS against GEANT4 Monte Carlo dose calculations for a three-beam liver treatment plan for axial, coronal, and sagittal slices through isocenter, as well as a dose profile along the $y$-axis through isocenter, in the presence of (a) $\mathrm{B}_{0}=0.5 \mathrm{~T}$ parallel, (b) $\mathrm{B}_{0}=1.5 \mathrm{~T}$ perpendicular.


Figure 6.11: Liver Patient 2. Isodose contours comparing deterministic GBBS against GEANT4 Monte Carlo dose calculations for a three-beam liver treatment plan for axial, coronal, and sagittal slices through isocenter, as well as a dose profile along the y -axis through isocenter, in the presence of (a) $\mathrm{B}_{0}=0.5 \mathrm{~T}$ parallel, (b) $\mathrm{B}_{0}=1.5 \mathrm{~T}$ perpendicular.

Table 6.4: Gamma pass-rates and runtimes for deterministic patient calculations

| Patient Label / Anatomical Site | Comment | Avg. spatial FEM elements per Beam | $\mathrm{B}_{0}=0.5 \mathrm{~T}$ parallel |  |  | $\mathrm{B}_{0}=1.5 \mathrm{~T}$ perpendicular |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
|  |  |  | $\gamma 1 \% / 1 \mathrm{~mm}$ | $\gamma 2 \% / 2 \mathrm{~mm}$ | Avg. Runtime | $\gamma 1 \% / 1 \mathrm{~mm}$ | $\gamma 2 \% / 2 \mathrm{~mm}$ | Avg. Runtime |
| Lung 1 | $\begin{gathered} \text { higher density lung } \\ \bar{\rho}_{\text {lung }}=0.246 \mathrm{~g} / \mathrm{cm}^{3} \end{gathered}$ | 78512 | 96.7\% | 99.9\% | 8 m 51 s | 94.6\% | 99.8\% | 11m38s |
| Lung 2 | intermediate density lung $\bar{\rho}_{\text {lung }}=0.188 \mathrm{~g} / \mathrm{cm}^{3}$ | 76318 | 94.3\% | 99.9\% | 8m19s | 94.0\% | 99.6\% | 10m40s |
| Lung 3 | lower density lung $\bar{\rho}_{\text {lung }}=0.118 \mathrm{~g} / \mathrm{cm}^{3}$ | 72724 | 96.6\% | 100.0\% | 7m04s | 94.8\% | 99.9\% | 10m32s |
| Brain 1 | central tumor | 70959 | 96.2\% | 100.0\% | 6m56s | 95.5\% | 99.9\% | 9 m 15 s |
| Brain 2 | peripheral tumor | 55848 | 95.8\% | 99.9\% | 6m02s | 95.6\% | 99.9\% | 7m23s |
| Liver 1 | patient with air cavities | 125542 | 94.4\% | 99.9\% | 11m52s | 93.9\% | 99.8\% | 14m49s |
| Liver 2 | normal liver | 78045 | 97.0\% | 100.0\% | 7 m 41 s | 96.4\% | 99.9\% | 9 m 35 s |

### 6.4 Discussion

### 6.4.1 Accuracy of Deterministic Hybrid Approach for Patient Dose Calculations

Figures 6.5-6.11, as well as the quantitative gamma pass rates in Table 6.4, show that the techniques and conventions developed for the deterministic calculation provide very high accuracy across a range of patient anatomies and clinical magnetic field configurations. This is especially relevant for lung and abdominal patients, where MRI-guided deliveries have a major potential benefit due to the management of breathing motion. Lung is also a challenging case dosimetrically, where electrons traversing large volumes of low density media exhibit greater sensitivity to deflection by magnetic fields. Gamma $1 \% / 1 \mathrm{~mm}$ pass rates approached or exceeded $94 \%$ in all cases evaluated for both parallel and perpendicular magnetic fields, indicating the robustness of the deterministic formalism and parameters chosen for these cases.

Conditioning of the transport sweep matrix remained well controlled at less than 1000 in all cases, thus its inversion did not noticeably contribute to the numerical error or stability in the present framework, enabling a focus on minimizing the error of discrete density material assignment through $k$-means. Conventions in Tables 6.2 and 6.3 offer reasonable hyperparameters to accommodate problem complexity for each category of anatomy, yielding very close agreement with Monte Carlo parameterized with continuous densities. $k$-means maximizes flexibility to optimally allocate limited degrees of freedom, especially useful for lung regions often having significant variability in their density distribution.

The distinct and contrasting dose distribution of parallel and perpendicular magnetic field configurations is particularly evident in the dose profiles along the $y$-axis for lung patients, demonstrating the nontrivial interplay of magnetic field dose perturbations from multiple intersecting beams which the deterministic GBBS is able to account for in clinical scenarios, matching GEANT4 closely in all cases. Compared to Discrete Ordinates, solution quality for a DFEM discretization in angle benefits from the absence of ray-effect artifacts and exhibits unconditional stability in the presence of strong magnetic fields.

### 6.4.2 Utility of Bulk Density Transport Sweep

Results of patient dose calculations show that a bulk-density pre-inverted matrix batched transport sweep approach is capable of exceptionally high accuracy in clinical scenarios. The utility and rationale is to greatly reduce computational complexity for rapid patient dose calculations. It was found that performing element-by-element matrix assembly, source term construction, and gauss elimination to solve each elemental equation serially took on average 216 times longer than our proposed method. The observed two orders of magnitude speedup confirms that batched matrix-matrix multiplication as a BLAS primitive is vastly more efficient than looping over elemental systems to be solved one at a time for patient dose calculations. Although this study was performed using a serial execution, it is expected that there would still be computational benefits when moving towards a parallel implementation where parallelization could be performed over batched elements. This is especially relevant to a DFEM model in angle where a larger transport sweep matrix arises due to the space-angle Kronecker product for linear, quadratic, or cubic angular basis functions. Any computational savings for an individual transport sweep are multiplicative, given the iterative nature of the solution.

Ultimately the batched formalism was made possible by discretization conventions of spatial voxels on a Cartesian grid, having the same size and orientation, aligned to the angular mesh along octant boundaries. Thus over the directions subtended by a given angular element, the transport sweep matrix ends up being identical, differing only as a function of material parameterization. Moreover, it guarantees three faces will be upwind and three faces downwind when advancing through spatial sweep groups enabling batched memory searches of spatial dependencies. This simplification would not be possible for unstructured tetrahedral elements where the transport operator would be different for each element and thus require a unique construction and inversion. Assembly of the right hand side benefits similarly from batched operations over the entire domain for all voxels sharing the same bulk material.

Equally important to the overall deterministic approach is to leverage the separation of the primaries and scatter photon fluence calculation. In the context of radiotherapy, the solution is very sensitive to the accurate computation of the primary photon fluence for which the continuous density information is preserved during raytracing, a one-time calculation having
minimal impact on total computation time. This paradigm is similar to kernel based approximation techniques such as convolution superposition, in their accurate yet computationally efficient raytracing coupled to the use of pre-calculated scattering kernels scaled to resemble the local conditions. In the GBBS, secondary scatter, including the effect of magnetic fields, are calculated more rigorously through a space-angle transport sweep.

### 6.4.3 Factors Affecting Runtime, and Pathways for Future Development

Runtime scales primarily with the number of voxels. This is expected due to the serial dependencies involved in the spatial transport sweep being a communication-bound problem ${ }^{14}$. The adaptive spatial voxel generator developed for this work allocates the finest elements to the entire beam plus a fixed margin of 12 mm . Additional flexibility to more efficiently allocate degrees of freedom to regions of dosimetric interest could be achieved through development of a more advanced mesh generator. Alternatively, spatial sweeping can be parallelized through the Koch-Baker-Alcouffe (KBA) scheduling approach ${ }^{15}$, where subdomains are solved independently. Overall, parallelization of our batched transport sweep method is expected to further reduce calculation times.

Secondly, complexity scales with the angular mesh. Calculations in the presence of perpendicular magnetic fields took longer as a result of needing an isotropic angular mesh at higher energies, containing more elements than if a forward peaked mesh was used ${ }^{7}$. This involves solving more angular elements in total, which preserves accuracy, but at additional computational cost.

The number of discrete material densities also affects overall efficiency and runtime. Allocating more density bins reduces the approximation error, but as the number of density bins increase, more memory is required to store the pre-inverted matrices. Additionally, runtime operation of the transport sweep is done on a greater number of smaller batches, reducing vectorization while requiring more memory search operations. In this work we have found that 10 bins are required for treatment sites that include lung within the primary beam, and four bins are required for other sites containing significantly less low density media. Although the number of discrete densities
could be further increased, we found that there is only a marginal gain in the dose calculation accuracy while reducing calculation efficiency.

### 6.5 Conclusions

Feasibility of a transport sweep for a deterministic GBBS dose calculation with magnetic fields based on batched multiplication by pre-inverted matrices has been demonstrated to yield accurate results on patient cases for both parallel and perpendicular magnetic field configurations. Specifically, primary fluence was ray-traced using the full underlying density information from the CT, while secondary scatter was reasonably approximated using bulk material densities determined through $k$-means clustering. Batched multiplication by a pre-inverted transport sweep matrix was shown to be two orders of magnitude faster than solving each elemental system of equations in a serial application. The key hypothesis validated is that with relatively few bulk materials, a deterministic GBBS framework is able to use our new transport sweep and achieve $94 \%$ agreement at a $1 \% / 1 \mathrm{~mm}$ gamma criterion compared to continuous density Monte Carlo calculations for anatomical sites including lung in the presence of 0.5 T parallel and 1.5 T perpendicular magnetic fields. Reasonable runtimes on a prototype non-parallel workstation implementation show promise towards an accurate and efficient deterministic patient dose calculation for MRI-guided radiotherapy.

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## Chapter 7 Summary and Future Investigation

### 7.1 Summary of Results

With the goal of reducing the margin of healthy tissue irradiated and escalating dose to the tumor, Magnetic Resonance Imaging guided Radiotherapy (MRIgRT) offers the ability for intrafractional motion tracking and inter-fractional plan adaptation. Clinical deliveries introduce a strong magnetic field $\left(\mathrm{B}_{0}\right)$ either parallel or perpendicular to a megavoltage photon beam causing non-trivial deflection of secondary dose-depositing electrons by the Lorentz force. Changes in the dose distribution, sometimes exceeding $40 \%$, requires rigorous simulation of radiation transport across heterogeneous media in the presence of magnetic fields. This work pursued a deterministic solution, directly solving 6 -dimensional phase-space of the Linear Boltzmann Transport Equation (LBTE) with magnetic fields ${ }^{1,2}$ towards the goal of developing an accurate and efficient patient dose calculation for MRIgRT.

Initial attempts to maximize explicit parallelization by reformulating the problem using the Least Squares Continuous Finite Element Method (LS-CFEM) yielded novel algorithms on GPU for sparse matrix assembly, Kronecker tensor product, and leveraged BLAS operations ideally suited for the SIMD architecture of the GPU. Despite immense computational speedup, continuous finite elements in space were found unsuitable to model the abrupt transition in material properties (such as bone to air) needed for the most challenging radiotherapy cases ${ }^{3}$.

Returning to discontinuous finite elements, a restructuring of discretization conventions to curvilinear angular elements on the unit-sphere aligned to hexahedral spatial elements on a Cartesian grid enabled an acyclic directed sweep graph in space and angle, such that the number of angular elements was reduced by an order of magnitude, while retaining the highest levels of accuracy. A novel technique for angular upwind stabilization across curvilinear elements, along with space-angle rotational formalism enabled simulation of oblique magnetic field orientations without re-gridding the underlying geometry. Correctness of the framework is verified by MMS to exhibit the correct order of convergence ${ }^{4}$.

Further reduction in the inherent degrees of freedom of a nested iterative solution was hypothesized based on the physics governing the anisotropy of scatter and realized through an energy-adaptive forward-peaked angular meshing architecture. Techniques were developed to transfer fluence between hemispheres having different $h$ and $p$ refinement, as well as retain an acyclic space-angle sweep graph at all gantry angles, overcoming complications associated with angular advection introduced by magnetic fields. With appropriate meshing schemes for parallel and perpendicular magnetic fields, the number of angular elements was further reduced by half ${ }^{5}$.

Finally, a novel technique to orchestrate the most computationally intensive primitive of the spatial transport sweep was proposed based on batched multiplication of pre-inverted matrices and integrated into a hybrid runtime architecture where primary fluence was raytraced with continuous densities while iterative scatter calculations were performed using a limited number of bulk material densities assigned using $k$-means clustering. The accuracy of this technique was investigated for multi-beam plans at patient anatomical sites of lung, liver, and brain, for clinical magnetic field configurations. Sites including lung required approximately 10 discrete $k$-means to model the density gradient for scatter calculations, while other sites required only 4 discrete $k$ means as most tissue densities were clustered near water. Bulk densities were also used to perform efficient hierarchical batched assembly of the scatter source ${ }^{6}$.

The development of these novel algorithmic frameworks reduced runtime from days to minutes. Flexibility to calculate multi-field plans on patient geometries, in the presence of clinical magnetic field configurations was maintained in this development. Accuracy was retained at $>99 \%$ ( $>94 \%$ ) of points passing a $2 \% / 2 \mathrm{~mm}(1 \% / 1 \mathrm{~mm})$ gamma criterion against reference GEANT4 Monte Carlo calculations, yet without statistical uncertainty.

The resulting prototype code demonstrated feasibility for accurate and efficient deterministic patient MRIgRT patient dose calculations, a new paradigm compared to mainstream Monte Carlo approaches, benefitting from the absence of statistical uncertainty.

Further developments have the potential to accelerate towards realtime adaptive treatment planning as well as clinical deployment.

### 7.2 Future Investigation

### 7.2.1 Data Driven Hybrid Dose Inferencing Scheme

An overarching limitation to any fast implementation of the current algorithmic framework is the inherent slow convergence of the numerical iterative scheme in the presence of magnetic fields. Recall that advection in angle involves sweeping between elements on the unit sphere which require the application of Periodic Boundary Conditions (PBCs) shown to affect the convergence rate of the solution ${ }^{7}$.

Convergence of Source Iteration as characterized by the spectral radius $\rho_{s}$, was shown to approach the worst case scenario $\left(\rho_{s}=1\right)$ in the presence of $\mathrm{PBCs}^{7}$. Although the solution is unconditionally stable, splitting the magnetic field operator with components on the right hand side of the system of equations as required for upwind stabilization degrades the convergence rate ${ }^{7}$. Practically, we observe certain energy groups requiring more than 50 source iterations to converge, compared to a maximum of 20 in the absence of magnetic fields. Typically, Discrete Ordinates transport codes apply Diffusion Synthetic Acceleration (DSA) ${ }^{8}$ to expedite convergence of the $0^{\text {th }}$ angular flux moment which is slowest to converge (in the absence of magnetic fields), and associated with isotropic diffusion of particles. In contrast, magnetic fields hinder convergence by advection (anisotropic bulk transport) of charged particles in angle, thus is theorized to require a different acceleration technique than DSA (although DSA could still be applied to the photon calculation). Having established a flexible, accurate, unconditionally stable upwind stabilized space-angle discontinuous Galerkin FEM framework, development of an acceleration scheme unique to magnetic fields would be of great benefit from an algorithmic standpoint.

Deep Learning has demonstrated remarkable versatility to encode complex relations in underlying datasets. Its application to Medical Physics has primarily focused on imaging tasks such as segmentation, and classification. Although images are the most abundant source of data, an emerging paradigm leverages deep learning techniques to learn complex non-linear interactions of physics ${ }^{9}$. This derives from the flexibility of neural networks as universal function approximators ${ }^{10}$, with the benefit of extreme dimensionality reduction to efficiently
model a class of problems using far fewer degrees of freedom than required in a traditional deterministic framework. A prime example of where industry is heading is Nvidia's physicsbased machine-learning accelerated architecture for raytracing ${ }^{11}$, a hybrid model for the propagation of light through reflection, refraction, scattering, and dispersion to render qualitatively photorealistic scenes in realtime. Beyond presenting qualitatively realistic visuals, radiotherapy dose calculation requires quantitative accuracy, recommended to be within $\pm 2 \%$ of delivered dose to achieve acceptable tumor control ${ }^{12}$. The key challenge is developing an efficient well-integrated mechanism to correct the neural network's qualitatively close inference towards a confident quantitatively accurate dose distribution. Existing attempts to model radiotherapy dose using neural networks have lacked robustness precisely on account of this difficulty. The NeuRad code ${ }^{13}$ was trained using Monte Carlo to model a 2D dose distribution in homogeneous water (and absence of magnetic fields). As a result, these were the only cases leading to inferences having quantitative accuracy. In essence it had learned the feature space of correction-based methods in uniform water. Such end-to-end training to infer the final dose distribution implicates that if the neural network produced an inference that was out of tolerance, to correct it using Monte Carlo would be equally time consuming as running Monte Carlo from the outset. Had the objective been to obtain a fast, approximate solution, existing model-based algorithms such as convolution superposition exist and are better characterized in where and how errors occur. This elusive tradeoff highlights the challenge that quantitative accuracy poses.

In contrast to Monte Carlo, the way our deterministic framework arrives at dose (through intermediate multigroup angular fluence) offers unique opportunities for a robust neural network accelerated hybrid architecture. By training compartmentalized neural networks for the convergence of Source Iteration (SI) in each energy multigroup, an enhanced inference can be generated at runtime to greatly reduce the number of SI (involving computationally intensive sweeping through space and angle) needed to converge on the accurate solution for angular fluence. Preliminary experimentation showed that initializing with the previous group's converged angular fluence $\left(\Psi_{g}^{0}(\vec{r}, \hat{\Omega})=\Psi_{g-1}^{\text {converged }}(\vec{r}, \hat{\Omega})\right)$ reduced SI by $40 \%$ in certain groups, and reduced overall runtime by $\sim 20 \%$ compared to initialization with $\Psi_{g}^{0}(\vec{r}, \hat{\Omega})=0$. Although fluence between adjacent electron groups can differ by an order of magnitude, the effect of not sweeping from 0 at the wraparound edge significantly improves convergence of SI, therefore an
even better initial inference $\Psi_{g}^{0}(\vec{r}, \hat{\Omega})$ derived from a trained neural network is anticipated to accelerate convergence even further.

A potential deep learning architecture could use a $3 \times 3 \times 3$ spatially translatable DFEM grid of spatial elements, with each node embedding the full angular degrees of freedom. For each energy multigroup, this space-angle kernel is trained to infer the converged scatter-fluence given the primary fluence and underlying material composition. A spatially translatable kernel can maximize data re-use. Any successful machine-learning application requires an abundance of data, in this case generated by our baseline deterministic code, which is accurate, flexible, and reasonably fast. By shifting the trainable kernel across an underlying calculation grid, each new position provides a new training case where the kernel learns the scattering behaviors in each part of the beam. This yields 2 orders of magnitude more training cases from a single baseline dose calculation. Also, a translatable kernel enables flexibility of deployment across various underlying geometries. Conventional neural networks constrain themselves to a fixed calculation grid whose size must remain invariant during training and inference. Such a limitation is overcome by training and inferring using a shiftable kernel deployable at every position within the underlying calculation grid, regardless of its overall dimension. This approach is justified by electron scatter behaving as a localized phenomenon in radiotherapy, propagating only within 12 cm of the primary fluence for the energies used in our calculation. This is the same rationale behind convolution superposition algorithms with finite sized kernels ${ }^{14}$. Nodes of the trainable kernel can be connected to a multilayer perceptron whose width, depth, activation functions, and cost function can be investigated to determine suitable hyperparameters.

What distinguishes the proposed architecture from using Monte Carlo to train a final dose distribution is the application of deep learning to accelerate the convergence and work in synergy with an existing framework proven to be highly accurate. Variability in the quality of inferencing can be corrected for at all intermediate stages of the solution using our existing finite element framework, retaining quantitative accuracy while accelerating convergence.

### 7.2.2 Source Modeling

For the current dose calculation engine to be used in clinical treatment planning, a realistic distributed source model is needed to replace the idealized point source used in this work. Efforts have begun to characterize variation of the primary fluence energy spectrum and intensity as a function of position for the Elekta Unity system ${ }^{15}$. Model parameters incorporated into the codebase developed in this work were validated to be in excellent agreement with measurement in homogeneous water for field sizes ranging from $5 \times 5 \mathrm{~cm}^{2}$ to $57 \times 22 \mathrm{~cm}^{2}$ in the presence of a 1.5 T perpendicular magnetic field ${ }^{15}$. Once calibrated through reference dosimetry, the code will be able to compute dose per output unit of the machine, as opposed to the current convention of dose per arbitrary unit of fluence.

### 7.2.3 Task-Level Parallelization

The prototype dose calculation developed through chapters 4,5 , and 6 was implemented as an unparallelized Matlab codebase running on a single workstation. Algorithmic techniques were developed to add flexibility and reduce computational degrees of freedom at the outset, which confers speedup invariant to implementation platform. From this starting point, which used physics principles and algorithmic architectures to establish the fundamentals of an efficient code, further parallelization strategies can be deployed, the simplest being task-level parallelism. Each beam can be calculated independently. Within each calculation, energy groups can be calculated concurrently based on their upstream dependencies. For example, higher energy electron groups can begin without waiting for lower energy photons which they do not depend on. Elements within an angular sweep group and even in different sweep groups can be solved concurrently, with the potential for overall speedup ${ }^{7}$, while converging to the correct solution provided upwind stabilization is correctly implemented. Likewise, launching spatial sweep groups simultaneously is the basis of the KBA algorithm used in massively parallel nuclear reactor transport codes ${ }^{16}$. Other parallelization techniques including leveraging the GPU in a different manner than Chapter 3 will need to be investigated on a more powerful programming language such as C. Such efforts are underway at the University of Iowa, in part using techniques developed in this work.

### 7.2.4 Integration with Radiotherapy Outcomes Modeling

The algorithmic underpinnings and resulting codebase of this work models the physics of radiation transport at a fundamental level, however the limiting uncertainty may no longer be physical dose, but rather radiobiological or contouring aspects which are not considered when treating the patient as a rigid geometry. A potential avenue for future investigation would be to incorporate radiobiological outcomes modeling and data-driven plan adaptation into a next generation oncology platform where the microstructure of dose delivered is one of several factors guiding optimal radiotherapy outcomes. Still further developments such as FLASH-RT ${ }^{17}$ may require completely different considerations such as alteration of the underlying media at extremely high dose rates, or the time structure of pulsed deliveries, all affecting treatment outcomes, with exciting potential for deterministic dose calculation models to play a key role.

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