Adaptive Discrete-Ordinates Quadratures Based on Discontinuous Finite Elements over Spherical Quadrilaterals

Thesis Proposal

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1 Introduction

The linear Boltzmann transport equation is used to model neutral-particle transport [1]:

$$\frac{1}{v(E)}\frac{\partial \Psi\left(\vec{r},\vec{\Omega},E,t\right)}{\partial t}+\vec{\Omega}\cdot\vec{\nabla}\Psi\left(\vec{r},\vec{\Omega},E,t\right)+\sigma_t\left(\vec{r},E,t\right)\Psi\left(\vec{r},\vec{\Omega},E,t\right) = \int_{4\pi}d\Omega'\int_0^\infty dE'\sigma_s\left(\vec{r},\vec{\Omega}'\cdot\vec{\Omega},E'\rightarrow E,t\right)\Psi\left(\vec{r},\vec{\Omega}',E',t\right)+q\left(\vec{r},\vec{\Omega},E,t\right) \tag{1}$$

Eqn. 1 has seven independent variables: three in position, two in direction, one in energy and one in time. Analytic solutions only exist for trivial problems. In practice the independent variables are discretized to form a set of algebraic equations that can be solved using an iterative method. The search for new discretization techniques increasing solution accuracy and computational efficiency is an active area of research.

We focus on the discretization of the direction variable, specifically angular quadratures used in the discrete-ordinates (D-O) method. The D-O method approximates angular integrals using a finite sum:

$$\int_{\Delta\Omega}d\Omega f\left(\vec{\Omega}\right)\approx\sum_{m=1}^{M}w_m f\left(\vec{\Omega}_m\right) \tag{2}$$

The set of directions and weights $(\vec{\Omega}_m, w_m), m = 1, ..., M$ in Eqn. 2 forms an angular quadrature over $\Delta\Omega$. Directions can be expressed in terms of directional cosines:

$$\Omega_x = \mu = cos(\gamma)sin(\theta) = cos(\gamma)\sqrt{1-\xi^2} \tag{3}$$

$$\Omega_y = \eta = sin(\gamma) sin(\theta) = sin(\gamma)\sqrt{1-\xi^2} \tag{4}$$

$$\Omega_z = \xi = cos(\theta) \tag{5}$$

where γ is the azimuthal angle in the x-y plane and θ is the polar angle relative to the z-axis. It is important for angular quadratures to accurately integrate spherical harmonics (SH) which are polynomials in the directional cosines. Consider Eqn. 1 after applying the multi-group energy and D-O angular discretizations [1]:

$$\begin{aligned} \frac{1}{v_g}\frac{\partial \Psi_{mg}\left(\vec{r},t\right)}{\partial t} + \vec{\Omega}_m \cdot \vec{\nabla}\Psi_{mg}\left(\vec{r},t\right) + \sigma_{tg}\left(\vec{r},t\right)\Psi_{mg}\left(\vec{r},t\right) \quad = \\ \sum_{g'}\sum_{l=0}^{L}\frac{2l+1}{4\pi}\sigma_{sl,g'\to g}\left(\vec{r},t\right)\sum_{n=-l}^{l} Y_{ln}\left(\vec{\Omega}_m\right)\phi_{ln,g'}\left(\vec{r},t\right) + q_{mg}\left(\vec{r},t\right) \end{aligned} \tag{6}$$

where m is the angular quadrature index, g is the energy group index, L is the anisotropic scattering order, $\sigma_{sl,g'\to g}$ is the lth coefficient of the $\sigma_{s,g'\to g}$ Legendre expansion, Y_{ln} is the spherical harmonic of degree l and order n, and $\phi_{ln,g'}$ is the angular flux moment given by:

$$\phi_{ln,g'}\left(\vec{r},t\right) = \sum_m w_m \psi_{mg'}\left(\vec{r},t\right) Y^*_{ln}\left(\vec{\Omega}_m\right) \tag{7}$$

If the scattering cross section and angular flux can be represented by Legendre and SH expansions of order L and K, respectively, then Eqn. 6 only requires angular flux moments through order $\min\left(L,K\right)$. Eqn. 7 shows forming these moments requires accurate integration of SH through order $2\cdot\min\left(L,K\right)$. Error in the angular flux moments as a result of angular quadrature integration may lead to loss of particle balance.

Traditional angular quadratures are generated over the entire 4π angular domain (Level Symmetric, Gauss-Chebyshev) or over octants (Quadruple Range) [1, 2, 3, 4]. These quadratures perform well when the angular flux is smooth over the angular domain for which they are derived. However in practice the angular flux is often discontinuous or near-discontinuous over sub-octant angular regions as illustrated in Fig. 1 showing the angular flux as a function of azimuthal angle at a fixed location in an infinite square lattice of circular fuel pins in water. An ideal angular quadrature should accurately integrate the angular flux moments of such functions requiring accurate SH integration over increasingly smaller angular regions.

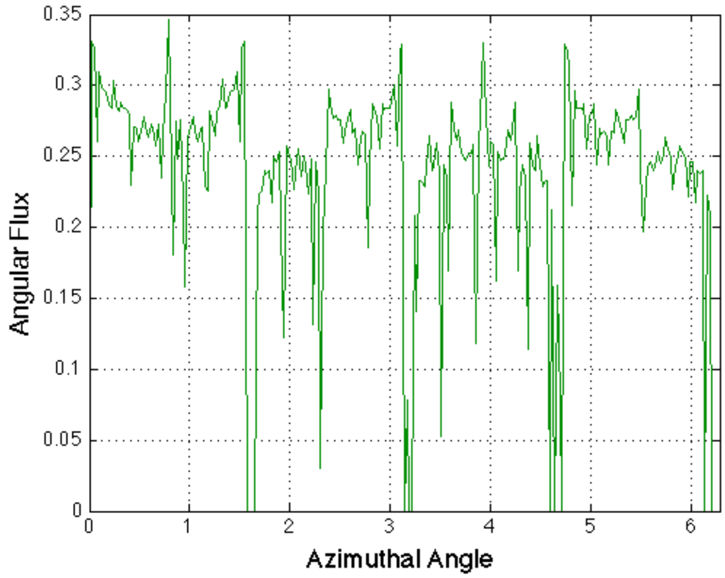

Figure 1: Angular flux solution as a function of azimuthal angle at a fixed location in an infinite square lattice of circular fuel pins in water.

Traditional angular quadratures are also computationally inefficient when the angular flux is discontinuous or near-discontinuous only for local angular regions. An ideal angular quadrature should only refine in the angular regions requiring additional resolution.

Stone and Adams [6, 7, 8] developed angular quadratures for use in two-dimensional cartesian geometry based on discontinuous finite elements (DFEM) over the azimuthal angular domain. The Stone-Adams angular quadratures overcome the deficiencies of the traditional quadratures by accurately integrating SH over increasingly smaller angular regions and supporting local refinement. The Stone-Adams angular quadratures are also adaptive i.e., local angular regions are refined based on adaptive rules applied to the current iterative solution. The Jarrell-Adams LDFE-ST quadratures [5] extend the DFEM-based angular quadrature methodology to three-dimensional cartesian geometry by defining linear discontinuous finite element (LDFE) basis functions over spherical triangles (ST) on the unit sphere. The LDFE-ST quadratures accurately integrate SH (exact integration of 0th and 1st-order and 4th-order accuracy for higher orders) and have superior performance over traditional quadratures for several benchmark problems. A major challenge for using the

LDFE-ST quadratures adaptively is the need for accurate mapping algorithms to pass the angular flux solution between two spatial regions with differently-refined LDFE-ST quadratures. Ideal mapping algorithms should retain the shape of the original angular flux solution while preserving the 0th and 1st angular flux moments.

We propose here to develop a new family of quadratures based on LDFE and quadratic discontinuous finite element (QDFE) basis functions defined over spherical quadrilaterals (SQ) on the unit sphere. The use of SQ instead of ST provides a more uniform distribution of quadrature ordinates reducing local integration variability. The use of SQ has been successful in other applications such as discontinuous Galerkin (DG) transport for weather modeling [9]. The QDFE-SQ quadratures demonstrate the use of higher-order basis functions in the DFEM-based quadrature methodology allowing exact integration of higher-order (above 0th and 1st) SH and the preservation of higher-order (above 0th and 1st) angular flux moments for mapping algorithms. The new family of LDFE/QDFE-SQ quadratures and associated mapping algorithms constitute this research.

2 Current State of the Problem

2.1 DFEM-Based Angular Quadrature Methodology

The discrete-ordinates (D-O) method approximates angular integrals using a finite sum:

$$\int_{\Delta\Omega} d\Omega f\left(\vec{\Omega}\right) \approx \sum_{m=1}^{M} w_m f\left(\vec{\Omega}_m\right) \tag{8}$$

The set of directions and weights $(\vec{\Omega}_m, w_m), m = 1, ..., M$ in Eqn. 8 forms an angular quadrature over $\Delta\Omega$. DFEM-based angular quadratures divide the global 4π angular domain into regions $\Delta\Omega_i$. The integrated function in each region is expanded as:

$$f_i\left(\vec{\Omega}\right) \approx \sum_{j=1}^{J} f_{ij} b_{ij}\left(\vec{\Omega}\right) \tag{9}$$

where i is the region index, j is the degree of freedom index, f_{ij} are basis function coefficients, and $b_{ij}\left(\vec{\Omega}\right)$ are basis functions in the directional cosines. The number of degrees of freedom depends on the basis function order. For example the linear basis function has four degrees of freedom:

$$b_j\left(\vec{\Omega}\right) = c_{c,j} + c_{\mu,j}\mu + c_{\eta,j}\eta + c_{\xi,j}\xi,\ j = 1,..,4 \tag{10}$$

The basis functions are defined by our requirement that each is a cardinal function and by the placement of the quadrature directions $\vec{\Omega}_{ij}$. Since the basis functions are cardinal:

$$f_{ij} = f_i\left(\vec{\Omega}_{ij}\right) \tag{11}$$

Inserting Eqns. 9 and 11 into the analytic integral (left side of Eqn. 8):

$$\int_{\Delta\Omega_i} d\Omega f_i\left(\vec{\Omega}\right) \approx \sum_{j=1}^{J} f_i\left(\vec{\Omega}_{ij}\right)\int_{\Delta\Omega_i} d\Omega b_{ij}\left(\vec{\Omega}\right) \tag{12}$$

Eqn. 12 can be expressed in the D-O form by defining the weights as:

$$w_{ij} = \int_{\Delta\Omega_i} d\Omega b_{ij}\left(\vec{\Omega}\right) \tag{13}$$

Inserting Eqn. 13 into Eqn. 12:

$$\int_{\Delta\Omega_i} f_i\left(\vec{\Omega}\right) d\Omega \approx \sum_{j=1}^{J} w_{ij} f_i\left(\vec{\Omega}_{ij}\right) \tag{14}$$

The set of directions and weights $(\vec{\Omega}_{ij}, w_{ij}), j = 1, ..., J$ in Eqn. 14 forms the DFEM-based angular quadrature for angular region $\Delta\Omega_i$.

2.2 LDFE-ST Quadratures

The LDFE-ST quadratures apply the DFEM-based angular quadrature methodology to linear discontinuous finite elements (LDFE) over spherical triangles (ST) on the unit sphere [5]. The constuction of the LDFE-ST quadratures begin by inscribing an octahedron into the unit sphere and projecting each face onto the unit sphere forming ST over each octant. Four quadrature ordinates are placed in each ST to satisfy the degrees of freedom for the underlying LDFE basis functions. The quadrature weights are the integral of the basis functions over the ST. For uniform refinement each ST is divided into four additional ST. For local refinement only selected ST are refined (either by the user or an adaptive algorithm). The LDFE-ST quadratures have accurate spherical harmonic integration (exact for 0th and 1st-order and 4th-order accurate for higher orders) and superior performance relative to traditional angular quadratures for scalar flux calculation in several benchmark problems. The LDFE-ST quadratures are well-suited for adaptivity since they have strictly positive weights, can be generated for large numbers of directions and support local refinement.

2.3 LDFE-ST Mapping

In order to support adaptivity the LDFE-ST quadratures require mapping algorithms to pass the angular flux solution between spatial regions with differently-refined LDFE-ST quadratures. Jarrel and Adams define an ideal mapping algorithm as one retaining the shape of the original angular flux solution while preserving the 0th and 1st angular flux moments [5]. Several mapping algorithms were developed by Jarrell and Adams but none were ideal. The final mapping algorithm selected by Jarrell and Adams interpolates the original angular flux solution using the underlying LDFE basis functions and preserves *either* the 0th or 1st angular flux moment using a conservation factor. If negativities or extrema relative to the original angular flux solution are present in the mapped solution then the mapping algorithm switches to constant discontinuous finite element interpolation. This results in strictly positive mapped angular flux solutions but loses the shape of the original angular flux solution. Jarrell and Adams found the selected mapping algorithm significantly degrades the accuracy of the LDFE-ST quadratures.

2.4 Limitations

The use of spherical triangles to divide the unit sphere results in non-uniform quadrature ordinate distributions causing local integration variability. Consider the integration of a constant function over a local angular region. The result significantly changes when the local angular region is rotated between angular regions with varying densities of quadrature ordinates. Fig. 2 shows the 108-point LDFE-ST quadrature revealing a non-uniform, ring-like distribution of ordinates which visually appear to have holes. An alternative unit sphere tessellation may produce more uniform quadrature ordinate distributions.

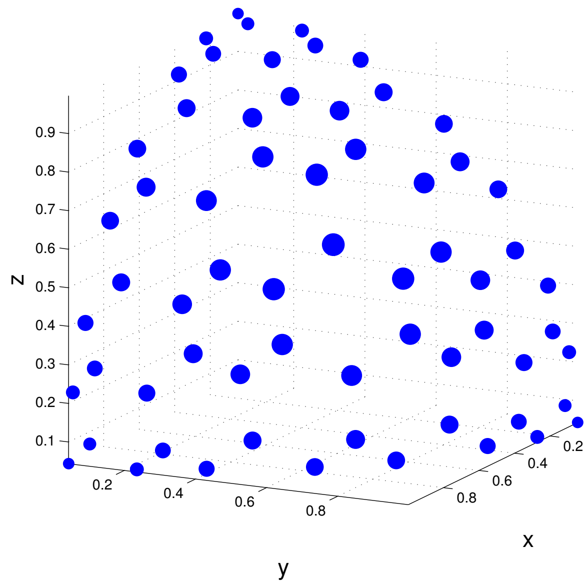

Figure 2: 108-point LDFE-ST angular quadrature showing non-uniform, ring-like distribution of ordinates. Weights are proportional to the ordinate size.

The use of higher-order (above linear) basis functions was also never investigated. Higher-order basis functions require more quadrature ordinates per angular region. The additional degrees of freedom allow exact integration of higher-order (above 0th and 1st) spherical harmonics and the preservation of higher-order (above 0th and 1st) angular flux moments for mapping algorithms.

The accuracy of using the LDFE-ST quadratures adaptively was limited by the error introduced by the mapping algorithms. An ideal mapping algorithm should retain the shape of the original angular flux solution while preserving the 0th and 1st angular flux moments.

3 Proposed Research

3.1 LDFE/QDFE-SQ Quadratures

We propose here to develop DFEM-based angular quadratures using linear and quadratic discontinuous finite elements over spherical quadrilaterals (LDFE/QDFE-SQ). The construction of the LDFE/QDFE-SQ quadratures begin by inscribing a cube into the unit sphere and allocating one corner to each octant. The faces of the cube are projected onto the unit sphere forming spherical quadrilaterals (SQ) over each octant as shown in Fig. 3. The use of SQ instead of spherical triangles (ST) provides a more natural and uniform distribution of quadrature ordinates. Consider LDFE basis functions which require four quadrature ordinates per angular region. For SQ the quadrature ordinates can be uniformly distributed on a 2x2 grid. However for ST we must place one quadrature ordinate in the center and the other three near each vertex leading to the non-uniform, ring-like LDFE-ST ordinate distribution shown in Fig. 2. Similarly QDFE basis functions require nine quadrature ordinates per angular region. For SQ the quadrature ordinates can be uniformly distributed on a 3x3 grid. However for ST there is no obvious uniform distribution.

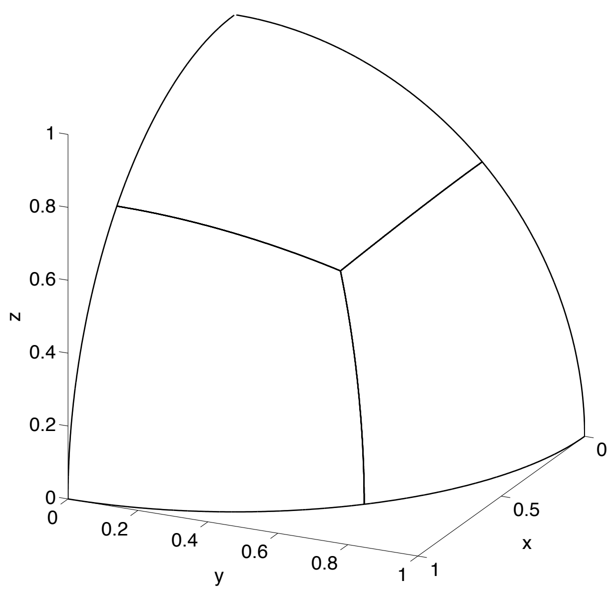

Figure 3: Spherical quadrilaterals over the first octant.

The degrees of freedom for the underlying basis functions and subsequently the quadrature weights are determined by the placement of the quadrature ordinates. The method for placing the quadrature ordinates leads to different LDFE/QDFE-SQ quadrature types. Ideal LDFE/QDFE-SQ quadratures should produce strictly positive weights and uniform weight and ordinate distributions.

For uniform refinement each SQ is divided into four SQ. The level-n LDFE/QDFE-SQ quadratures contain $3 \cdot (n+1)^2$ SQ per octant. Fig. 4 shows the SQ for the level-1

LDFE/QDFE-SQ quadratures over the first octant. For local refinement only selected SQ (either by the user or an adaptive algorithm) are refined. Local LDFE-SQ (resp. QDFE-SQ) refinement divides the selected SQ into four (resp. nine) SQ. Fig. 5 shows the SQ over the first octant after two local refinements of the level-1 LDFE-SQ quadrature over an arbitrary cone of angle.

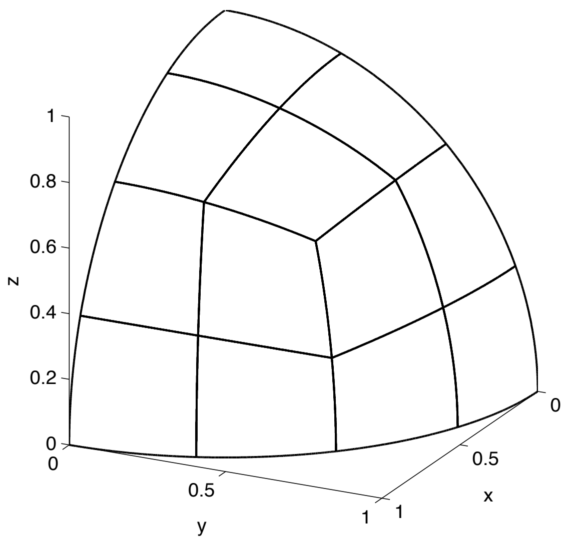

Figure 4: Spherical quadrilaterals over the first octant for the level-1 LDFE/QDFE-SQ quadratures.

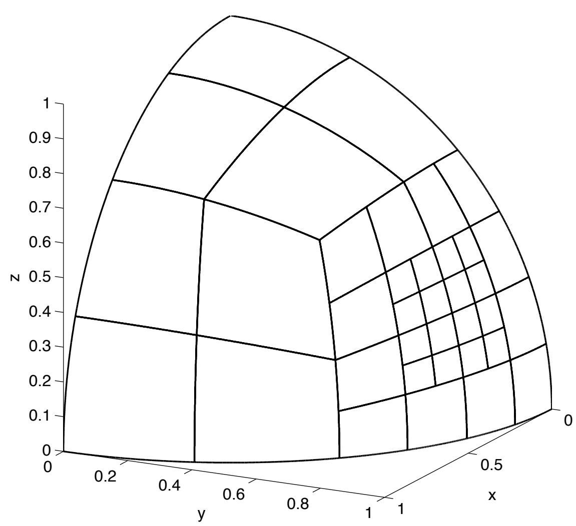

Figure 5: Spherical quadrilaterals over the first octant for the level-1 LDFE-SQ quadratures after two local refinements over an arbitrary cone of angle.

The performance of the LDFE/QDFE-SQ quadratures will be measured by accuracy in both spherical harmonic integration and scalar flux calculation for several benchmark problems (e.g., Kobayashi [10]).

3.2 Mapping Algorithms

We propose here to develop mapping algorithms to pass the angular flux solution between spatial regions with differently-refined LDFE/QDFE-SQ quadratures. An ideal mapping algorithm should retain the shape of the original angular flux solution while preserving the 0th and 1st angular flux moments [5]. In order to preserve the 0th and 1st angular flux moments we must satisfy:

$$\sum_{m=1}^{N_f} w_{f,m}\psi_{f,m} = \sum_{n=1}^{N_c} w_{c,n}\psi_{c,n} \tag{15}$$

$$\sum_{m=1}^{N_f} w_{f,m}\psi_{f,m}\Omega_{x_{f,m}} = \sum_{n=1}^{N_c} w_{c,n}\psi_{c,n}\Omega_{x_{c,n}} \tag{16}$$

$$\sum_{m=1}^{N_f} w_{f,m}\psi_{f,m}\Omega_{y_{f,m}} = \sum_{n=1}^{N_c} w_{c,n}\psi_{c,n}\Omega_{y_{c,n}} \tag{17}$$

$$\sum_{m=1}^{N_f} w_{f,m}\psi_{f,m}\Omega_{z_{f,m}} = \sum_{n=1}^{N_c} w_{c,n}\psi_{c,n}\Omega_{z_{c,n}} \tag{18}$$

where m is the fine quadrature index, n is the coarse quadrature index, w are the quadrature weights, ψ are the angular flux solutions, and Ω_x, Ω_y and Ω_z are the directional cosines defined in Eqns. 3 through 5.

For LDFE-SQ quadratures each coarse SQ has four overlapping fine SQ resulting in $N_c = 4$ and $N_f = 16$ (four ordinates per SQ). For fine-to-coarse mapping Eqns. 15 through 18 can be directly solved (four equations and four unknowns $\psi_{c,n}, n = 1, ..., 4$). For coarse-to-fine mapping Eqns. 15 through 18 form an under-determined system (four equations and

16 unknowns $\psi_{f,m}, m = 1, ..., 16$). We close the system by projecting the fine angular flux solutions onto the coarse basis functions:

$$\psi_{f,m} \approx \sum_{n=1}^{N_c} \tilde{\psi}_{c,n} b_{c,n} \left(\vec{\Omega}_{f,m} \right) \tag{19}$$

resulting in four equations and four unknowns $\tilde{\psi}_{c,n}, n = 1, ..., 4$.

For QDFE-SQ quadratures each coarse SQ has nine overlapping fine SQ resulting in $N_c = 9$ and $N_f = 81$ (nine ordinates per SQ) . For fine-to-coarse mapping Eqns. 15 through 18 is an under-determined system (four equations and nine unknowns $\psi_{c,n}, n = 1, ..., 9$). We close the system by requiring the mapping algorithm to conserve the remaining 2nd-order spherical harmonics moments (i.e., $\Omega_x\Omega_y$, $\Omega_x\Omega_z$, $\Omega_y\Omega_z$, Ω_z^2, and $\Omega_x^2 - \Omega_y^2$). For coarse-to-fine mapping Eqns. 15 through 18 and the additional 2nd-order spherical harmonics requirements form an under-determined system (nine equations and 81 unknowns $\psi_{f,m}, m = 1, ..., 81$). We close the system by projecting the fine angular flux solutions onto the coarse basis functions as shown in Eqn. 19.

The previous mapping algorithm preserves the 0th and 1st (including 2nd for QDFE-SQ) angular flux moments. However negativities or extrema relative to the original angular flux solution may exist in the mapped angular flux solution when discontinuities or near-discontinuities occur in the original angular flux solution. For these cases we apply a fix-up algorithm preserving as much of the original angular flux shape and as many angular flux moments as possible while removing all negativities and extrema.

4 Summary

The LDFE-ST angular quadratures showed DFEM-based angular quadratures are well-suited for adaptive D-O. The LDFE-ST quadratures demonstrated accurate spherical harmonic integration and superior performance relative to traditional angular quadratures for several benchmarks. The LDFE-ST quadratures are strictly positive, can be generated for large numbers of directions and locally refinable. The accuracy of using LDFE-ST quadratures for adaptive D-O was limited by errors introduced by the mapping algorithms and ordinate non-uniformity. We propose:

1. To create a new family of LDFE-SQ quadratures defining linear discontinuous finite elements over spherical quadrilaterals (instead of spherical triangles) to produce more uniform ordinate distributions leading to less local integration variability,

2. To extend the LDFE quadrature methodology to QDFE in order to demonstrate the use of higher-order basis functions leading to the exact integration of higher-order (above 0th and 1st) spherical harmonics and the preservation of higher-order (above 0th and 1st) angular flux moments for mapping algorithms,

3. To create mapping algorithms preserving the maximum degree angular flux moment possible while not introducing non-physical extrema, and

4. To implement and test the LDFE/QDFE-SQ quadratures and associated mapping algorithms on difficult 1D, 2D and 3D problems. Performance will be based on the convergence rates of particle balance and solution error as a function of the total number of ordinates.

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