

# Quadratic Serendipity Discontinuous Finite Element Discretization for $S_N$ Transport on Arbitrary Polygonal Grids

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## Abstract

In this paper, we present a quadratic serendipity discontinuous finite element (DFEM) discretization of the  $S_N$  transport equation for arbitrary polygonal grids. The quadratic functions are constructed from products of the linear Generalized Barycentric Coordinates (GBC) and are compatible with polygonal mesh elements. They span the  $\{1, x, y, x^2, xy, y^2\}$  space of functions and grow by  $2n$  on a mesh element where  $n$  is the number of the polygon's vertices. Numerical tests confirm that the functions capture exactly quadratic solutions and appropriate convergence rates are observed, including a test case involving spatial adaptive mesh refinement. Finally, the functions are analyzed for diffusive problems and retain full resolution in the thick diffusion limit.

*Key words:* Radiation Transport, Arbitrary Polygonal Grids, Discontinuous Finite Element, Serendipity Basis Functions

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## 1. Introduction

The solution of the radiation transport equation is important for the fields of reactor physics, high density energy physics, astrophysics, medical imaging and treatment, and others. High-fidelity solutions are difficult to obtain because of the large phase space of the radiation distribution: three for space, two for angular direction on the unit sphere, one for energy, and one for time for unsteady problems [1]. The angular flux solution of the radiation transport equation,  $\psi(\vec{r}, \vec{\Omega}, E)$ , about position  $\vec{r}$ , about energy  $E$ , and traveling in a cone about direction  $\vec{\Omega}$  is given by

$$\begin{aligned} \vec{\Omega} \cdot \vec{\nabla} \psi(\vec{r}, \vec{\Omega}, E) + \sigma_t(\vec{r}, E) \psi(\vec{r}, \vec{\Omega}, E) &= Q(\vec{r}, \vec{\Omega}, E) \\ &+ \int_0^\infty dE' \int_{4\pi} d\Omega' \sigma_s(\vec{r}, \vec{\Omega}' \rightarrow \vec{\Omega}, E' \rightarrow E) \psi(\vec{r}, \vec{\Omega}', E'), \end{aligned} \quad (1)$$

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where  $\sigma_t$  and  $\sigma_s$  are the total and scattering cross sections,  $Q$  is an angularly-dependent distributed source, and we have omitted temporal dependence. Various numerical techniques have been developed to appropriately discretize Eq. (1) in space, energy, and angle.

In this work, we focus on using solution techniques developed for Eq. (1), also referred to as the first-order form of the transport equation. Namely, we restrict ourselves to the one-speed transport equation, the discrete ordinates ( $S_N$ ) approximation in angle, and the discontinuous Galerkin finite element method (DGFEM) in space. The DGFEM discretization of the  $S_N$  transport equation dates back to Reed and Hill [2] as well as Lesaint and Raviart [3]. It is a common spatial discretization of the transport equation because it is amenable to efficient iterative techniques [4] and scales well on massively parallel architectures [5]. Most of the DGFEM  $S_N$  codes use first-order (linear) functions on simplicial (triangles and tetrahedra) and tensor (quadrilaterals and hexahedra) grids, including DENOVO [6], PARTISN [7], and ATTILA [8]. PDT [5] and Jaguar [9] use up to first-order functions, but differ from other codes by solving the transport equation on unstructured polytope grids.

Primarily, only linear basis functions have been employed with the DFEM transport equation (see previously listed transport codes). Moving away from finite difference methods required solving local linear systems of equations. With computational limits of the time, researchers did not want to solve these larger local system when using higher-order basis functions. Furthermore, there was a focus on the robustness of the spatial discretization, which is well characterized for linear functions especially in the thick diffusive limit [10]. The thick diffusion limit is an important asymptotic limit of the transport equation that requires the use of spatial discretizations with certain properties [10]. Much research has been performed with linear functions for multidimensional calculations, but limited to simplicial and tensor mesh cells [11, 12, 13, 14]. The piecewise linear (PWL) functions are the only discretization technique for arbitrary polygonal cells and DFEM transport [15, 16]. Our work includes using these PWL functions, along with other linear polygonal functions.

While linear basis functions have been primarily utilized, there has been a push to analyze the DFEM transport equation with higher-order basis functions. Maginot et. al [17, 18] and Hennart and De Valle [19, 20] have analyzed higher-order functions for 1D slab problems. In 2D, the TRIPLET code [21] used higher-order Lagrange elements on triangles and Wang and Ragusa [22, 23] used hierarchical triangular elements. Other methods besides the DFEM discretization have utilized higher-order approximations including AHOT for nodal and characteristic transport [24, 25] and Wachspress' functions for curved mesh cell boundaries [26].

In this paper, we seek to analyze the DFEM  $S_N$  transport equation with a higher-order quadratic serendipity spatial discretization on arbitrary polygonal grids. With advancements in computer architectures, computations are becoming cheaper than data movement in memory along with communication times between processors for parallel problems. For this reason, along with higher-order functions achieving equivalent accuracy than linear functions on larger mesh cells, there is a growing benefit to using higher-order

functions for the DFEM transport equation. Likewise, we seek to analyze DFEM transport equation on arbitrary polygonal grids because of the flexibility and benefits they provide:

1. Polygonal mesh cells are now being employed in other physics communities - notably computational fluid dynamics (CFD) [27] and solid mechanics [28];
2. They can reduce cell/face counts which can reduce algorithm wallclock times depending on the solution method;
3. They can allow for transition elements between different portions of the domain (e.g., triangular elements bordering quadrilateral elements at the border of the boundary layer);
4. They can easily be split along cut planes - allowing the mesh to be partitioned into regular or irregular divisions as well as be generated by simplicial meshing techniques across processor sets in parallel;
5. Hanging nodes from non-conforming meshes, like those that naturally arise from locally refined/adapted meshes using spatial adaptive mesh refinement (AMR) as seen in Figure 1, are not necessary.

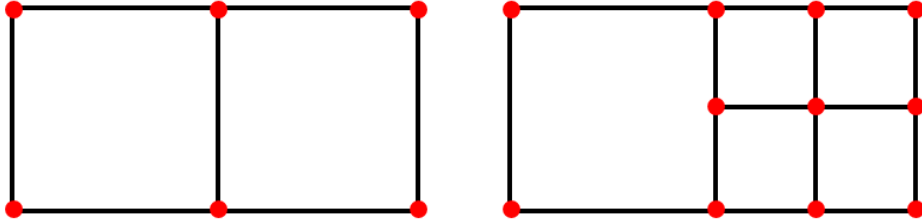


Figure 1: Local mesh refinement of an initial quadrilateral cell (left) leads to a degenerate pentagonal cell (right) without the use of a hanging node.

The higher-order discretization that we employ uses the quadratic serendipity space of functions developed by Rand et al. [29]. They proposed a process where linear functions, compatible with polygonal mesh elements, are converted into a quadratic serendipity space of functions that span  $\{1, x, y, x^2, xy, y^2\}$  on strictly-convex polygons. Their procedure used an intermediate step to form  $O(n^2)$  pairwise quadratic products in 2D, where  $n$  is the number of the polygon's vertices. Because the number of functions grows large for large vertex counts, these pairwise functions were then converted to  $2n$  serendipity functions, drastically reducing the number of functions. We summarize their process in this work, and provide our methodology that is compatible with weakly-convex polygons (*i.e.*, collinear vertices) so that we could perform AMR calculations using degenerate polygons without hanging nodes. Finally, we note that the basis functions derived in this work are not solely compatible with the first-order form of the transport equation, but can be used with the second-order form of the transport equation, such as the self-adjoint and even-parity forms [30, 31].

The remainder of the paper is as follows. We provide a brief description of the DGFEM  $S_N$  transport equation along with its theoretical spatial convergence rate in Section 2. We then describe a family of functions that are linearly-complete on polygons in Section 3. We then present in Section 4 the methodology

to convert the linear polygonal basis functions presented in Section 3 into a serendipity space of basis functions with quadratic-completeness. Section 5 briefly describes the methodology that will be employed to perform spatial AMR with the DGFEM transport equation. Finally, Section 6 provides a set of numerical experiments to verify the polynomial interpolation of the functions as well as their ability to retain full resolution in the thick diffusion limit.

## 2. The DGFEM $S_N$ Discretization of the Transport Equation

In this section, we review the DGFEM  $S_N$  transport equation. Given an angular quadrature set,  $\{\vec{\Omega}_m, w_m\}_{m=1}^M$ , the monoenergetic  $S_N$  transport equation with isotropic scattering is defined within an open, convex spatial domain  $\mathcal{D}$ , with boundary,  $\partial\mathcal{D}$ , as

$$\left(\vec{\Omega}_m \cdot \vec{\nabla} + \sigma_t(\vec{r})\right) \psi_m(\vec{r}) = \frac{\sigma_s(\vec{r})}{4\pi} \phi(\vec{r}) + Q_m(\vec{r}), \quad (2)$$

where  $\psi_m(\vec{r}) = \psi(\vec{r}, \vec{\Omega}_m)$  is the angular flux at position  $\vec{r}$  and in direction  $\vec{\Omega}_m$  and  $Q_m$  is a distributed source for angle  $m$ . The scalar flux is defined as

$$\phi(\vec{r}) = \int_{4\pi} d\Omega \psi(\vec{r}, \vec{\Omega}) \approx \sum_{m=1}^M w_m \psi_m(\vec{r}). \quad (3)$$

We then lay down an unstructured mesh,  $\mathbb{T}_h \in \mathbb{R}^d$ , over the spatial domain, where  $d$  is the spatial dimension of the problem (for this work,  $d = 2$ ). This mesh consists of non-overlapping spatial elements to form a complete union over the entire spatial domain:  $\mathcal{D} = \bigcup_{K \in \mathbb{T}_h} K$ . The 2D domain is meshed with arbitrary polygonal elements.

As is standard in the discontinuous Galerkin scheme, the angular flux unknown of Eq. (2) is expanded using discontinuous basis functions over each mesh cell  $K$ :

$$\psi_m(\vec{r}) \approx \sum_{j=1}^{n_K} \psi_{m,j} b_j(\vec{r}). \quad (4)$$

The basis functions are nonzero over a single element and discontinuous across the element interfaces. The DGFEM weak form for the transport equation is obtained by multiplying Eq. (2) by any test function  $b$ , integrating over element  $K$ , applying the divergence theorem to the streaming term, and using the standard upwind technique for the angular flux at the element's boundaries. A compact notation for the weak form over element  $K$ , for an angular direction  $\vec{\Omega}_m$ , is as follows:

$$\begin{aligned} & \left\langle (\vec{\Omega}_m \cdot \vec{n}) b, \psi_m \right\rangle_{\partial K^+} - \left( \vec{\Omega}_m \cdot \vec{\nabla} b, \psi_m \right)_K + \left( \sigma_t b, \psi_m \right)_K \\ & = \left( \frac{\sigma_s}{4\pi} b, \phi \right)_K + (b, Q_m)_K - \left\langle (\vec{\Omega}_m \cdot \vec{n}) b, \psi_m^\uparrow \right\rangle_{\partial K^-}. \end{aligned} \quad (5)$$

91 In Eq. (5),  $\partial K^\pm$  represents the outflow/inflow boundary of element  $K$  (with respect to direction  $\vec{\Omega}_m$ ),

$$\partial K^\pm = \left\{ \vec{r} \in \partial K \mid \vec{\Omega}_m \cdot \vec{n}_K(\vec{r}) \gtrless 0 \right\}, \quad (6)$$

92 with  $\vec{n}_K(\vec{r})$  the outward unit normal vector at location  $\vec{r}$ ,  $\psi_m^\uparrow$  are the angular flux values on an inflow face  
93 taken from the upwind neighbor element, and the inner products

$$(u, v)_K \equiv \int_K u v d\vec{r} \quad \text{and} \quad \langle u, v \rangle_{\partial K} \equiv \int_{\partial K} u v ds \quad (7)$$

94 correspond to integrations over the cell volume and faces, respectively, where  $d\vec{r} \in \mathbb{R}^d$  is within the cell and  
95  $ds \in \mathbb{R}^{d-1}$  is along the cell boundary. In Eq. (5), all angular flux unknowns “live on” element  $K$ , except for  
96 the upwind values which are taken from the upwind neighboring element:

$$\psi_m^\uparrow(\vec{r}) = \lim_{s \rightarrow 0^+} \psi_m(\vec{r} + s\vec{n}_K(\vec{r})), \quad \vec{r} \in \partial K^-. \quad (8)$$

97 The spatial convergence of DGFEM methods for hyperbolic systems has been extensively studied [3, 32,  
98 33, 22]. With the discretized flux solution,  $\phi_h \in W_D^h$ , corresponding to our unstructured mesh,  $\mathbb{T}_h$ , we can  
99 define an error for our DGFEM transport solution with the  $L_2$ -norm as

$$\|\phi_h - \phi_{exact}\|_{L_2} \leq C \frac{h^q}{(p+1)^{q-1/2}}. \quad (9)$$

100 In Eq. (9),  $q = \min(p+1, r)$ ,  $h$  is the maximum diameter of all the mesh elements,  $p$  is the polynomial  
101 completeness of the finite element function space,  $r$  is the regularity index of the transport solution, and  
102  $C$  is a constant that is independent of the mesh employed. Therefore, the DGFEM transport convergence  
103 rates are limited by the regularity,  $r$ , of the solution space. If we have sufficiently smooth data, then we  
104 have, at most, a solution regularity of  $r = 3/2$ . However, in the case of a pure absorber or void, the solution  
105 regularity diminishes to  $r = 1/2$ . From these indices, one would think that the transport solution regularity  
106 would impede the use of higher-order finite element spaces. We note, however, that these regularity indices  
107 only apply to the asymptotic convergence range, which usually only applies to very fine meshes that are  
108 much smaller than typically employed meshes. Therefore, we expect to capture up to order  $(p+1)$  in  
109 preasymptotic ranges that would be employed for a wide variety of transport problems.

110 We can also define the DGFEM transport solution convergence rates in terms of the total number of  
111 spatial degrees of freedom,  $N_{dof}$ , instead of the maximum element diameter,  $h$ . We first relate the total  
112 number of mesh elements,  $N_{ele}$ , to the maximum element diameter:  $N_{ele} \propto h^{-d}$ , where we assume that the  
113 polygonal elements are strictly-convex. We then assume that the finite element functional space on each  
114 element is the serendipity space [34]. This means that the number of degrees of freedom per element is  
115 proportional to the polynomial order:  $N_{dof} \propto p h^{-d}$  or  $h \propto \left(\frac{N_{dof}}{p}\right)^{-1/d}$ . Substituting this relation into

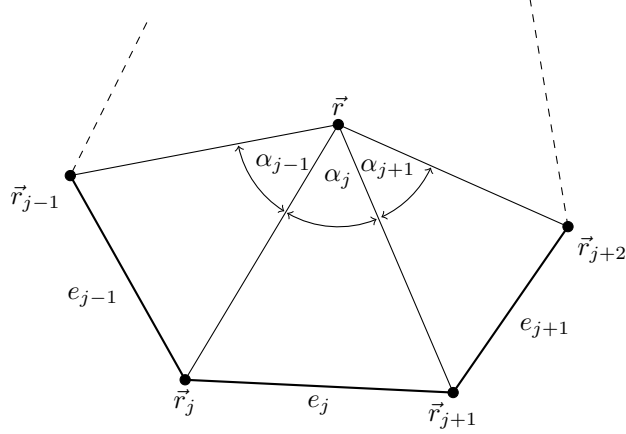


Figure 2: Arbitrary polygon with geometric properties used for 2D basis function generation.

Eq. (9), yields an  $L_2$ -norm convergence rate in terms of the problem's total number of spatial degrees of freedom,

$$\|\phi_h - \phi_{exact}\|_{L_2} \leq C(p) (N_{dof})^{-q/d}, \quad C(p) = \frac{p^{q/d}}{(p+1)^{q-1/2}}. \quad (10)$$

### 3. Linear Polygonal Basis Functions

We now describe the linear polygonal functions that we will analyze where any geometric notations are given by Figure 2. To achieve the maximum possible solution convergence rate of Eq. (9), these functions need to exactly interpolate the  $\{1, x, y\}$  span of functions. For this work, we will utilize a family of linear functions known as Generalized Barycentric Coordinates (GBC) [35]. In particular, we investigated the Wachspress functions, the piecewise linear functions, the mean value functions, and the maximum entropy functions. These functions (denoted as  $\{\lambda_j\}_{j=1}^n$  on a polygon with  $n$  vertices) have the following properties:

1. Positivity:  $\lambda_j \geq 0$ ;
2. Partition of unity:  $\sum_{j=1}^n \lambda_j = 1$ ;
3. Affine combination:  $\sum_{j=1}^n \vec{r}_j \lambda_j(\vec{r}) = \vec{r}$ ;
4. Lagrange property:  $\lambda_i(\vec{r}_j) = \delta_{ij}$ ;
5. Piecewise boundary linearity:  $\lambda_j((1-\mu)\vec{r}_j + \mu\vec{r}_{j+1}) = (1-\mu)\lambda_j(\vec{r}_j) + \mu\lambda_j(\vec{r}_{j+1})$ ,  $\mu \in [0, 1]$ .

We can see from properties 2 and 3 that the GBCs span the  $\{1, x, y\}$  space and can exactly interpolate constant and linear functions.

### 3.1. Wachspress Rational Functions

The first linearly-complete polygonal functions that we consider are the Wachspress rational functions [36]. These rational functions were originally derived for 2D polygons and possess all the properties of the barycentric functions. However, they are only valid interpolants over strictly-convex polygons. Weakly-convex polygons (containing colinear vertices) lose piecewise linearity on the boundary. Concave polygons have regions within their domain that are undefined and divide-by-zero occurs. The Wachspress functions (which we denote as  $\lambda^W$ ) have the following form

$$\lambda_j^W(\vec{r}) = \frac{w_j(\vec{r})}{\sum_{i=1}^n w_i(\vec{r})}, \quad (11)$$

where the Wachspress weight function for vertex  $j$ ,  $w_j$ , has the following definition:

$$w_j(\vec{r}) = \frac{A(\vec{r}_{j-1}, \vec{r}_j, \vec{r}_{j+1})}{A(\vec{r}, \vec{r}_{j-1}, \vec{r}_j) A(\vec{r}, \vec{r}_j, \vec{r}_{j+1})}. \quad (12)$$

In Eq. (12), the terms  $A(\vec{a}, \vec{b}, \vec{c})$  denote the signed area of the triangle with vertices  $\vec{a}$ ,  $\vec{b}$ , and  $\vec{c}$ . Each of these signed areas can be computed by

$$A(\vec{a}, \vec{b}, \vec{c}) = \frac{1}{2} \begin{vmatrix} 1 & 1 & 1 \\ x_a & x_b & x_c \\ y_a & y_b & y_c \end{vmatrix}. \quad (13)$$

Through observation of Eq. (12), we can see that the denominator of  $w_j$  goes to zero on faces  $e_j$  and  $e_{j+1}$ . This makes numerical evaluation of the Wachspress functions impossible on the boundary of the element boundary. However, the functions do have valid limits on the boundary as shown in Appendix A.

### 3.2. Piecewise Linear Functions

The second linearly-complete 2D polygonal functions that we will analyze are the piecewise linear (PWL) functions proposed by Stone and Adams [37, 15]. The 2D PWL functions are defined as combinations of linear triangular functions, with some of them only having measure within a subregion of a polygon. These subregions are formed by triangulating the arbitrary 2D polygon into a set of sub-triangles. Each sub-triangle is defined by two adjacent vertices of the polygon and the polygon's centroid,  $\vec{r}_c$ . The polygon's centroid can be defined by

$$\vec{r}_c = \sum_{j=1}^n \alpha_j \vec{r}_j, \quad (14)$$

where  $\alpha_j$  are the vertex weights functions and,

$$\sum_{j=1}^n \alpha_j = 1. \quad (15)$$

For this work, we continue to use the definition for the vertex weight functions from previous works [37, 15, 16]:  $\alpha_j = 1/n$ . Therefore, the vertex weight functions are the same for every vertex, and the cell centroid simply becomes the average position of all the vertices. Using these vertex weight functions, the PWL basis function for vertex  $j$ ,  $\lambda_j^{PWL}$ , is defined as

$$\lambda_j^{PWL}(\vec{r}) = t_j(\vec{r}) + \alpha_j t_c(\vec{r}). \quad (16)$$

In Eq. (16),  $t_j$  is the standard 2D linear function with unity at vertex  $j$  that linearly decreases to zero at the cell center and each adjoining vertex.  $t_c$  is the 2D cell “tent” function located at  $\vec{r}_c$  which is unity at the cell center and linearly decreases to zero at each cell vertex. The functional form of Eq. (16) with identical vertex weights means that the PWL function for vertex  $j$ , within the domain of the polygon, linearly decreases to a value of  $1/n$  at the polygonal center. From there, the function linearly decreases to zero on all faces that are not connected to vertex  $j$ .

### 3.3. Mean Value Functions

The third linearly-complete 2D polygonal functions that we will analyze are the mean value functions (MV) [38]. These functions were derived to approximate harmonic maps on a polygon by a set of piecewise linear maps over a triangulation of the polygon for use in computer aided graphic design. The mean value function at vertex  $j$ ,  $\lambda_j^{MV}$ , is defined as

$$\lambda_j^{MV}(\vec{r}) = \frac{w_j(\vec{r})}{\sum_{i=1}^n w_i(\vec{r})}, \quad (17)$$

where the mean value weight function for vertex  $j$ ,  $w_j$ , has the following definition:

$$w_j(\vec{r}) = \frac{\tan(\alpha_{j-1}/2) + \tan(\alpha_j/2)}{|\vec{r}_j - \vec{r}|}. \quad (18)$$

Similar to the Wachspress functions, we can observe from Eq. (18) that the numerator of  $w_j$  tends to infinity on faces  $e_j$  and  $e_{j+1}$  as  $\alpha_j \rightarrow \pi/2$ . Again, the MV functions have valid limits on the boundary as shown in Appendix A.

### 3.4. Maximum Entropy Functions

The final linearly-complete 2D polygonal functions that we investigate are the maximum entropy functions (ME) [39]. The principle of maximum entropy stems from the concept of Shannon entropy [40], where the maximum of the Shannon entropy function,  $H$ , will lead to the least-biased statistical inference for



176 some set of testable constraints [41]. In FEM analysis, these testable constraints are the partition of unity  
 177 and the affine combination properties of the barycentric functions. For  $n$  discrete probability functions  
 178 (corresponding to the  $n$  vertex functions), the functional form for the Shannon entropy can be given by

$$H(\vec{b}, \vec{m}, \vec{r}) = - \sum_{j=1}^n b_j(\vec{r}) \log \left( \frac{b_j(\vec{r})}{m_j(\vec{r})} \right), \quad (19)$$

179 where  $m_j$  is called the prior distribution. If  $(\lambda_j^{ME}(\vec{x}), j = 1, \dots, n)$  is the solution of the following constrained  
 180 optimization problem

$$\max_{\vec{b}(\vec{r})} H(\vec{b}, \vec{m}, \vec{r}), \quad (20)$$

181 then the maximum entropy functions can be given by

$$\lambda_j^{ME}(\vec{r}) = \frac{w_j(\vec{r})}{\sum_{i=1}^n w_i(\vec{r})}, \quad (21)$$

182 where the maximum entropy weight function for vertex  $j$ ,  $w_j$ , has the following definition,

$$w_j(\vec{r}) = m_j(\vec{r}) \exp(-\vec{\kappa} \cdot (\vec{r}_j - \vec{r})), \quad (22)$$

183 and  $\vec{\kappa}$  is a vector value of dimension  $d$  that will be explained shortly. In the context of Eq. (22), the  
 184 prior distribution,  $m_j$ , can be viewed as a weight function associated with vertex  $j$ . This means that there  
 185 is variability that one can employ for these weight functions. For FEM applications [42], an appropriate  
 186 functional form for the prior distribution is given by

$$m_j(\vec{r}) = \frac{\pi_j(\vec{r})}{\sum_{k=1}^n \pi_k(\vec{r})}, \quad (23)$$

187 where

$$\pi_j(\vec{r}) = \prod_{k \neq j-1, j}^n \rho_k(\vec{r}) = \rho_1(\vec{r}) \dots \rho_{j-2}(\vec{r}) \rho_{j+1}(\vec{r}) \dots \rho_n(\vec{r}), \quad (24)$$

188 and

$$\rho_j(\vec{r}) = \|\vec{r} - \vec{r}_j\| + \|\vec{r} - \vec{r}_{j+1}\| - \|\vec{r}_{j+1} - \vec{r}_j\|. \quad (25)$$

189 In Eqs. (24) and (25), we have defined a new function,  $\rho_j$ , that corresponds to face  $e_j$  between vertices  $j$   
 190 and  $j + 1$ . These face functions are zero along face  $e_j$ , but strictly positive elsewhere due to the triangle  
 191 inequality. This means that the vertex function,  $\pi_j$ , is also non-negative and vanishes on all faces that are  
 192 not adjacent to vertex  $j$ . We note that  $m_j(\vec{r}_j) = 1$ .

To complete the definition of the ME functions, we now explain how the  $\vec{\kappa}$  vector in Eq. (22) is computed. We can see that once  $\vec{\kappa}$  is known, the ME functions can be directly calculated. To obtain  $\vec{\kappa}$ , we solve the constrained optimization problem of Eq. (20) through the use of Lagrange multipliers with a Newton's method. Let  $\kappa_0$  be the Lagrange multiplier for the constant constraint and  $\vec{\kappa}$  be the Lagrangian multiplier for the affine constraint, then the Lagrangian for the problem of Eq. (20) is given by

$$\mathcal{L}(\vec{b}; \kappa_0, \vec{\kappa}) = - \sum_{j=1}^n b_j \log \left( \frac{b_j}{m_j} \right) - \kappa_0 \left( \sum_{j=1}^n b_j - 1 \right) - \vec{\kappa} \cdot \left( \sum_{j=1}^n b_j (\vec{r}_j - \vec{r}) \right), \quad (26)$$

where we omitted the spatial parameter  $\vec{r}$  for brevity and differentiate between  $\vec{b}$  and  $\vec{\kappa}$  being vectors of lengths  $n$  and  $d$ , respectively. If we define  $W = \sum_{j=1}^n w_j(\vec{r})$ , then the solution of Eq. (21) is equivalent to solving the following dual unconstrained optimization problem [43]:

$$\vec{\kappa}^* = \min_{\vec{\kappa}} F(\vec{\kappa}), \quad F(\vec{\kappa}) = \log W(\vec{\kappa}). \quad (27)$$

### 3.5. Summary of the Linear Polygonal Basis Functions

For this work, we are analyzing four different linear barycentric functions for use as our FEM basis functions: the Wachspress rational functions, the piecewise linear functions, the mean value functions, and the maximum entropy functions. Table 1 provides a summary of the properties for the different functions. The PWL, MV, and ME functions can interpolate degenerate-convex and concave polygons while the Wachspress functions can only interpolate strictly-convex polygons. Using geometric information for a given polygonal cell, the Wachspress, PWL, and MV functions can be directly evaluated, whereas the ME functions require an iterative approach with Newton's method since their functional form constitutes a non-linear optimization problem. Finally, the elementary matrices of Eq. (5) can be integrated analytically with the PWL functions. The Wachspress, MV, and ME functions need to be integrated numerically.

We conclude our discussion of the linear barycentric functions by providing some example contour plots. Figure 3 provides the contour plots of the different functions located at vertex  $(0, 1)$  on the unit square. Figure 4 provides the contour plots on the degenerate pentagon that is formed by inserting a vertex at  $(1/2, 1)$  into the unit square. This re-emphasizes that the Wachspress functions are only valid interpolatory functions on strongly-convex polygons. Finally, Figure 5 provides the contour plots of the PWL, MV, and ME functions on the L-shaped domain at the  $(0, 1)$  and  $(1/2, 1/2)$  vertices.

## 4. Quadratic Serendipity Polygonal Basis Functions

We have fully-defined the linearly-complete generalized barycentric functions that will be used to derive the quadratic serendipity functions. These 2D serendipity functions can exactly interpolate the  $\{1, x, y, x^2, xy, y^2\}$

Table 1: Summary of the properties of the 2D barycentric functions.

Basis Function	Polygon Type	Evaluation	Integration
Wachspress	Convex	Direct	Numerical
Piecewise Linear	Convex/Concave	Direct	Analytical
Mean Value	Convex/Concave	Direct	Numerical
Max Entropy	Convex/Concave	Iterative	Numerical

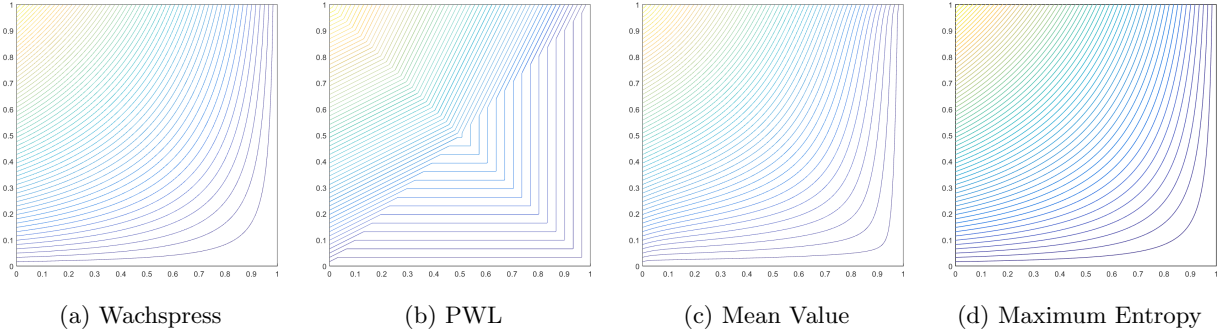


Figure 3: Contour plots of the different linear basis function on the unit square located at vertex (0,1).

span of functions. Next, we describe how to convert any generalized barycentric function into the quadratic serendipity space of functions to yield quadratic precision based on the work of Rand et al. [29]. The linear maximum entropy functions were independently converted into the quadratic serendipity space by other researchers [44, 45].

Figure 6 gives a visual depiction of this conversion process. For a polygon with  $n$  vertices, we can summarize this procedure as the following:

1. For a point  $\vec{r}$ , compute the  $n$  linear barycentric functions  $\{\lambda_i(\vec{r})\}$  (*e.g.*, Wachspress, mean value, or maximum entropy);
2. Take all non-repeating pairwise products of the linear functions to obtain  $\frac{n(n+1)}{2}$  quadratic functions  $\{\mu_{ab}(\vec{r})\}$ ;
3. Form the linear transformation matrix  $\mathbb{A}$  through the use of monomial constraint equations;
4. Use the  $\mathbb{A}$  matrix to reduce the  $\{\mu_{ab}(\vec{r})\}$  function set to the  $2n$  serendipity basis set  $\{\xi_{ij}(\vec{r})\}$ .

We begin by computing the  $(i = 1, \dots, n)$  linear barycentric functions,  $\{\lambda_i(\vec{r})\}$ , and their gradients,  $\{\vec{\nabla}\lambda_i(\vec{r})\}$ , for a point  $\vec{r}$ . These evaluation points will correspond to spatial quadrature points to compute the FEM integrals of Eq. (5). These linearly-complete barycentric functions can be converted immediately to barycentric-like functions with quadratic precision. Taking all non-repeating pairwise products of the linear functions yields a total of  $N_Q = \frac{n(n+1)}{2}$  quadratic functions:  $\mu_{ab} = \lambda_a \lambda_b$  ( $1 \leq a \leq n; 1 \leq a \leq b$ ).

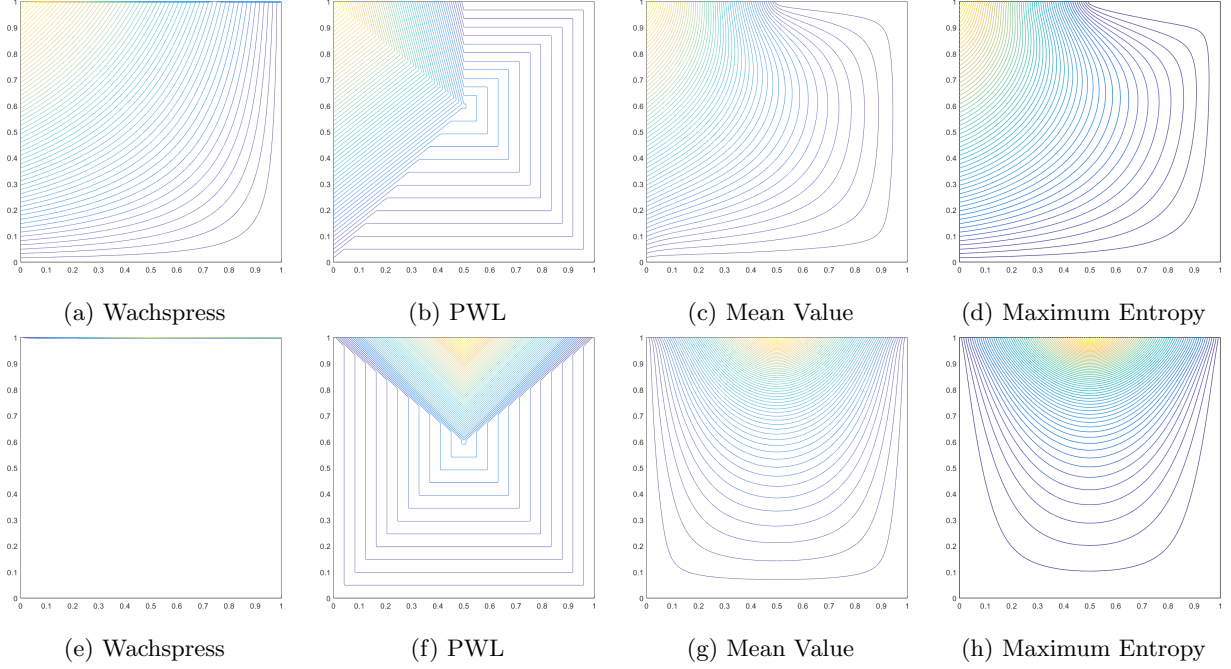


Figure 4: Contour plots of the different linear basis function on the degenerate pentagon located at vertex (0,1) (a-d) and vertex (1/2,0) (e-h). The Wachspress functions clearly fail for the weakly convex case.

237 Doing this generates functions that either live on the polygon's vertices, mid-face points, or midpoints of  
 238 the polygon's interior diagonals between two vertices as seen in Figure 6. The set of  $n$  vertex functions  
 239 is denoted as  $V$  ( $a = b$ ), the set of  $n$  mid-face (mid-edge) functions is denoted as  $E$  ( $|a - b| = 1$ ), and  
 240 the set of  $\frac{n(n-3)}{2}$  interior functions is denoted as  $I$  ( $|a - b| > 1$ ). For the mid-edge and interior functions,  
 241 only 1 combination of  $ab$  is kept since  $\mu_{ab} = \mu_{ba}$ . We also define the abbreviated notation of  $\vec{r}_{ab} = \frac{\vec{r}_a + \vec{r}_b}{2}$ .  
 242 Using these various notations, we can write the precision properties of the  $\mu_{ab}$  functions for the constant  
 243 constraint,

$$\sum_{aa \in V} \mu_{aa}(\vec{r}) + \sum_{ab \in E \cup I} 2\mu_{ab}(\vec{r}) = 1, \quad (28)$$

244 for the linear constraint,

$$\sum_{aa \in V} \mu_{aa}(\vec{r}) \vec{r}_a + \sum_{ab \in E \cup I} 2\mu_{ab}(\vec{r}) \vec{r}_{ab} = \vec{r}, \quad (29)$$

245 and for the quadratic constraint,

$$\sum_{aa \in V} \mu_{aa}(\vec{r}) (\vec{r}_a \otimes \vec{r}_a) + \sum_{ab \in E \cup I} \mu_{ab}(\vec{r}) (\vec{r}_a \otimes \vec{r}_b + \vec{r}_b \otimes \vec{r}_a) = \vec{r} \otimes \vec{r}. \quad (30)$$

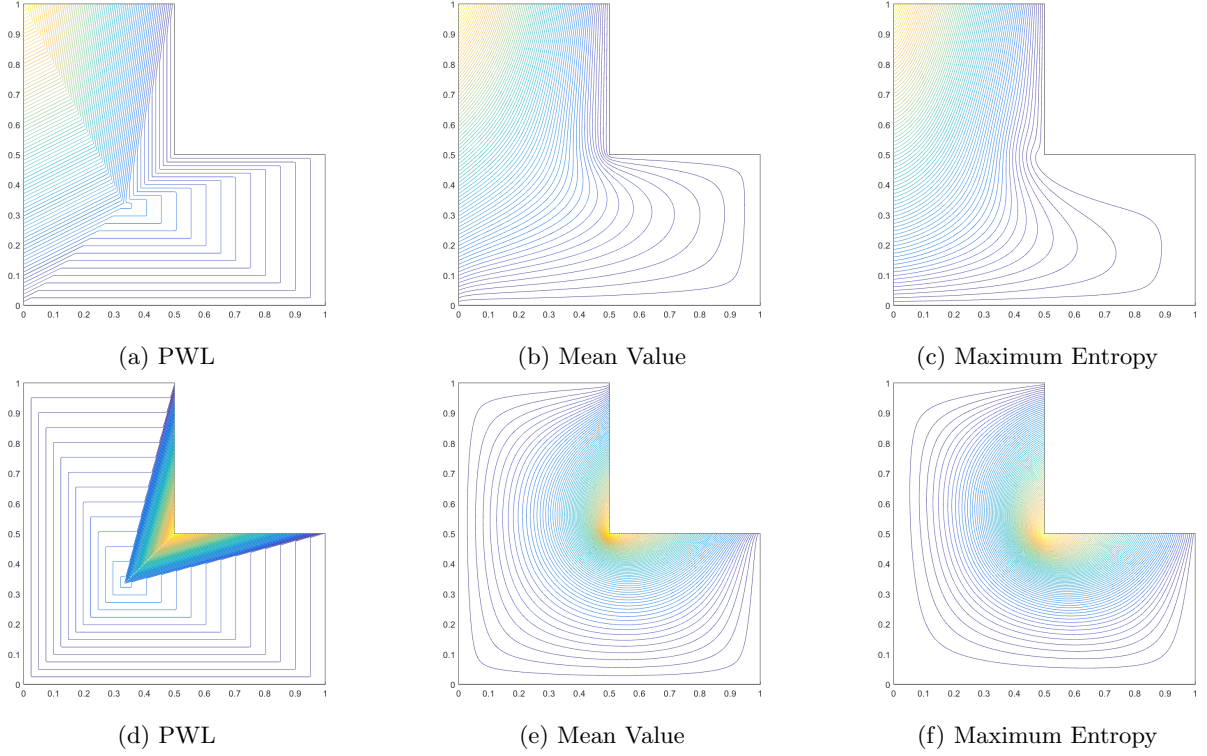


Figure 5: Contour plots of the mean value and maximum entropy functions on the L-shaped domain at vertex (0,1) (a-c) and vertex (1/2, 1/2) (d-f).

In Eq. (30),  $\otimes$  is the dyadic tensor product. We can immediately see that quadratic precision is ensured. However, the set of these pairwise quadratic functions grows quadratically. This means that as  $n$  grows large, the number of interpolatory functions grows as order  $O(n^2)$ , but still only maintains precision of the  $\{1, x, y, x^2, xy, y^2\}$  space of functions. Therefore, the computational work required to utilize these quadratic barycentric functions can become prohibitive for polygons with large vertex counts.

To minimize the number of interpolatory functions but still maintain the precision of the  $\{1, x, y, x^2, xy, y^2\}$  span of functions, we seek to convert the quadratic barycentric functions into the quadratic serendipity space of functions  $\{\xi_{ij}\}$ . This quadratic serendipity space only contains the vertex and mid-face functions (total of  $2n$ ) and has been extensively studied for tensor-based elements in the past [34]. This means that we seek to reduce the  $\{\mu_{ab}\}$  set of functions by removing the interior functions ( $ab \in I$ ) while still maintaining quadratic precision. If we define  $\xi_{ii}$  and  $\xi_{i(i+1)}$  as the serendipity functions that live at vertex  $i$  and the mid-face point between vertices  $i$  and  $i+1$ , respectively, then we can write the serendipity precision properties for the constant constraint,

$$\sum_{ii \in V} \xi_{ii}(\vec{r}) + \sum_{i(i+1) \in E} 2\xi_{i(i+1)}(\vec{r}) = 1, \quad (31)$$

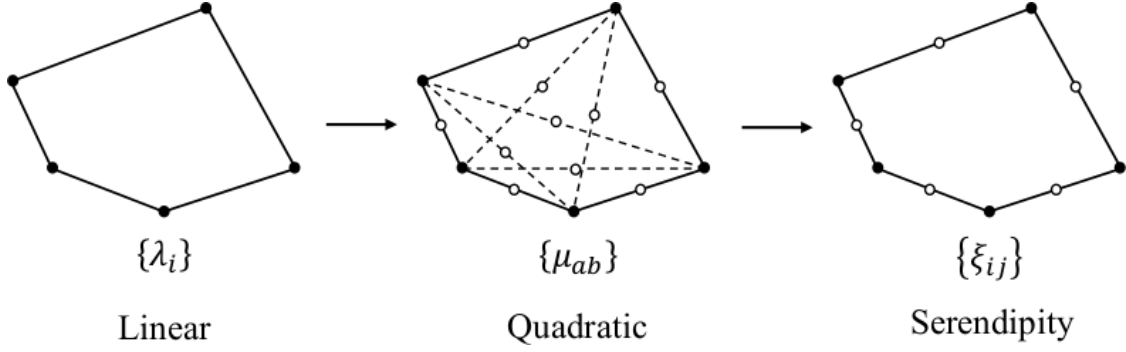


Figure 6: Overview of the process to construct the quadratic serendipity basis functions on polygons. The filled dots correspond to basis functions that maintain the Lagrange property while empty dots do not.

for the linear constraint,

$$\sum_{ii \in V} \xi_{ii}(\vec{r}) \vec{r}_{ii} + \sum_{i(i+1) \in E} 2\xi_{i(i+1)}(\vec{r}) \vec{r}_{i(i+1)} = \vec{r}, \quad (32)$$

and for the quadratic constraint,

$$\sum_{ii \in V} \xi_{ii}(\vec{r}) (\vec{r}_i \otimes \vec{r}_i) + \sum_{i(i+1) \in E} \xi_{i(i+1)}(\vec{r}) (\vec{r}_i \otimes \vec{r}_{i+1} + \vec{r}_{i+1} \otimes \vec{r}_i) = \vec{r} \otimes \vec{r}. \quad (33)$$

To remove the interior functions, we formalize this procedure by recasting it as a linear algebra problem. We seek a matrix  $\mathbb{A}$  such that the linear transformation,

$$\{\xi\} = \mathbb{A} \{\mu\}, \quad (34)$$

will satisfy the precision properties of Eqs. (31 - 33). It is easy to see that  $\mathbb{A}$  has dimension  $(2n \times N_Q)$ . We wish for this matrix to have constant entries for any point within the polygon's interior so that it does not have to be recalculated for each interpolatory quadrature point of interest. To ease the notation, we will assign specific basis orderings for the quadratic and quadratic serendipity functions. The serendipity basis is ordered such that all vertex functions ( $ii \in V$ ) in a counter-clockwise ordering are first, followed by a counter-clockwise ordering of the mid-face nodes ( $ij \in E$ ) starting with the node between vertices 1 and 2. This ordering can be succinctly stated by

$$\{\xi_{ij}\} = \left\{ [\xi_{11}, \xi_{22}, \dots, \xi_{nn}], [\xi_{12}, \xi_{23}, \dots, \xi_{(n-1)n}, \xi_{n(n+1)}] \right\}, \quad (35)$$

where  $n + 1$  is understood to be 1. The quadratic basis begins identically to the serendipity basis by first listing the vertex and mid-face functions. Then the interior functions are indexed in lexicographical order. This gives the following ordering for the quadratic functions

$$\{\mu_{ab}\} = \left\{ [\mu_{11}, \mu_{22}, \dots, \mu_{nn}], [\mu_{12}, \mu_{23}, \dots, \mu_{(n-1)n}, \mu_{n(n+1)}], \right. \\ \left. [\mu_{13}, \dots, (\text{lexicographical}), \dots, \mu_{(n-2)n}] \right\}. \quad (36)$$

273 With these basis orderings, we can now denote the entries of  $\mathbb{A}$  (given by  $c_{ab}^{ij}$ ) as

$$\mathbb{A} = \begin{bmatrix} c_{11}^{11} & \dots & c_{ab}^{11} & \dots & c_{(n-2)n}^{11} \\ \dots & \ddots & \vdots & \ddots & \vdots \\ c_{11}^{ij} & \dots & c_{ab}^{ij} & \dots & c_{(n-2)n}^{ij} \\ \dots & \ddots & \vdots & \ddots & \vdots \\ c_{11}^{n(n+1)} & \dots & c_{ab}^{n(n+1)} & \dots & c_{(n-2)n}^{n(n+1)} \end{bmatrix}, \quad (37)$$

274 A sufficient set of constraints for the entries in  $\mathbb{A}$  to ensure the precision properties of Eqs. (31 - 33) can  
275 be written for the constant constraint,

$$\sum_{ii \in V} c_{aa}^{ii} + \sum_{i(i+1) \in E} 2c_{aa}^{i(i+1)} = 1, \quad \forall aa \in V \\ \sum_{ii \in V} c_{ab}^{ii} + \sum_{i(i+1) \in E} 2c_{ab}^{i(i+1)} = 2, \quad \forall ab \in E \cup I \quad (38)$$

276 for the linear constraint,

$$\sum_{ii \in V} c_{aa}^{ii} \vec{r}_{ii} + \sum_{i(i+1) \in E} 2c_{aa}^{i(i+1)} \vec{r}_{i(i+1)} = \vec{r}_{aa}, \quad \forall aa \in V \\ \sum_{ii \in V} c_{ab}^{ii} \vec{r}_{ii} + \sum_{i(i+1) \in E} 2c_{ab}^{i(i+1)} \vec{r}_{i(i+1)} = 2\vec{r}_{ab}, \quad \forall ab \in E \cup I \quad (39)$$

277 for the  $a \in V$  vertex quadratic constraints,

$$\sum_{ii \in V} c_{aa}^{ii} \vec{r}_{ii} \otimes \vec{r}_{ii} + \sum_{i(i+1) \in E} c_{aa}^{i(i+1)} (\vec{r}_i \otimes \vec{r}_{i+1} + \vec{r}_{i+1} \otimes \vec{r}_i) = \vec{r}_{aa} \otimes \vec{r}_{aa}, \quad (40)$$

278 and for the  $ab \in E \cup I$  mid-face and interior quadratic constraints,

$$\sum_{ii \in V} c_{ab}^{ii} \vec{r}_{ii} \otimes \vec{r}_{ii} + \sum_{i(i+1) \in E} c_{ab}^{i(i+1)} (\vec{r}_i \otimes \vec{r}_{i+1} + \vec{r}_{i+1} \otimes \vec{r}_i) = (\vec{r}_a \otimes \vec{r}_b + \vec{r}_b \otimes \vec{r}_a). \quad (41)$$

279 For  $n > 3$ , there are more coefficients than the six constraint equations. This means that there is flexibility  
280 in the construction of the solution to the constraint equations. Therefore, we choose a simple structure for  
281  $\mathbb{A}$  that consists of the following,

$$\mathbb{A} = [\mathbb{I} \mid \mathbb{A}'], \quad (42)$$

where  $\mathbb{I}$  is the  $(2n \times 2n)$  identity matrix, and  $\mathbb{A}'$  is a full  $(2n \times \frac{n(n-3)}{2})$  matrix. This means that the vertex and face midpoint serendipity functions,  $\xi_{ij}$ , are formed by taking their corresponding quadratic function and adding some linear combination of the interior functions. Therefore, we only need to determine the  $\frac{n(n-3)}{2}$  columns of the  $\mathbb{A}'$  matrix to complete this linear transformation.

In their work, Rand et al. proposed a methodology where only six coefficients are chosen to be non-zero and can be directly calculated through geometric expressions. However, their approach is only valid for strictly-convex polygons. This will not work for our analysis since we wish to also analyze degenerate polygons that will arise in our AMR calculations. Therefore, we will use a least squares method to calculate each of the columns of  $\mathbb{A}'$ . We note that the coefficients calculated with this least squares method and that of Rand will be identical only for rectangles. If we isolate the column  $(ab)$  from  $\mathbb{A}'$ , then we can form the following system of equations,

$$\mathbb{B}\vec{c}_{ab} = \vec{q}_{ab}, \quad (43)$$

where  $\mathbb{B}$  is a matrix of dimension  $(6 \times 2n)$ ,  $\vec{c}_{ab}$  is a vector of length  $2n$ , and  $\vec{q}_{ab}$  is a vector of length 6. The entries of  $\mathbb{B}$  correspond to coefficients given in the left-hand-side terms of Eqs. (38), (39), and (41). The values of  $\vec{q}_{ab}$  are given by the right-hand-sides of these same equations. To invert  $\mathbb{B}$ , we use the Moore-Penrose pseudoinverse (denoted as  $\mathbb{B}^*$ ) [46]. For an under-determined system of equations, the pseudoinverse is given by,

$$\mathbb{B}^* = \mathbb{B}^T (\mathbb{B}\mathbb{B}^T)^{-1}. \quad (44)$$

We note that we have only tested this methodology on convex and weakly-convex polygons. Once all of the coefficients for the  $\mathbb{A}'$  matrix are known, each of the quadratic serendipity functions can be computed by

$$\xi_{ij} = \lambda_i \lambda_j + \sum_{ab \in D} c_{ab}^{ij} \lambda_a \lambda_b, \quad (45)$$

where  $j = i$  for the vertex functions and  $j = i + 1$  for the mid-face functions. From Eq. (45), we can clearly see that the quadratic functions,  $\mu_{ab}$ , act as an intermediate step and do not ever need to be explicitly computed.

We now present some example contour plots of the different quadratic serendipity functions. Figure 7 provides contour plots of the functions on the unit square. Then, Figure 8 provides the contour plots of the PWL, MV, and ME functions on the degenerate square that is formed by inserting a vertex at  $(1/2, 1)$  onto the unit square.



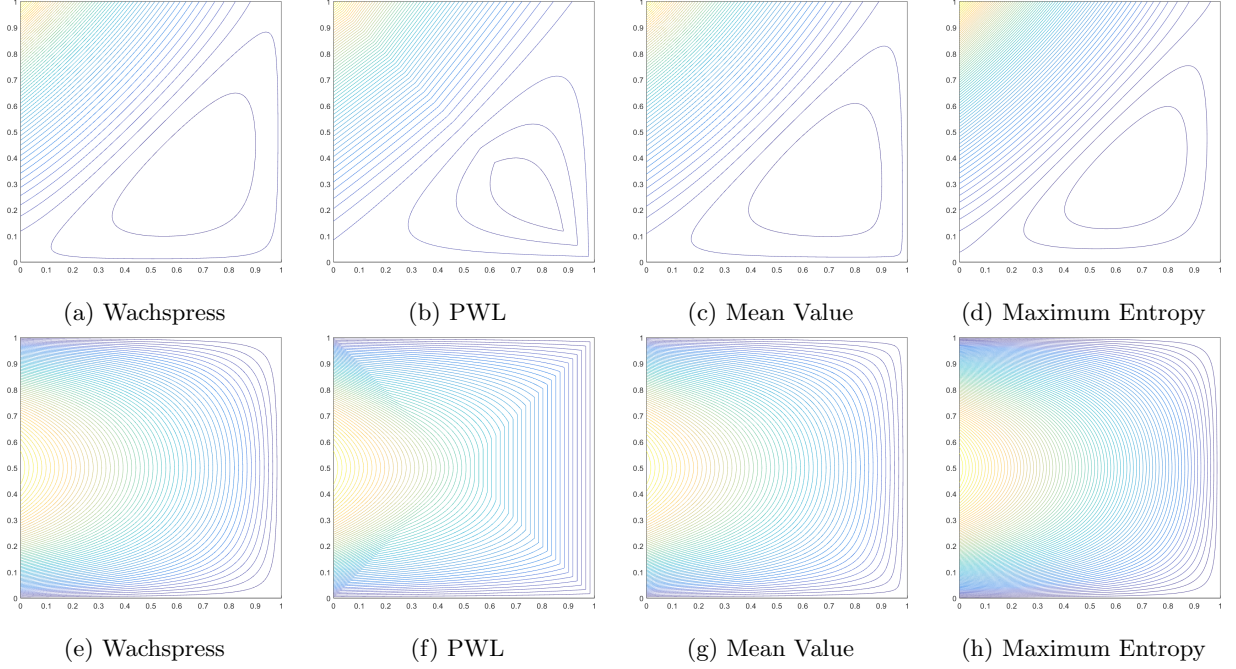


Figure 7: Contour plots of the different quadratic serendipity basis function on the unit square located at vertex (0,1) (a-d) and vertex (0,1/2) (e-h).

## 5. Adaptive Mesh Refinement Using Polygonal Basis Functions

Mesh adaptivity is a methodology that can accurately and efficiently capture solutions with strong and rapid spatial variations [47]. With spatial AMR, the mesh at refinement level  $r$ ,  $\mathbb{T}_h^\ell$ , is formed by selectively refining mesh cells from  $\mathbb{T}_h^{\ell-1}$  based on local error estimates. Using discontinuous functions, the magnitude of the solution jump across cell faces is proportional to the degree of spatial variation. Therefore, a heuristic local error indicator can monitor the interfacial jumps [48]. We define this jump-based error indicator for cell  $K$  and refinement level  $\ell$  as

$$\eta_K^\ell = \int_{\partial K} \llbracket \phi^\ell \rrbracket^2 ds = \int_{\partial K} \left( \sum_m w_m \llbracket \psi_m^\ell \rrbracket \right)^2, \quad (46)$$

where  $\llbracket \cdot \rrbracket$  is the jump operator along a face defined as

$$\llbracket \phi(\vec{r}) \rrbracket = \phi^+(\vec{r}) - \phi^-(\vec{r}), \quad (47)$$

and  $\phi^\pm(\vec{r}) = \lim_{s \rightarrow 0^\pm} \phi(\vec{r} + s\vec{n})$ . With the error estimates defined for all cells  $K \in \mathbb{T}_h^\ell$ , the criterion to determine the cells flagged for refinement is

$$\eta_K^\ell \geq \alpha \max_{K' \in \mathbb{T}_h^\ell} (\eta_{K'}^\ell), \quad (48)$$

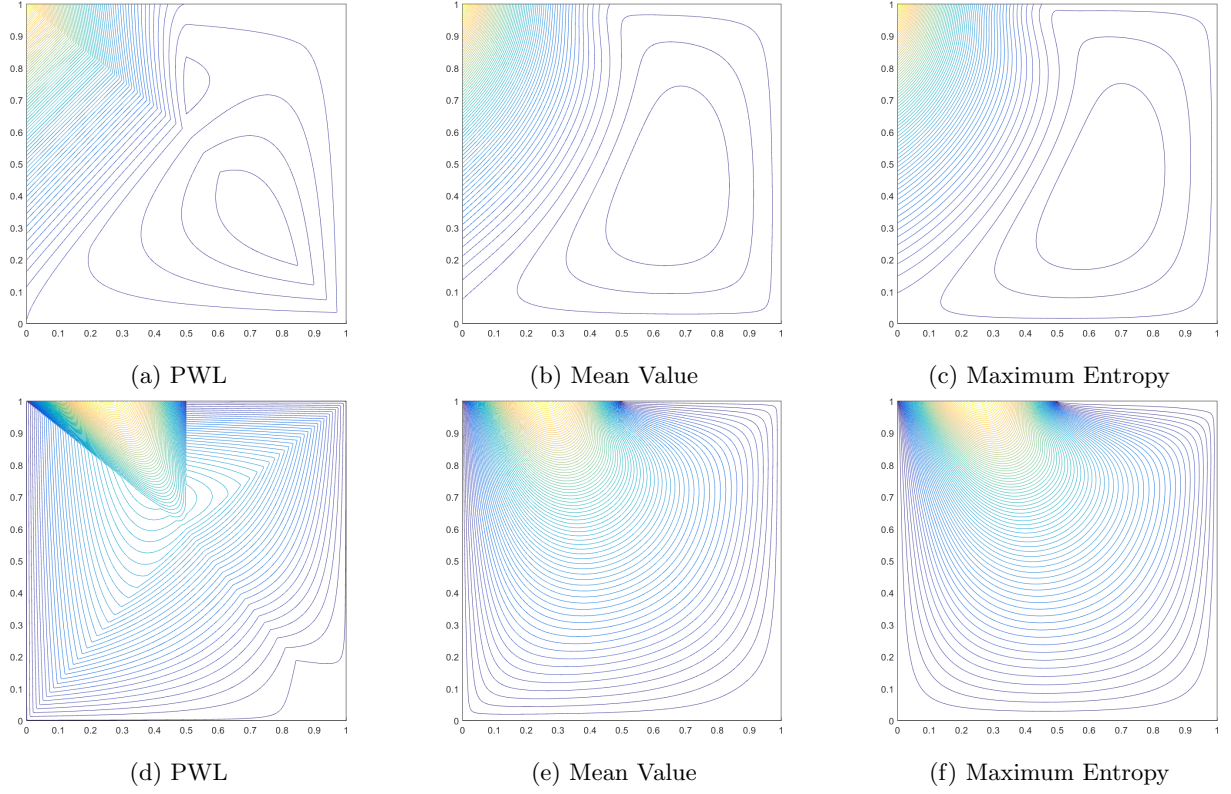


Figure 8: Contour plots of the different quadratic serendipity basis function on the unit degenerate pentagon located at vertex (0,1) (a-c) and mid-face node (1/4,1) (d-f).

where  $\alpha$  is a user-defined value (0,1). Equation (48) states that cells selected for refinement have error, normalized to the cell with the largest magnitude error, that is greater than or equal to  $\alpha$ .

For this work, we will only utilize  $h$ -type refinement strategies for 2D transport problems on initial meshes containing only quadrilateral cells. Refined parent cells are subdivided into four daughter cells where each daughter cell contains four vertices: one of the corner vertices of its parent, the midpoint of the two faces containing that corner, and the parent centroid.

## 6. Numerical Results

### 6.1. Exactly-Linear Transport Solutions

We first verify that the linear polygonal finite element basis functions capture an exactly-linear solution space. We will show this by the method of manufactured solutions (MMS) [49]. We build our exact solution by investigating the 2D, one energy group transport problem with no scattering and an angle-dependent distributed source,

$$\mu \frac{\partial \psi}{\partial x} + \eta \frac{\partial \psi}{\partial y} + \sigma_t \psi = Q(x, y, \mu, \eta), \quad (49)$$

where the streaming term was separated into the corresponding two-dimensional terms. We then define an angular flux solution that is linear in both space and angle along with the corresponding scalar flux solution:

$$\begin{aligned} \psi(x, y, \mu, \eta) &= ax + by + c\mu + d\eta + e \\ \phi(x, y) &= 4\pi (ax + by + e). \end{aligned} \quad (50)$$

Inserting the angular flux solution of Eq. (50) into Eq. (49) yields the following functional form for the distributed source:

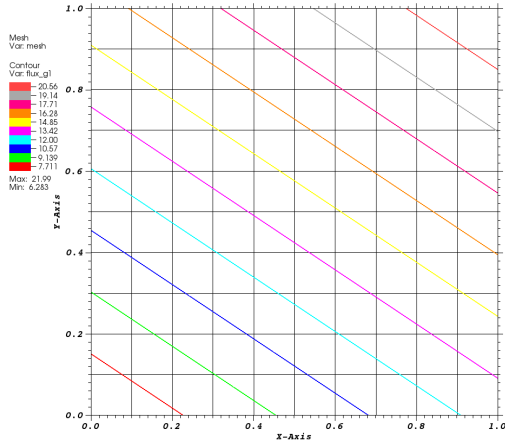
$$Q(x, y, \mu, \eta) = a\mu + b\eta + \sigma_t (c\mu + d\eta) + \sigma_t (ax + by + e). \quad (51)$$

Our boundary conditions for all inflow boundaries are uniquely determined by the angular flux solution of Eq. (50). We test the linear functions on six different mesh types, including triangular, quadrilateral, and polygonal meshes:

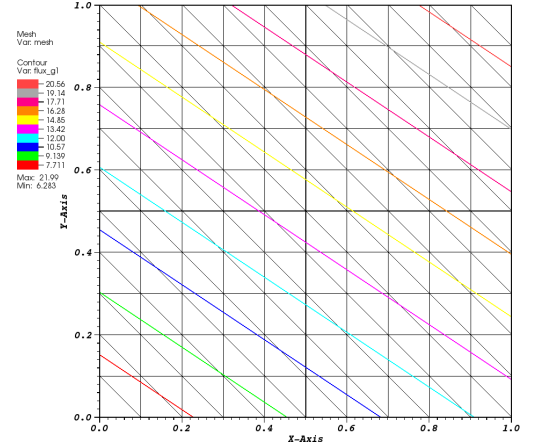
1. Orthogonal Cartesian mesh formed by the intersection of 11 equally-spaced vertices in both the  $x$  and  $y$  dimensions. This forms a 10x10 array of quadrilateral mesh cells.
2. Ordered-triangular mesh formed by the bisection of the previous orthogonal Cartesian mesh (forming 200 triangles all of the same size/shape).
3. Polygonal Shestakov grid formed by the randomization of vertices based on a skewness parameter [50, 51]. With a certain range of this skewness parameter, highly distorted meshes can be generated.
4. Sinusoidal polygonal grid that is generated by the transformation of a uniform orthogonal grid based on a sinusoid functional [52].
5. Kershaw's quadrilateral z-mesh [53]. This mesh is formed by taking an orthogonal quadrilateral grid and displacing certain interior vertices only in the  $y$  dimension.
6. A polygonal variant of the quadrilateral z-mesh.

The polygonal Shestakov grid, sinusoidal polygonal grid, and the polygonal z-mesh grid are formed by the conversion of an underlying quadrilateral grid into a corresponding polygonal grid by computing a bounded Voronoi diagram.

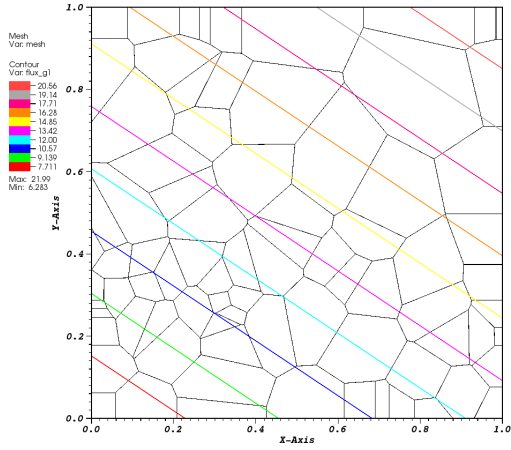
For this example, we use  $\sigma_t = a = c = d = e = 1.0$  and  $b = 1.5$ . The solution has a tilt in space ( $a \neq b$ ) so that it would not align with the triangular mesh. An  $S_8$  level-symmetric (LS) quadrature set [54] is used for all combinations of basis functions and mesh types. Figure 9 provides contour plots of the scalar flux solution for the Wachspress functions on the different meshes. We can see that an exactly-linear solution is captured as shown by the unbroken nature of the contour lines. The PWL, MV, and ME functions provide identical results and are not shown for brevity.



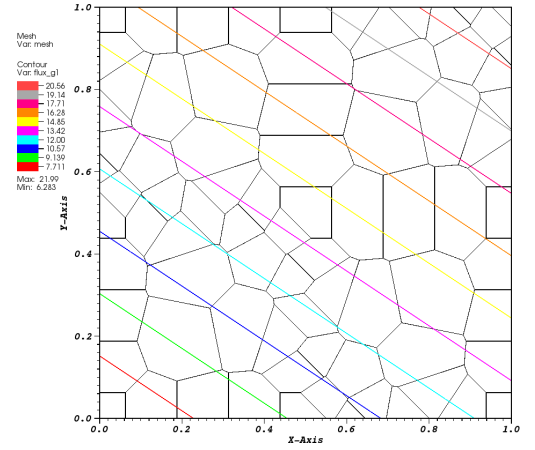
(a) Cartesian



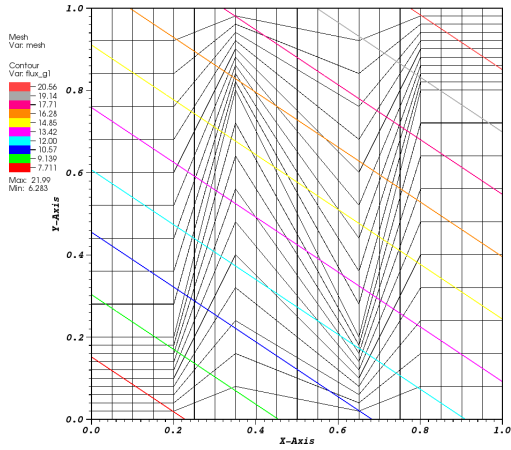
(b) Triangular



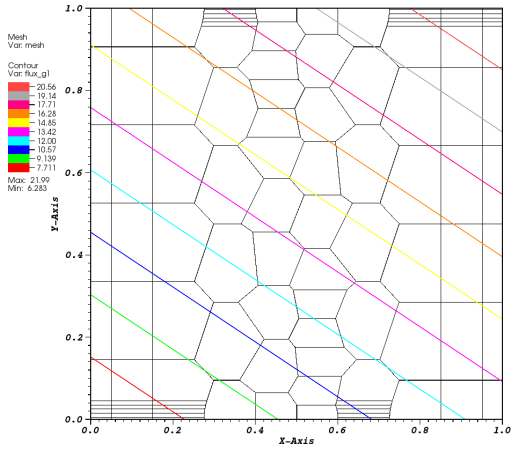
(c) Shestakov Polygons



(d) Sinusoid Polygons



(e) Z-Quadrilaterals



(f) Z-Polygons

Figure 9: Contour plots of the exactly-linear solution with the Wachspress basis functions. The PWL, MV, and ME functions yield identical results.

## 6.2. Exactly-Quadratic Transport Solutions

We next demonstrate that the quadratic serendipity basis functions capture the appropriate functional space, using two different MMS solutions. The first problem interpolates the  $\{1, x, y, x^2, xy, y^2\}$  span of functions, which we denote with the following exactly-quadratic spatial solution,  $\{\psi_q, \phi_q\}$ :

$$\begin{aligned}\psi_q(x, y, \mu, \eta) &= a + bx + cy + dxy + ex^2 + fy^2 + g\mu + h\eta + i\mu\eta + j\mu^2 + k\eta^2 \\ \phi_q(x, y) &= 4\pi \left( a + \frac{j+k}{3} + bx + cy + dxy + ex^2 + fy^2 \right).\end{aligned}\tag{52}$$

We clearly see that any combination of positive or negative (non-zero) values for the coefficients  $a - k$  will span the quadratic serendipity space, if the angular quadrature set can exactly integrate the  $\{\mu, \eta, \mu^2, \mu\eta, \eta^2\}$  functions. The second problem contains terms up to  $x^2y^2$ . This higher-order functional form has a solution,  $\{\psi_{x2y2}, \phi_{x2y2}\}$ , given by the following

$$\begin{aligned}\psi_{x2y2}(x, y) &= x(L_x - x)y(L_y - y) \\ \phi_{x2y2}(x, y) &= 4\pi x(L_x - x)y(L_y - y),\end{aligned}\tag{53}$$

where  $L_x$  and  $L_y$  are the dimensions of the domain in  $x$  and  $y$ . For this problem, we set  $L_x = L_y = 1$  and use the  $S_8$  LS quadrature set.

From the methodology presented in Section 4, we expect the quadratic serendipity functions to exactly capture the  $\phi_q$  solution but not the  $\phi_{x2y2}$  solution. For both problems, we use the same meshes utilized for the exactly-linear problem in Section 6.1. Tables 2 and 3 give the  $L_2$ -norm of the error for the quadratic and  $x^2y^2$  solutions, respectively. We can clearly see from the machine precision results, that the quadratic serendipity functions exactly capture the  $\phi_q$  solution. We note that the ME functions have higher norms since a tolerance value of  $10^{-14}$  was used for the Newton iterations to compute the linear ME functions. Likewise, we can see from Table 3 that the functions clearly do not capture the  $\phi_{x2y2}$  solution.

## 6.3. Convergence Rate Analysis Using MMS

After verifying the interpolation space of the linear and quadratic serendipity functions, we now demonstrate that the functions capture the appropriate theoretical convergence rates, by again using MMS. We demonstrate this on polygonal meshes generated by Voronoi diagrams in Section 6.3.1 and by polygonal meshes generated by spatial AMR in Section 6.3.2.

### 6.3.1. MMS on Voronoi Polygonal Meshes

For the first MMS example, we will analyze convergence rates on polygonal meshes generated from Voronoi diagrams. We use the PolyMesher mesh generator [55] to generate all of our polygonal grids. The functional form of the MMS solution is a sinusoid,  $\{\psi_s, \phi_s\}$ , having the following parameterized form,

Table 2:  $L_2$ -norm of the error in the quadratic solution spanning  $\{1, x, y, x^2, xy, y^2\}$  for the different quadratic serendipity basis functions on different mesh types.

	Basis Functions			
Mesh Type	Wachspress	PWL	Mean Value	Max. Entropy
Cartesian	8.53E-16	1.31e-15	1.70e-15	2.73e-14
Triangular	9.14E-16	2.03e-15	1.41e-15	7.38e-14
Shes. Poly	1.14e-15	1.59e-15	1.51e-15	3.95e-13
Sine Poly	1.20e-15	1.45e-15	1.48e-15	1.05e-13
Z-Poly	1.08e-15	2.08e-15	2.44e-15	1.77e-14
Z-Quad	1.13e-15	2.79e-15	1.89e-15	3.99e-13

Table 3:  $L_2$ -norm of the error in the quadratic solution containing the  $x^2y^2$  term for the different quadratic serendipity basis functions on different mesh types.

	Basis Functions			
Mesh Type	Wachspress	PWL	Mean Value	Max. Entropy
Cartesian	3.5e-06	2.72e-05	8.29e-06	3.86e-05
Triangular	5.13e-05	5.13e-05	5.13e-05	5.13e-05
Shes. Quad	3.97e-04	3.37e-04	2.81e-04	3.91e-04
Sine Poly	3.75e-05	1.22e-04	7.62e-05	1.39e-04
Z-Poly	2.93e-05	3.07e-05	2.6e-05	3.46e-05
Z-Quad	2.98e-05	8.73e-05	5.08e-05	1.17e-04

$$\begin{aligned}
\psi_s(x, y) &= \sin(\nu \frac{\pi x}{L_x}) \sin(\nu \frac{\pi y}{L_y}), \\
\phi_s(x, y) &= 4\pi \sin(\nu \frac{\pi x}{L_x}) \sin(\nu \frac{\pi y}{L_y}),
\end{aligned} \tag{54}$$

where  $\nu$  is a frequency parameter ( $\nu = 1, 2, 3, \dots$ ) that we have set to 3 for this problem. The domain is  $[0, 1]^2$ , which makes  $L_x = L_y = 1$ . The domain is filled with a pure absorber that has a total cross section of  $\sigma_t = 1$ . A  $S_8$  LS quadrature is used.

We first provide examples of the polygonal meshes that are employed for this problem along with the

corresponding MV isoline solutions in Figure 10. Upon convergence, PolyMesher provides grids with mesh cells composed of approximately regular polygons. From the isolines, it is apparent that the quadratic functions better capture the sinusoid solution than the linear functions. This result is obvious since the curvature of the quadratic functions can better reproduce the smoothly varying nature of the sinusoid solution. Then, Figure 11 provides the convergence rates for all of the functions in terms of the global number of degrees of freedom. The expected  $p + 1$  convergence rates are observed with slopes of  $-(p + 1)/2$  per Eq. (10).

### 6.3.2. MMS using Adaptive Mesh Refinement

For the second MMS example, we will analyze convergence rates on polygonal meshes generated from spatial AMR. The functional form of the MMS solution that will be analyzed is a localized Gaussian. This Gaussian solution space,  $\{\psi_g, \phi_g\}$ , that has its local maximum centered at  $(x_0, y_0)$  has the parameterized form,

$$\begin{aligned}\psi_g(x, y) &= C_M x(L_x - x)y(L_y - y) \exp\left(-\frac{(x - x_0)^2 + (y - y_0)^2}{\gamma}\right), \\ \phi_g(x, y) &= 4\pi C_M x(L_x - x)y(L_y - y) \exp\left(-\frac{(x - x_0)^2 + (y - y_0)^2}{\gamma}\right),\end{aligned}\tag{55}$$

where the constants in the equations are:

$$C_M = \frac{100}{L_x^2 L_y^2} \quad \gamma = \frac{L_x L_y}{100}.\tag{56}$$

We again choose the dimensionality of our problem to be  $[0, 1]^2$  which makes  $L_x = L_y = 1$ . We set the local maximum to be  $x_0 = y_0 = 0.75$ . The domain consists of a pure absorber with  $\sigma_t = 1$ , and the quadrature is again the  $S_8$  LS set.

Because we are using AMR for this Gaussian problem, we will only analyze the PWL, MV, and ME functions since the Wachspress functions cannot handle degenerate polygons. For both the linear and quadratic AMR runs, the refinement criterion,  $\alpha$ , was set to 0.1. Figure 12 gives the convergence history of the MMS error in the  $L_2$ -norm. We plot the different AMR cases with their corresponding uniform refinement case ( $\alpha = 0$ ) for comparison. We can clearly see that we obtain the proper convergence rates for all cases, and the AMR sets provide better solution accuracy with fewer spatial degrees of freedom. Finally, we provide an example of a pair of AMR meshes and solutions in Figure 13 using the ME basis functions. We can see a clear difference in how the linear and quadratic basis functions will refine, with the quadratic functions causing much smoother refinement to occur.

### 6.4. Convergence Rate Analysis Bounded by the Solution Regularity

Our next numerical example involves studying the convergence rates of transport solutions in a purely-absorbing medium. Specifically, we seek to analyze the effects of mesh alignment along the solution discon-

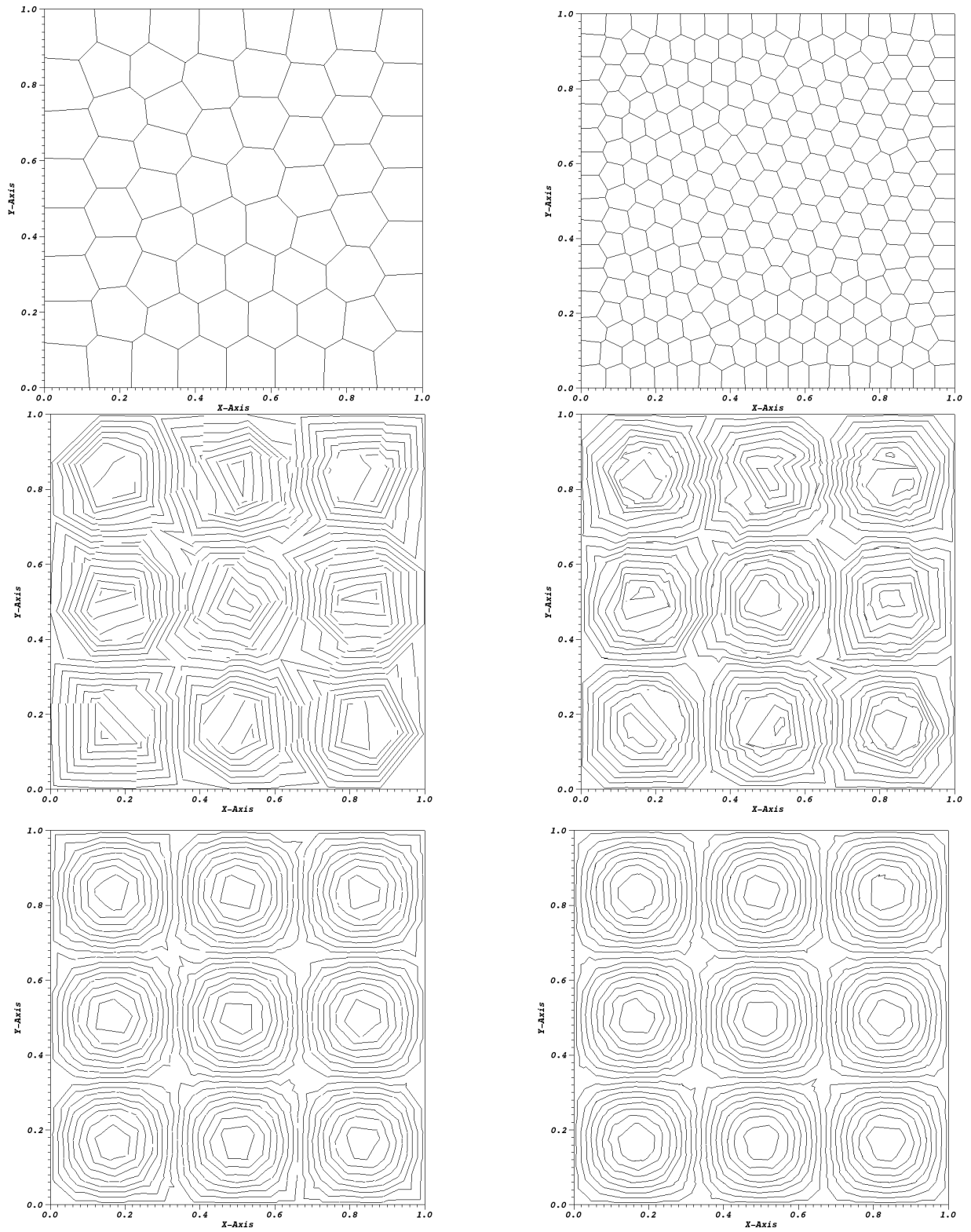


Figure 10: Examples contour plots of the sinusoid solution on polygonal meshes (top) using the linear mean value functions (middle) and the quadratic mean value functions (bottom).



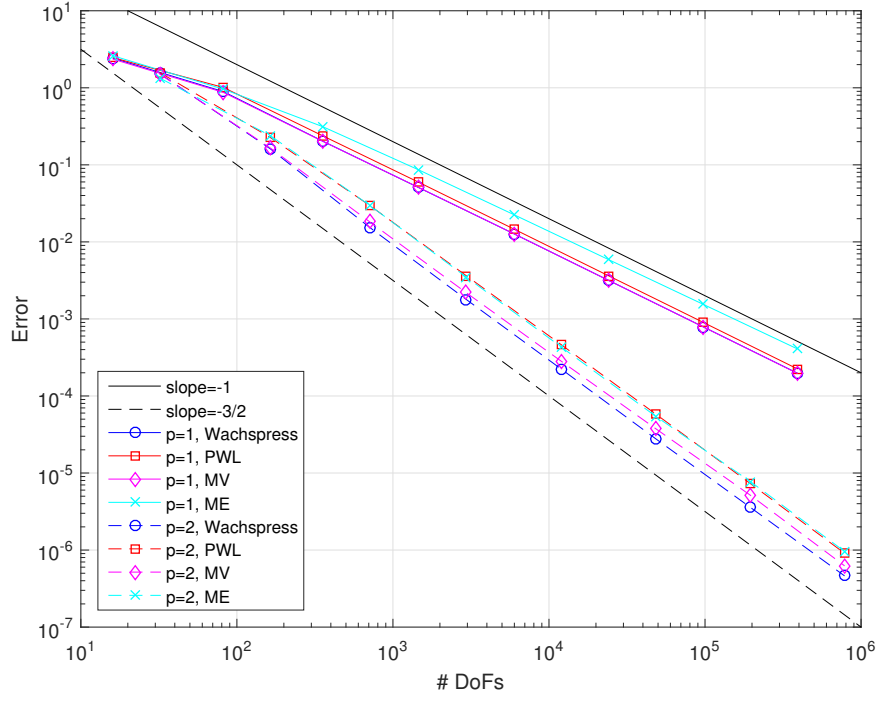


Figure 11: Convergence rates for the 2D Sinusoid MMS problem.

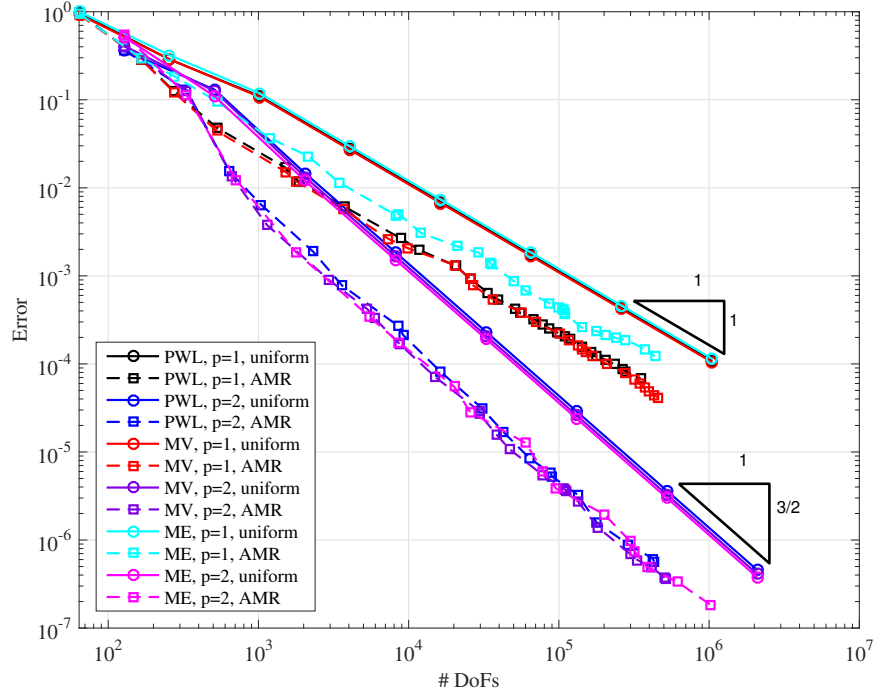


Figure 12: Convergence rates for the 2D Gaussian MMS problem.

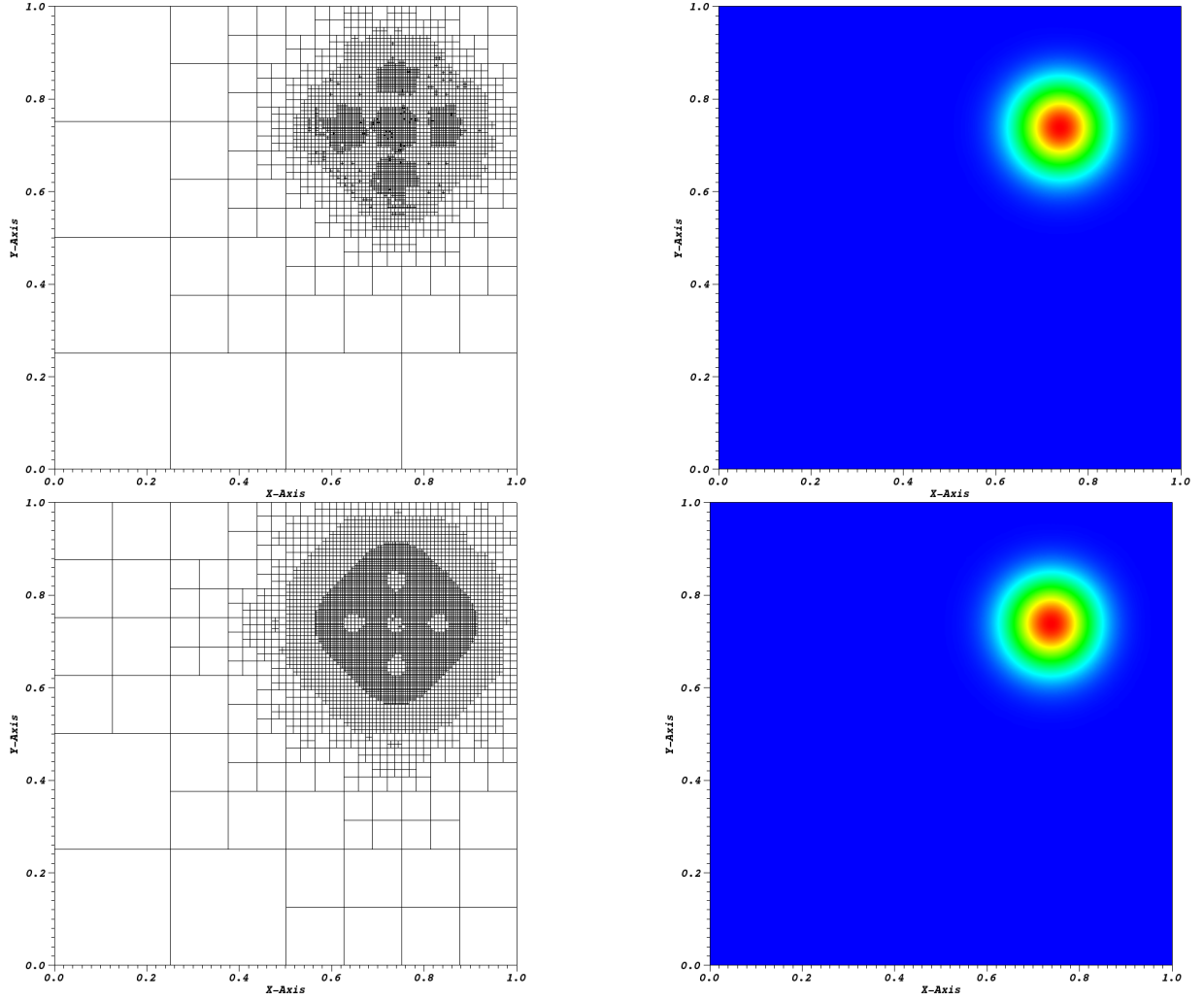


Figure 13: AMR meshes and solutions for the Gaussian MMS problem using the maximum entropy functions: (top) linear basis functions at cycle 15 and (bottom) quadratic serendipity basis functions at cycle 08.

tinuities for problems that will be constrained by the solution regularity. From Section 2, we noted that if the mesh does not align with the discontinuities of the transport solution, then the solution convergence is restricted by the regularity,  $r$ . However, if the mesh aligns with all of the solution discontinuities, then the maximum  $p + 1$  convergence rates can be observed.

For this example, we analyze a transport problem without scattering ( $\sigma_s = 0$ ) and no volumetric distributed source ( $q = 0$ ). We use a domain consisting of the unit square,  $[0, 1]^2$ , where an incident angular flux is imparted on the left face at a downward  $45^\circ$  angle. This means that there is a solution discontinuity along the line from the point  $(0, 1)$  to point  $(1, 0)$  and the upper-right portion of the domain contains no particles. Therefore, this transport solution has a regularity of  $r = 1/2$ .

Two different mesh types are analyzed for this example. The first mesh type is a polygonal mesh that is

again generated with the PolyMesher software. The second mesh type is a split-polygonal mesh where the mesh elements that fall on the line  $(0,1)$  to  $(1,0)$  are bisected. This bisection aligns with the discontinuity of the transport solution. Therefore, we expect convergence rates of  $1/2$  on the polygonal mesh and  $p + 1$  on the split-polygonal mesh.

We first give an example solution of this problem on the two mesh types using the linear Wachspress functions in Figure 14. The solution does not “see” the transport discontinuity with the split-polygonal mesh, but the polygonal mesh contains numerical dispersion across the transport discontinuity from the non-aligned boundary outflow. The convergence rates in the  $L_2$ -norm are given in Figures 15 and 16 for the split-polygonal and polygonal meshes, respectively. With the discontinuity-aligned, split-polygonal mesh, we can clearly see that convergence rates of  $p + 1$  are obtained. With the polygonal mesh, we see that convergence rates of about  $1/2$  are obtained for optically thin meshes. However, for thicker domains in the pre-asymptotic range, higher convergence rates (without quite obtaining  $p + 1$  values) are observed.

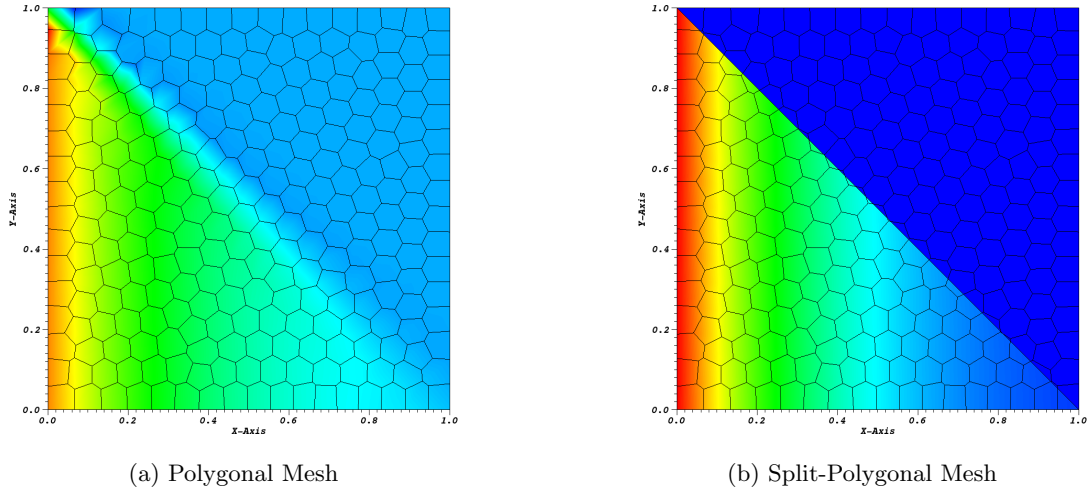


Figure 14: Example solution of the purely-absorbing medium case with left-face incidence and  $\sigma_t = 1$  using the linear Wachspress basis functions.

### 6.5. Thick Diffusion Limit Problem

So far, we have only presented numerical examples without scattering. Adams showed that the choice of spatial basis functions for the DGFEM transport equation is important in the thick diffusive limit [10]. Therefore, we conclude our numerical examples by demonstrating the applicability of the linear and quadratic polygonal functions for this limit. Our problem consists of a homogeneous square domain  $[0, 1]^2$  with isotropic scattering, an isotropic distributed source, and vacuum boundary conditions. The cross sections are scaled to reflect the properties of the thick diffusion limit. If we introduce a scaling parameter,  $\epsilon$ , then the total cross section, absorption cross section, and distributed source scale as  $1/\epsilon$ ,  $\epsilon$ , and  $\epsilon$ , respectively. Using these scaled parameters yields transport and diffusion equations of

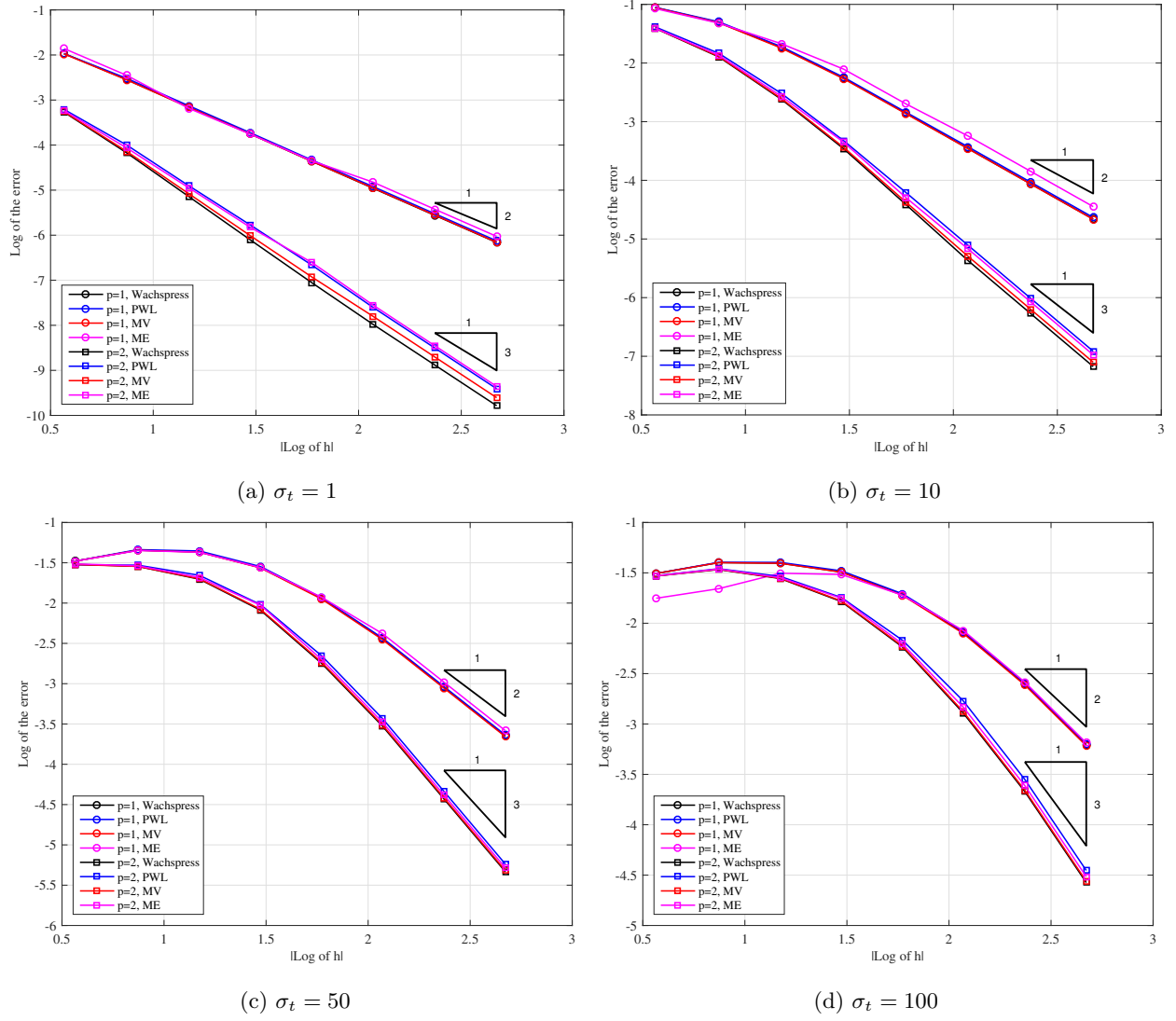


Figure 15: Convergence rates for the pure absorber problem with left-face incidence on split-polygonal meshes with different values of  $\sigma_t$ .

$$\vec{\Omega} \cdot \vec{\nabla} \psi + \frac{1}{\epsilon} \psi = \left( \frac{1}{\epsilon} - \epsilon \right) \frac{\phi}{4\pi} + \frac{\epsilon}{4\pi}, \quad (57)$$

445 and

$$-\frac{\epsilon}{3} \nabla^2 \phi + \epsilon \phi = \epsilon, \quad (58)$$

446 respectively. We have kept the scaling terms in Eq. (58) for completeness, even though the diffusion

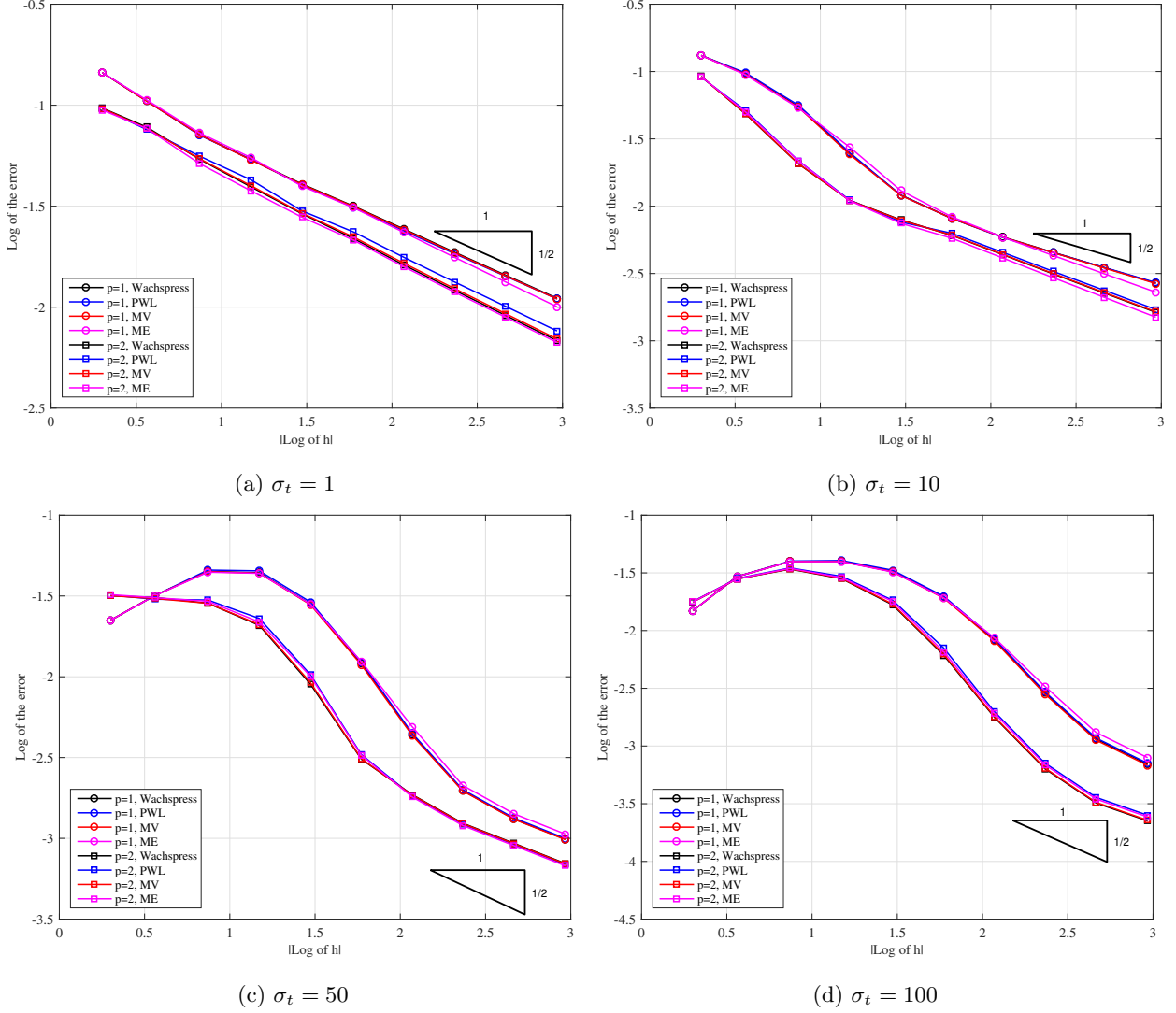


Figure 16: Convergence rates for the pure absorber problem with left-face incidence on polygonal meshes with different values of  $\sigma_t$ .

solution is invariant to the value of  $\epsilon$ . The transport equation is discretized according to Eq. (5), while the diffusion equation is discretized using a continuous finite element (CFEM) form. The diffusion equations use a homogeneous Dirichlet boundary condition, and the  $S_8$  quadrature is used for the transport equations.

With the chosen boundary conditions, the transport and diffusion solutions will converge only as  $\epsilon$  gets small. Figure 17 provides the transport and diffusion solutions of the linear and quadratic maximum entropy functions. We can see that as  $\epsilon$  goes from  $10^{-1}$  to  $10^{-5}$ , the transport solutions qualitatively converge to their corresponding diffusion solutions. Figure 18 then provides the convergence rates of the discretized transport,

$\phi_T$ , and diffusion,  $\phi_D$ , solutions under the  $L_2$ -norm ( $\|\phi_T - \phi_D\|_{L_2}$ ). We can see that the transport solutions for the linear and quadratic Wachspress, MV, and ME functions converge to the diffusion solution at a rate of  $\epsilon$ . However, the linear and quadratic PWL functions plateau because their gradients do not live in the same functional space. Both of these behaviors are expected from [10].

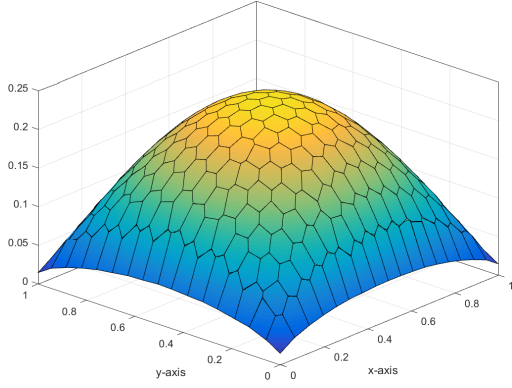
## 7. Conclusions

A higher-order discontinuous Galerkin finite element discretization using the quadratic serendipity space of functions has been applied to  $S_N$  transport equation on arbitrary polygonal grids. The quadratic serendipity functional space is formed by combinations of pairwise products of linear polygonal barycentric functions, of which we utilized the Wachspress functions, mean value functions, and maximum entropy functions in this work. The quadratic serendipity functions preserve the thick diffusion limit of the  $S_N$  transport equation as predicted by the theory of [10]. Third-order convergence was numerically verified for transport problems on polygonal grids that were not bound by the solution regularity. Asymptotic convergence rates of  $1/2$  were appropriately obtained for problems bounded by the solution regularity. Spatial adaptive mesh refinement was also used to solve the transport equation on polygonal grids, where degenerate polygons were used in place of hanging nodes. We verified that third-order convergence was retained while achieving greater solution accuracy with fewer unknowns than grids that were uniformly refined.

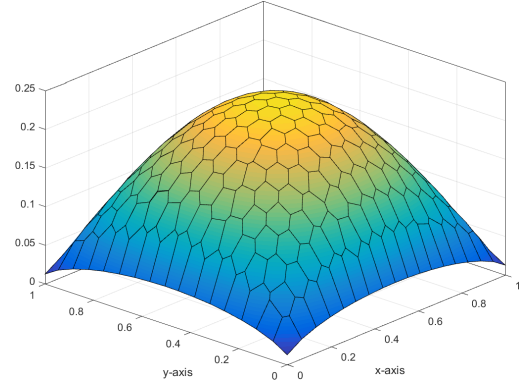
This paper shows that the  $S_N$  transport equation can be effectively discretized on arbitrary polygonal meshes using a higher-order DGFEM spatial discretization. However, we are not constrained to just the first order form of the  $S_N$  transport equation. The basis functions presented here can be employed with other forms of the transport equation including the self-adjoint angular flux equation, the least-squares equation, and the even-parity equations, as well as the  $P_N$  method in angle.

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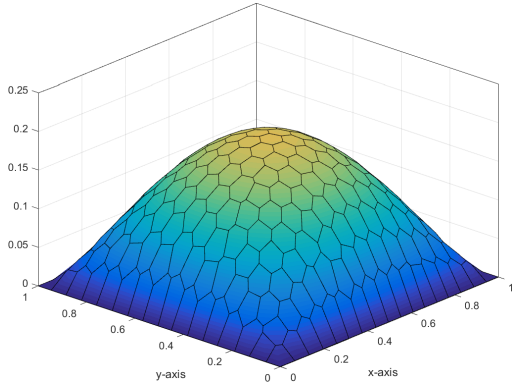
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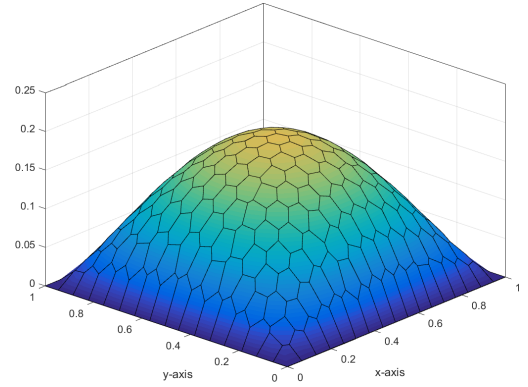
(a) Linear,  $\epsilon = 10^{-1}$



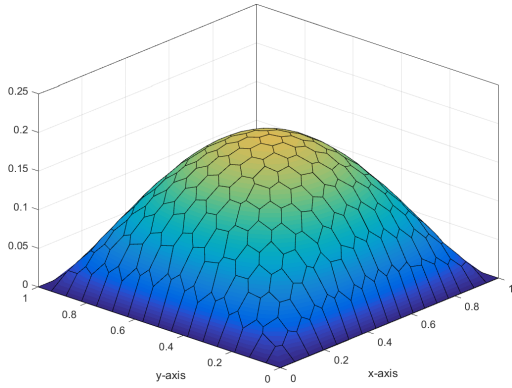
(b) Quadratic,  $\epsilon = 10^{-1}$



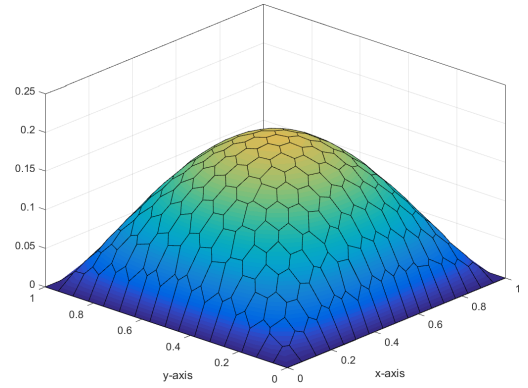
(c) Linear,  $\epsilon = 10^{-5}$



(d) Quadratic,  $\epsilon = 10^{-5}$



(e) Linear, Diffusion



(f) Quadratic, Diffusion

Figure 17: Solutions of the thick diffusion limit problem using the maximum entropy basis functions. The top and middle rows show the linear and quadratic transport solutions for  $\epsilon = 10^{-1}$  and  $\epsilon = 10^{-5}$ , respectively. The bottom row shows the corresponding diffusion solutions.

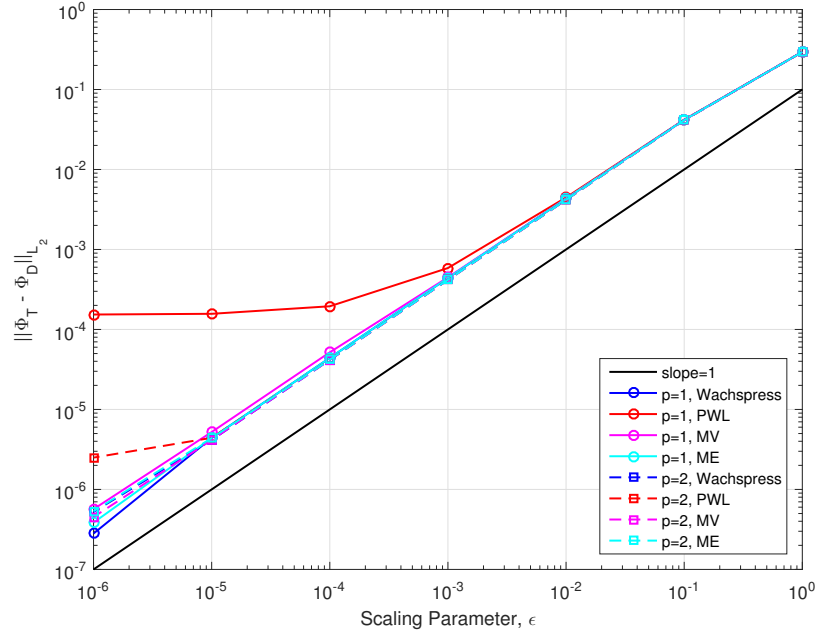


Figure 18: Convergence rates for the diffusion limit problem on a polygonal mesh.

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## A. Limits of the Barycentric Functions on the Boundary

Each of the four basis functions presented in this paper satisfies the definitions of the general barycentric functions given in Section 3. These functions can be written for a polygonal element  $K$  with  $n$  vertices using the general form:

$$\lambda_i(\vec{r}) = \frac{w_i(\vec{r})}{\sum_{j=1}^n w_j(\vec{r})}. \quad (59)$$

The differences between the functions lie with the definition of the weight functions,  $w$ . Unfortunately, for the Wachspress, MV, and ME functions, there is a sub-set of the element boundary,  $\partial K$ , where some of the weight functions are undefined (divide-by-zero numerical evaluations). However, these functions do have valid limits, which can be directly evaluated to compute the surface integrals in Eq. (5). For this analysis, we will evaluate the limits of the barycentric functions on face  $e_j$  connected by vertices  $j$  and  $j + 1$ . The limits of the functions  $\lambda_j$  and  $\lambda_{j+1}$  for position  $\vec{r}^* \in e_j$  are given by

$$\lim_{\vec{r} \rightarrow \vec{r}^* \in e_j} \lambda_j(\vec{r}) = \frac{w_j(\vec{r})}{w_j(\vec{r}) + w_{j+1}(\vec{r})} \quad (60)$$

and

$$\lim_{\vec{r} \rightarrow \vec{r}^* \in e_j} \lambda_{j+1}(\vec{r}) = \frac{w_{j+1}(\vec{r})}{w_j(\vec{r}) + w_{j+1}(\vec{r})}, \quad (61)$$

respectively, where the denominators contain the two terms because all the other weight functions are zero along  $e_j$ . The affine property then states the following:

$$w_j(\vec{r}) (\vec{r}_j - \vec{r}) + w_{j+1}(\vec{r}) (\vec{r}_{j+1} - \vec{r}) = \vec{0}. \quad (62)$$

If we take the norm of Eq. (62) and rearrange terms, then we obtain

$$\frac{w_{j+1}}{w_j} = \frac{|\vec{r}_j - \vec{r}|}{|\vec{r}_{j+1} - \vec{r}|}. \quad (63)$$

Inserting Eq. (63) into Eqs. (60 - 61) obtains the limits of the barycentric functions on face  $e_j$ :

$$\lim_{\vec{r} \rightarrow \vec{r}^* \in e_j} \lambda_i(\vec{r}) = \begin{cases} \frac{|\vec{r}_{j+1} - \vec{r}|}{|\vec{r}_{j+1} - \vec{r}_j|}, & i = j \\ \frac{|\vec{r}_j - \vec{r}|}{|\vec{r}_{j+1} - \vec{r}_j|}, & i = j + 1 \\ 0, & \text{otherwise} \end{cases} \quad (64)$$

From Eq. (64), we can see that the Lagrange property and the piecewise boundary linearity property are satisfied. Using the limits of  $\lambda_j$  and  $\lambda_{j+1}$  on face  $e_j$ , we can explicitly write the surface integral for all linear functions as

$$\langle \vec{n} b, b \rangle_{e_j} = \frac{L_j \vec{n}_j}{6} \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix}, \quad (65)$$

where  $b = [b_j, b_{j+1}]$ ,  $\vec{n}_j$  is the outward unit normal of face  $e_j$ , and  $L_j$  is the edge length of face  $e_j$ . It is assumed that  $\vec{n}_j$  is constant along  $e_j$ .

## B. Conversion of the Serendipity Functions to the Lagrange Space

The serendipity functions are formed from the pairwise products of vertex-based linear functions. Therefore, these functions will not satisfy the Lagrange property like their linear parent functions as can be seen in Figure 19a along an arbitrary polygonal face. We can convert the quadratic serendipity functions to a Lagrange basis,  $\{\chi(\vec{r})\}$ , which have the same functional form as the  $\mathbb{Q}_9$  functions on a face as seen in Figure 19b. The Lagrange basis spans the same functional space as the quadratic serendipity functions,  $\{1, x, y, x^2, xy, y^2\}$ , and is formed by:

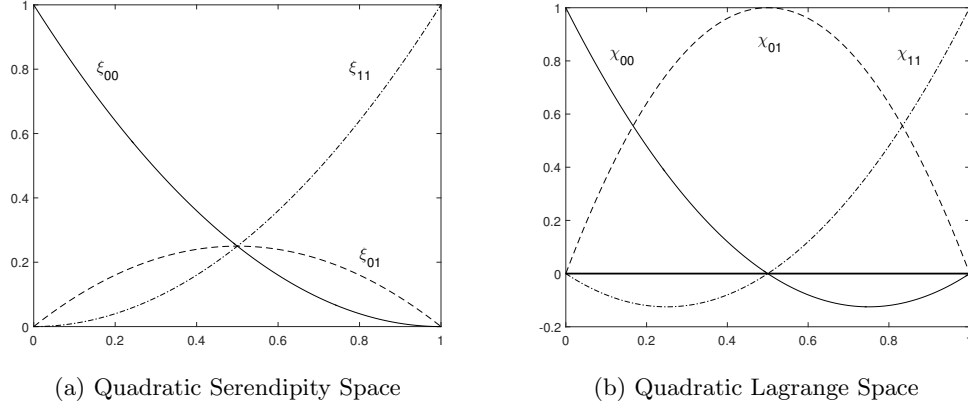


Figure 19: Comparison on a polygonal face of the quadratic basis (left) and the standard Lagrange basis (right).

$$\chi_{ii} = \xi_{ii} - \xi_{i,i+1} - \xi_{i-1,i} \quad \text{and} \quad \chi_{i,i+1} = 4\xi_{i,i+1}. \quad (66)$$

607 We can see from Eq. (66) that the Lagrange functions are a linear combination of the quadratic serendipity  
 608 functions, which we can formally define as  $\{\chi\} = \mathbb{L}\{\xi\}$ . The transformation matrix,  $\mathbb{L}$ , has a simple structure  
 609 as seen in Eq. (67).

$$\mathbb{L} = \left[ \begin{array}{c|cccc} 1 & & & & \\ & \ddots & & & \\ & & \ddots & & \\ & & & \ddots & \\ & & & & 1 \\ \hline & & & & 4 \\ & & & & \ddots \\ & & & & & \ddots \\ & & & & & & \ddots \\ & & & & & & & 4 \end{array} \right] \quad (67)$$