# HIGHER ORDER DISCONTINUOUS FINITE ELEMENT METHODS FOR DISCRETE ORDINATES THERMAL RADIATIVE TRANSFER

#### A Dissertation

by

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#### ABSTRACT

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# DEDICATION

To my wife, Kelli, for traveling with me along all the unforeseen curves of life.

To my mom and dad, for providing my foundation and inspiration.

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# NOMENCLATURE

B/CS Bryan/College Station

HSUS Humane Society of the United States

P Pressure

T Time

TVA Tennessee Valley Authority

TxDOT Texas Department of Transportation

This page is optional.

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#### 1. INTRODUCTION

This dissertation is dedicated to the solution of thermal radiative transfer (TRT) equations. The TRT equations:

$$\frac{1}{c}\frac{dI}{dt} + \vec{\Omega} \cdot \vec{\nabla}I + \sigma_t I = \int_0^\infty \int_{4\pi} \sigma_s(\vec{\Omega}' \to \vec{\Omega}, E' \to E)I, d\vec{\Omega}' dE' + \sigma_a B \quad (1.1a)$$

$$C_v \frac{dT}{dt} = \int_0^\infty \sigma_a \left(\phi - 4\pi B\right) dE, \quad (1.1b)$$

are a nonlinear system of equations that describe the exchange of energy between a photon radiation field and a non-moving material. The radiation intensity, I, is a seven dimensional field dependent upon spatial location,  $\vec{x}$ ; photon energy, E; photon direction of travel,  $\vec{\Omega}$ ; and time t. c is the speed of light. Material opacities for all interactions,  $\sigma_t$ ; absorption,  $\sigma_a$ ; and scattering,  $\sigma_s$  are functions of photon energy and material temperature, T. Material heat capacity,  $C_v$ , is also a function of material temperature. The angle integrated radiation intensity is an integral over all photon directions of the the photon intensity and is a function of space and photon energy. Finally, the Planck function, B, is a function of photon energy and material temperature. While materials at all temperatures emit photon radiation, the radiation emission is proportional to  $T^4$ . Thus, solution of the radiative transfer equations is most important in situations where materials are very hot. Solving the thermal radiative transfer equations is an important component of the simulation of different scientific and engineering problems including astrophysics supernova explosions and high energy density laboratory physics experiments like those conducted at the National Ignition Facility.

## 1.1 Simplifications of the Thermal Radiative Transfer Equations

In this dissertation, we we make a number of simplifying assumptions to make solution of Eqs. (1.1) more tractable. First, we limit our focus to 1-D Cartesian (slab) geometry. The assumption of slab geometry is not required, but slab geometry radiation transport simulations require significantly less computational time. Further, any methods that have a possibility of being viable for radiation transport in multiple spatial dimensions must also work well in slab geometry.

Second, we approximate the continuous angle dependence of the intensity using the discrete ordinates  $(S_N)$  method. The  $S_N$  method approximates the true definition of the angle integrated intensity,

$$\phi(\vec{x}, E, t) = \int_{4\pi} I(\vec{x}, \vec{\Omega}, E, t) d\vec{\Omega},$$

using quadrature integration,

$$\phi(\vec{x}, E, t) \approx \sum_{d=1}^{N_{dir}} w_d I(\vec{x}, \vec{\Omega}_d, E, t). \tag{1.2}$$

In Eq. (1.2),  $\{w_d, \vec{\Omega}_d\}_{d=1,...N_{dir}}$  is the set of  $N_{dir}$  quadrature weights  $w_d$  and discrete directions,  $\vec{\Omega}_d$  and corresponding intensities  $I_d$ .

Finally, we treat the photon energy dependence using the multi-frequency method. The multi-frequency method approximates photon energy dependence by discretizing the continuous photon energy dependence with G discrete groups such that:

$$\int_0^\infty I(\vec{x}, \vec{\Omega}, t, E) dE = \sum_{g=1}^G I_g \,, \tag{1.3}$$

where

$$I(\vec{x}, \vec{\Omega}, t)_g = \int_{E_{q+1/2}}^{E_{g-1/2}} I(\vec{x}, \vec{\Omega}, t, E) dE, \qquad (1.4)$$

 $E_{g+1/2}$  is the lower photon energy bound of group g,  $E_{g-1/2}$  is the upper photon energy bound of group g, and we have maintained the traditional neutron transport number of higher energy particles belonging to lower number energy groups.

#### 1.2 Spatial and Temporal Discretization

To complete a description of the approach we will take to solve Eqs. (1.1), we now describe how we will discretize the spatial and temporal variables.

## 1.2.1 Time Integration

The appearance of the speed of light in Eq. (1.1) results in the TRT equations being very stiff. To solve the such a stiff system of equations would require either an impractically small time step, or the use of implicit methods. We elect to use Diagonally Implicit Runge-Kutta (DIRK) methods to advance our TRT solution in time. The simplest of DIRK scheme is the first order implicit Euler scheme, but more advanced DIRK higher order methods in time [5].

#### 1.2.2 Spatial Discretization with Discontinuous Finite Elements

The linear discontinuous finite element method (LDFEM) has long been used to solve the discrete ordinates neutron transport equation [21]. Through manipulation, the thermal radiative transfer equations can be transformed into a form that is equivalent to the neutron transport equation with pseudo-scattering, fission, and fixed sources. This makes it possible to use the same methods and techniques developed for neutron transport to assist in solving the thermal radiative transfer equations. LDFEM has achieved wide spread acceptance in the neutron transport community because it is accurate [12] and highly damped. Because it possesses the thick diffusion

limit [11], LDFEM has also been applied to the  $S_N$  TRT equations. Morel, Wareing, and Smith first considered the application of LDFEM to the  $S_N$  TRT equations in [17]. Mass matrix lumped LDFEM was shown to preserve the thick equilibrium diffusion limit [17]. This suggests that discontinuous finite element (DFEM) schemes can be used to accurately solve the TRT equations in both diffusive and transport effects dominated regions.

## 1.3 Progression Towards Higher Order DFEM Thermal Radiative Transfer

For higher order (quadratic and higher polynomial degree trial spaces) DFEM to be accurate and practical for solving Eqs. (1.1) we must demonstrate that higher order DFEM:

- 1. are "robust",
- 2. account for within cell spatial variation of opacity accurately, and
- 3. can be accelerated using appropriate iterative acceleration techniques.

By "robust", we mean that that calculated radiation outflow from a spatial cell is strictly positive for all cell widths and optical thicknesses.

In Section 2 we use a steady-state, mono-energetic, source-free pure absorber neutron transport problem with a cross section that is constant in space to examine the robustness of different radiation transport DFEM matrix lumping techniques. Next, we extend the techniques developed by Adams [2, 4], for a spatial discretization scheme related to LDFEM to address the within cell spatial variation of opacity, for higher order DFEM in Section 3. Then, we examine iterative acceleration techniques compatible with higher order DFEM spatial discretizations that account for the spatial variation of interaction cross (in neutron transport problems) or opacity (TRT simulations) in Section 4.

In preparation for solving the coupled, non-linear TRT equations, in Section 5 we combine all of the strategies we have developed in Sections 2-4 and apply them to a coupled system of linear equations. Section 5, is deveoted to the development and solution of a two-group fuel depletion problem that uses explicit Euler time differencing. Finally, in Section 6 we solve the energy integrated, or grey, thermal radiative transfer equations using higher order DFEM. We then provides solutions to analytic benchmarks to verify our methods [23], and use the method of manufactured solutions [22] to demonstrate the increased accuracy of applying higher order DFEM and DIRK time integration techniques to the grey TRT equations.

#### 2. DISCONTINUOUS FINITE ELEMENTS FOR RADIATION TRANSPORT

In Section 1, we briefly mentioned that through manipulation, the thermal radiative transfer equations can be put into a form equivalent to the neutron transport equations with pseudo- scattering, fission, and fixed sources. We will (repeatedly) go through this process in Section 6, but for now we take for granted that solving for the neutron transport equation's angular flux,  $\psi$ , is related to solving Eq. (1.1) for I. Additionally, we will assume that a steady-state neutron transport source-free pure absorber problem taxes DFEM schemes in a manner similar to the way DFEM schemes are tested in time-dependent thermal radiative transfer simulations, in particular Marshak wave type problems [19]

#### 2.1 History of DFEM for Neutron Transport

The linear discontinuous finite element method (LDFEM) for discrete ordinates neutron transport is widely used and has been extensively studied[10, 6, 15, 3]. However, the DFEM technique is not limited to linear trial spaces. Reed et. al [21] used arbitrary order DFEM  $S_N$  transport in TRIPLET but, due to data storage limitations at the time, only LDFEM was computationally practical. Possibly as a result of these historical computing limitations, the majority of reported DFEM radiation transport literature has focused on the LDFEM approximation. Higher order DFEM methods have received periodic attention; some older examples include the work of Walters [25] and Hennart and del Valle [8, 9]. More recent investigations of higher order DFEM trial spaces include those of Warsa and Prinja [28] and Wang and Ragusa [27, 26]. The primary focus of the work in [8, 9, 28, 27, 26] was the convergence rate of arbitrary order DFEM schemes.

Negative angular flux solutions of the neutron transport equation obtained with

LDFEM have been well documented in [6, 15, 3]. While these negativities do not affect the order of convergence and can be tolerated for certain applications [13], some nonlinear problems, particularly radiative transfer calculations, can diverge if the angular intensities are negative. As a result, several methods to eliminate or inhibit negative solutions have been developed and can be categorized into one of three categories: ad-hoc fix-ups [6], strictly non-negative solution representations [15], and matrix lumping [3]. The first two methods result in nonlinear systems of equations, while matrix lumping yields linear systems of equations. By definition, ad-hoc fix-ups and strictly non-negative solution representations yield non-negative outflows in 1-D, 2-D, and 3-D geometries, regardless of material properties. Mass matrix lumping (applied to LDFEM) yields strictly positive outflows only in 1-D geometries, though it does otherwise inhibit negativities [3]. Although not related to DFEM discretizations, we note that other approaches have been investigated to mitigate negativities; see, for instance, [7].

Solution positivity of even degree unlumped DFEM methods for 1-D problems has been noted previously [25, 8, 9]. In comparing DFEM methods to nodal transport methods, Walters derived the quadratic DFEM scheme from the nodal transport equations using the Padé(2,3) approximation to the exponential term and noted that this approximation would result in a strictly positive outflow, regardless of cell optical thickness [25]. Hennart and del Valle then showed for slab geometry that all even P degree polynomial DFEM schemes approximate the cell outflow angular flux as a Padé(P, P + 1) function, which is a strictly positive approximation of the exponential [8, 9]. The positivity of even degree unlumped DFEM for 1-D problems was also shown in [28].

## 2.2 Matrix Lumping Techniques to Study

In this Section, we examine the idea of mass matrix lumping and its ability to ensure positive angular flux solutions of the neutron transport equation for arbitrary degree DFEM trial spaces in non-scattering 1-D slab geometries. We consider traditional lumping (TL), that constructs a diagonal mass matrix by collapsing all off-diagonal entries onto the main diagonal [3], and quadrature-based self-lumping (SL) methods [20], that yield a diagonal mass matrix by numerically integrating the DFEM equations using the DFEM interpolatory points as quadrature points. Restricting ourselves to equally-spaced interpolation points, self-lumping numerical integration with the greatest degree of accuracy is achieved through the use of closed Newton-Cotes formulae [1]. However, Newton-Cotes formulas with a large number of integration points are known to be oscillatory and are of relatively low-order accuracy, integrating polynomials at most of degree equal to the number of integration points. By considering solution representations that employ quadrature points as the interpolatory points, for example Gauss-Legendre (hereafter Gauss) or Lobatto-Gauss-Legendre (hereafter Lobatto) quadrature points [1], we wish to find methods that are self-lumping with a significantly higher accuracy. We analyze the combinations of Lagrange interpolatory points and numerical integration strategies given in Table 2.1 for positivity of the angular flux solution, local truncation error order, and spatial convergence order as a function of trial space polynomial degree. We limit the consideration of exact numerical integration schemes to those with equally-spaced interpolatory points, due to the fact that exact integration with any particular set of interpolatory points will always yield the same DFEM solution)

It has long been noted that traditional lumping (TL) with equally-spaced interpolatory points for 1-D LDFEM is equivalent to using the trapezoidal quadrature

Table 2.1: Nomenclature of numerical schemes (TL=Traditional Lumping; SL=Self-Lumping).

Integration	Method					
Strategy	Short Hand Name					
Exact spatial integration,	TL					
with collapsing of mass matrix						
entries to the main diagonal						
Numerical integration via	SL Newton-Cotes					
Newton-Cotes quadrature restricted						
to interpolation points						
Numerical integration via	SL Gauss					
Gauss quadrature restricted						
to interpolation points						
Numerical integration via	SL Lobatto					
Lobatto quadrature restricted						
to interpolation points						
Exact spatial integration	Exact DFEM					
	Exact spatial integration, with collapsing of mass matrix entries to the main diagonal Numerical integration via Newton-Cotes quadrature restricted to interpolation points Numerical integration via Gauss quadrature restricted to interpolation points Numerical integration via Lobatto quadrature restricted to interpolation points					

rule to approximately integrate the mass matrix [24] while exactly integrating the gradient operator. Since the trapezoidal rule is identical to the closed Newton-Cotes formula with two points, we hypothesize that, for finite elements of arbitrary order using equally-spaced interpolatory points, traditional lumping is equivalent to using a closed Newton-Cotes formula to compute the mass matrix while exactly integrating the gradient operator. We demonstrate the equivalence between traditional lumping and closed Newton-Cotes formulae in the computation of the mass matrix.

Self-lumping (SL) based on Newton-Cotes formulae differs from traditional lumping in that SL Newton-Cotes generally does not exactly integrate the gradient operator. Coincidentally, the gradient operator is exactly integrated for linear/quadratic trial spaces using a 2-point/3-point Newton-Cotes formula, respectively. However, for higher degree polynomial trial spaces, the corresponding Newton-Cotes formula does not exactly integrate the gradient operator.

Self-lumping based on either Gauss or Lobatto quadratures exactly integrates the gradient operator in 1-D slab geometry for all degree of polynomial trial spaces; thus, there is no need to distinguish between exact integration and quadrature integration of the gradient operator for the SL Gauss and SL Lobatto schemes.

# 2.3 Lumping Techniques for the 1-D $S_N$ Neutron Transport Equation with Arbitrary Order DFEM

In Sec. 2.3, we provide the weak form for the 1-D  $S_N$  equations discretized with DFEM and define the different mass matrix lumping techniques.

#### 2.3.1 Weak Form Derivation

Consider the 1-D slab geometry  $S_N$  neutron transport equation:

$$\mu_d \frac{d\psi_d}{dx} + \sigma_t \psi_d = Q_d, \tag{2.1}$$

where  $\psi_d$  is the angular flux  $[1/[cm^2 - sec - ster]]$  in the  $\mu_d$  direction,  $\mu_d$  is the d'th directional cosine relative to the x-axis,  $\sigma_t$  is the total interaction cross section  $[cm^{-1}]$ , and  $Q_d$  is a total source (fixed+scattering+fission) angular source in the direction of  $\mu_d$   $[1/[cm^3 - sec - ster]]$ . In all that follows, we consider only non-scattering, non-fissioning media (pure absorbers), thus  $Q_d$  will only be non-trivial if a fixed source i present in the problem. The scalar flux  $\phi$   $[n/cm^2 - sec]$  is defined as

$$\phi(x) = 2\pi \int_{-1}^{1} \psi(x, \mu_d) \ d\mu_d. \tag{2.2}$$

For simplicity, we derive the DFEM equations for a single-cell domain, with  $x \in [x_L, x_R]$ . A known angular flux,  $\psi_{in,d}$ , is defined on the incoming face of the domain for all  $\mu_d$ . For  $\mu_d > 0$ ,  $\psi_{in,d}$  is defined only at  $x_L$  and for  $\mu_d < 0$ ,  $\psi_{in,d}$  is defined

at  $x_R$ . We begin our derivation by first transforming the physical geometry to a reference element,  $s \in [-1, 1]$ . This affine transformation is such that:

$$x = \bar{x} + \frac{\Delta x}{2}s \tag{2.3a}$$

$$dx = \frac{\Delta x}{2} ds \tag{2.3b}$$

with  $\bar{x} = \frac{x_L + x_R}{2}$  and  $\Delta x = x_R - x_L$ . We seek a numerical approximation to the true angular flux  $\psi_d$  using Lagrange polynomials of degree P:

$$\psi_d(s) \approx \widetilde{\psi}_d(s) = \sum_{j=1}^{N_P} \psi_{j,d} \mathbf{B}_{\mathbf{j}}(s) ,$$
 (2.4)

where the  $\widetilde{\phantom{a}}$  denotes the numerical approximation. The basis functions  $B_j$  are the canonical Lagrange polynomials

$$\mathbf{B_{j}}(s) = \prod_{\substack{k=1\\k\neq j}}^{N_{P}} \frac{s - s_{k}}{s_{j} - s_{k}},$$
(2.5)

and  $N_P = P + 1$ . To determine the  $N_P$  unknown coefficients of Eq. (2.4), we follow a standard discontinuous Galerkin procedure, successively multiplying Eq. (2.1) by weight function  $\mathbf{B_i}$  and integrating by parts, hence generating  $N_P$  moment equations  $(1 \le i \le N_P)$ . We assume that the cross sections are constant per cell. Inserting our solution representation  $\widetilde{\psi}_d$ , the *i*-th moment equation is given by:

$$\mu_{d} \left[ \mathbf{B}_{\mathbf{i}}(1)\widetilde{\psi}_{d}(1) - \mathbf{B}_{\mathbf{i}}(-1)\widetilde{\psi}_{d}(-1) - \int_{-1}^{1} \widetilde{\psi}_{d}(s) \frac{d\mathbf{B}_{\mathbf{i}}}{ds} ds \right] + \frac{\Delta x \sigma_{t}}{2} \int_{-1}^{1} \mathbf{B}_{\mathbf{i}}(s)\widetilde{\psi}_{d}(s) ds$$

$$= \frac{\Delta x}{2} \int_{-1}^{1} \mathbf{B}_{\mathbf{i}}(s)Q_{d}(s) ds. \quad (2.6)$$

We now introduce the upwind approximation to define the angular flux at the cell edges. For  $\mu_d > 0$  the angular flux at the cell interfaces is

$$\widetilde{\psi}_d(-1) = \psi_{in,d} \tag{2.7a}$$

$$\widetilde{\psi}_d(1) = \sum_{j=1}^{N_P} \psi_{j,d} \mathbf{B}_{\mathbf{j}}(1). \qquad (2.7b)$$

Similarly for  $\mu_d < 0$ :

$$\widetilde{\psi}_d(-1) = \sum_{j=1}^{N_P} \psi_{j,d} \mathbf{B}_{\mathbf{j}}(-1)$$
(2.8a)

$$\widetilde{\psi}_d(1) = \psi_{in,d}. \tag{2.8b}$$

In Eq. (2.7a) and Eq. (2.8b),  $\psi_{in,d}$  is either the known angular flux outflow from the upwind cell or a boundary condition. Inserting the definition of  $\widetilde{\psi}_d(s)$ , Eq. (2.6) becomes, for  $\mu_d > 0$ ,

$$\mu_{d} \left[ \mathbf{B_{i}}(1) \left( \sum_{j=1}^{N_{P}} \psi_{j,d} \mathbf{B_{j}}(1) \right) - \mathbf{B_{i}}(-1) \psi_{in,d} - \int_{-1}^{1} \left( \sum_{j=1}^{N_{P}} \psi_{j,d} \mathbf{B_{j}}(s) \right) \frac{d\mathbf{B_{i}}}{ds} ds \right] + \frac{\Delta x \sigma_{t}}{2} \int_{-1}^{1} \mathbf{B_{i}}(s) \left( \sum_{j=1}^{N_{P}} \psi_{j,d} \mathbf{B_{j}}(s) \right) ds = \frac{\Delta x}{2} \int_{-1}^{1} \mathbf{B_{i}}(s) Q_{d}(s) ds, \quad (2.9)$$

and, for  $\mu_d < 0$ ,

$$\mu_d \left[ \mathbf{B_i}(1)\psi_{in,d} - \mathbf{B_i}(-1) \left( \sum_{j=1}^{N_P} \psi_{j,d} \mathbf{B_j}(-1) \right) - \int_{-1}^1 \left( \sum_{j=1}^{N_P} \psi_{j,d} \mathbf{B_j}(s) \right) \frac{d\mathbf{B_i}}{ds} ds \right]$$

$$+ \frac{\Delta x \sigma_t}{2} \int_{-1}^1 \mathbf{B_i}(s) \left( \sum_{j=1}^{N_P} \psi_{j,d} \mathbf{B_j}(s) \right) ds = \frac{\Delta x}{2} \int_{-1}^1 \mathbf{B_i}(s) Q_d(s) ds. \quad (2.10)$$

Considering all of the  $N_P$  moment equations at once we can write both Eq. (2.9) and Eq. (2.10) in a single matrix form:

$$\left(\mu_d \mathbf{G} + \frac{\sigma_t \Delta x}{2} \mathbf{M}\right) \vec{\psi}_d = \frac{\Delta x}{2} \vec{Q}_d + \mu_d \psi_{in,d} \vec{f}.$$
 (2.11)

In Eq. (2.11) we have made use of the following definitions: the vector of unknowns is given by

$$\vec{\psi}_d = \left[\psi_{1,d} \dots \psi_{N_P,d}\right]^T, \qquad (2.12)$$

the mass matrix M is:

$$\mathbf{M}_{ij} = \int_{-1}^{1} \mathbf{B_i}(s) \mathbf{B_j}(s) \ ds \,, \tag{2.13}$$

the fixed source moment vector,  $\vec{Q}_d$ , is a column vector of length  $N_P$ :

$$\vec{Q}_{d,i} = \int_{-1}^{1} \mathbf{B_i}(s) Q_d(s) \ ds \,, \tag{2.14}$$

and  $\vec{f}$  is a column vector of length  $N_P$ :

$$\vec{f_i} = \begin{cases} \mathbf{B_i}(-1) & \text{for } \mu_d > 0 \\ -\mathbf{B_i}(1) & \text{for } \mu_d < 0 \end{cases}$$
 (2.15)

**G** is a  $N_P \times N_P$  matrix which we refer to as the gradient operator. When  $\mu_d > 0$ , **G** is given by:

$$\mathbf{G}_{ij} = \mathbf{B_i}(1)\mathbf{B_j}(1) - \int_{-1}^{1} \frac{d\mathbf{B_i}}{ds} \mathbf{B_j}(s) \ ds.$$
 (2.16a)

For  $\mu_d < 0$ , **G** is:

$$\mathbf{G}_{ij} = -\mathbf{B_i}(-1)\mathbf{B_j}(-1) - \int_{-1}^{1} \frac{d\mathbf{B_i}}{ds} \mathbf{B_j}(s) \ ds.$$
 (2.16b)

When interpolatory points are not located at the cell interfaces (i.e., at  $s = \pm 1$ ), it can be noted that

1.  $\vec{f}$  has  $N_P$  non-zero entries, and

2. 
$$\mathbf{B_i}(\pm 1)\mathbf{B_i}(\pm 1) \neq 0$$
 for all  $i, j = 1, ..., N_P$ .

When a Lagrange interpolatory point exists on the cell edges, then  $\vec{f}$  has only one non-zero entry and the product  $\mathbf{B_i}(\pm 1)\mathbf{B_j}(\pm 1) \neq 0$  only when  $i=j=N_P$  for  $\mu_d>0$  or when i=j=1 for  $\mu_d<0$ , as is the case when equally-spaced points or a Lobatto quadrature are used as interpolation points.

We evaluate the integrals of Eq. (2.13) and Eq. (2.16) using a numerical quadrature. A method exactly integrates a quantity when the quadrature rule used to evaluate the integral is accurate for polynomials of degree equal to or greater than the polynomial degree of the integrand. In general, the matrices are dense and their entries are computed as:

$$\mathbf{M}_{ij} \approx \sum_{q=1}^{N_q} w_q \mathbf{B_i}(s_q) \mathbf{B_j}(s_q)$$
 (2.17)

$$\mathbf{G}_{ij} \approx sg(\mu_d)\mathbf{B}_{\mathbf{i}}(sg(\mu_d))\mathbf{B}_{\mathbf{j}}(sg(\mu_d)) - \sum_{q=1}^{N_q} w_q \frac{d\mathbf{B}_{\mathbf{i}}}{ds} \bigg|_{s=s_q} \mathbf{B}_{\mathbf{j}}(s_q), \qquad (2.18)$$

where  $N_q$  is the number of quadrature points to be used,  $w_q$  are the weights associated with quadrature points  $s_q$ , and sg(a) is the sign function defined as

$$sg(a) = \begin{cases} +1 & \text{if } a > 0 \\ -1 & \text{if } a < 0 \end{cases}$$
 (2.19)

#### 2.3.2 Traditional Lumping

The traditional lumping (TL) scheme replaces  $\mathbf{M}$  with  $\widehat{\mathbf{M}}$ , the latter being formed by collapsing row entries onto the main diagonal via the following formula [3]:

$$\widehat{\mathbf{M}}_{ij} = \begin{cases} \sum_{j=1}^{N_P} \mathbf{M}_{ij} & \text{for } i = j \\ 0 & \text{otherwise} \end{cases}$$
 (2.20)

## 2.3.3 Quadrature-Based Lumping

An alternative method of mass matrix lumping restricts the quadrature points to the interpolatory points where:

$$\mathbf{B_i}(s_j) = \begin{cases} 1 & \text{if } s_i = s_j \\ 0 & \text{otherwise} \end{cases}, i = 1, \dots, N_P,$$
 (2.21)

and the quadrature integration of Eq. (2.17) reduces to:

$$\mathbf{M}_{ij} = \begin{cases} w_i & i = j \\ 0 & \text{otherwise} \end{cases}$$
 (2.22)

As mentioned previously, we refer to the implicit lumping of Eq. (2.22) as self-lumping (SL). Self-lumping is a method to automatically generate a diagonal mass matrix. We note that self-lumping does not imply that the quadrature formula inexactly integrates the mass matrix.

#### 2.3.4 Source Moment Evaluation

Historically, when discussing lumping techniques, the focus has been on matrix lumping [3] and little attention was paid to lumping source terms. For instance,

we consider  $\delta$ -shaped volumetric sources (i.e., equal to 0 everywhere except at one given point) as an example of a highly skewed volumetric source. In such a case, the evaluation of  $\vec{Q}_d$  using quadrature-based self-lumping schemes is an open question. Obviously, quadrature-based schemes cannot evaluate Eq. (2.14) for  $\delta$ -sources. To address this, we expand the source on a Legendre polynomial basis:

$$\widehat{S}_d(s) = \sum_{n=0}^P S_n P_n(s) \tag{2.23a}$$

with 
$$S_n = \frac{2n+1}{2} \int_{-1}^1 Q_d(s) P_n(s) ds$$
, (2.23b)

and evaluate  $\vec{Q}_d$  as follows

$$\vec{Q}_{d,i} = \int_{-1}^{1} \mathbf{B_i}(s) \hat{S}_d(s) \ ds \,. \tag{2.24}$$

Note that if the right-hand-side of Eq. (2.24) is exactly integrated, this is equivalent to exactly integrating Eq. (2.14).

## 2.4 Quadrature Point Selection

In Sec. 2.4, we discuss the properties of different numerical quadratures as applied to the 1-D DFEM  $S_N$  equations.

We consider three different types of interpolatory points: equally-spaced, Gauss quadrature, and Lobatto quadrature. On the [-1,1] interval, the  $N_P = P+1$  equally spaced interpolation points for a degree P polynomial trial space are:

$$s_j = -1 + (j-1)\frac{2}{P}, \quad j = 1, \dots, N_P.$$
 (2.25)

Self-lumping using equally-spaced interpolation points requires numerical integration with closed Newton-Cotes quadrature formulae. The  $N_P$  weights,  $w_j$ , used for Newton-Cotes numerical integration at the interpolation points do not follow a concise pattern, so we refer the reader to [1]. The Gauss quadrature points are the  $N_P$  roots of the Legendre polynomial,  $P_{N_P}(s)$  [1]. The corresponding weights are:

$$w_j = \frac{2}{(1 - s_j^2)} \left[ P'_{N_P}(s_j) \right]^2. \tag{2.26}$$

Lobatto quadrature points have fixed endpoints,  $s_1 = -1$ ,  $s_{N_P} = 1$ . The remaining  $N_P - 2$  points are the roots of  $P'_{N_P-1}(s)$  [1], with corresponding weights:

$$w_{j} = \begin{cases} \frac{2}{N_{P}(N_{P}-1)} & j = 1, \ j = N_{P} \\ \frac{2}{N_{P}(N_{P}-1)[P_{N_{P}-1}(s_{j})]^{2}} & \text{otherwise} \end{cases}$$
 (2.27)

The highest polynomial degree a particular self-lumping quadrature formula exactly integrates is given in Table 2.2 for Newton-Cotes, Gauss, and Lobatto quadratures. Also listed in Table 2.2 is the maximum polynomial degree of the integrands present in the gradient and mass matrices.

Table 2.2: Accuracy of self-Lumping quadratures for trial spaces of different polynomial degree P (each quadrature uses  $N_P = P + 1$  points).

miles degree i (eden quadrevare dece i i i i perio).										
Polynomial	$N_P =$	Degree of	Degree of	Accuracy of	Accuracy of	Accuracy of				
Degree of $\widetilde{\psi}$	P+1	M integrand	$\mathbf{G}$ integrand	Newton-Cotes	Gauss	Lobatto				
1	2	2	1	1	3	1				
2	3	4	3	3	5	3				
3	4	6	5	3	7	5				
4	5	8	7	5	9	7				
5	6	10	9	5	11	9				
$P \qquad P+1$		2P	2P - 1	Odd $\widetilde{\psi}$ : $P$	2P + 1	2P - 1				
				Even $\widetilde{\psi}$ : $P+1$						

Since the accuracy of an  $N_P = P + 1$  point Gauss quadrature integration exceeds the polynomial degree of the  $\mathbf{M}$  and  $\mathbf{G}$  integrands for a trial space of degree P, using the SL Gauss scheme will strictly yield the same numerical solution as any DFEM scheme that exactly integrates  $\mathbf{M}$  and  $\mathbf{G}$ . Thus, the SL Gauss scheme yields the same numerical solution as the Exact DFEM scheme.

For linear and quadratic trial spaces, self-lumping methods using either Lobatto or equally-spaced interpolation points will yield identical solutions. This is a direct result of the two- and three-point Lobatto quadrature formulae being identical to the two- and three-point closed Newton-Cotes quadratures. This equivalence does not hold for higher degree polynomial trial spaces because the Lobatto quadrature points will no longer correspond to the equally-spaced quadrature points.

By definition, TL uses equally-spaced interpolation points and exactly integrates the gradient operator. For cell-wise constant cross sections, TL is equivalent to a numerical integration scheme that:

- 1. uses equally-spaced interpolation points,
- 2. integrates the gradient operator exactly, and
- 3. uses a Newton-Cotes quadrature restricted to the DFEM interpolation points to compute the mass matrix.

The third point can easily be demonstrated. Indeed, with traditional lumping,  $\mathbf{M}_{ij}$  is exactly computed and then a row-sum operation is performed on the rows of  $\mathbf{M}$ ; thus the entries of the diagonal mass matrix computed for TL are

$$\widehat{\mathbf{M}}_{ii} = \sum_{j=1}^{N_P} \int_{-1}^{1} \mathbf{B}_{\mathbf{i}}(s) \mathbf{B}_{\mathbf{j}}(s) \ ds = \int_{-1}^{1} \mathbf{B}_{\mathbf{i}}(s) \left[ \sum_{j=1}^{N_P} \mathbf{B}_{\mathbf{j}}(s) \right] \ ds$$
$$= \int_{-1}^{1} ds \, \mathbf{B}_{\mathbf{i}}(s) \quad \forall i = 1, \dots, N_P,$$
(2.28)

because  $\sum_{j}^{N_P} \mathbf{B_j}(s) = 1 \ \forall s \in [-1, +1]$  by definition. The integral  $\int_{-1}^{1} ds \, \mathbf{B_i}(s)$  is exactly integrated using a closed Newton-Cotes formula with  $N_P = P + 1$  points since  $\mathbf{B_i}(s)$  is a polynomial of degree P. Finally, when the  $\mathbf{B_i}$  functions are defined using equally-spaced points, the use of a closed Newton-Cotes formula with  $N_P$  points yields

$$\widehat{\mathbf{M}}_{ii} = \int_{-1}^{1} ds \, \mathbf{B}_{\mathbf{i}}(s) = \sum_{q=1}^{N_P} w_q \mathbf{B}_{\mathbf{i}}(s_q) = w_i, \qquad (2.29)$$

because  $\mathbf{B_i}(s_q) = \delta_{iq}$ . Thus, the diagonal mass matrix computed using TL contains the closed Newton-Cotes weights as diagonal entries and is equivalent to approximating  $\mathbf{M}$  using closed Newton-Cotes quadrature in Eq. (2.22). We also numerically verify this in Table 2.3 for polynomial degrees up to 4.

Table 2.3: Equivalence of traditional lumping and Newton-Cotes approximation of

the mass matrix.

the mass matrix.									
$\mid P \mid$	Exact Integration of $M$	Row Sum of M	Newton-Cotes w						
	C		with $P+1$ points						
	F 1	F -	With 1   1 points						
1	$ \begin{array}{c ccccccccccccccccccccccccccccccccccc$								
1									
	$\frac{4}{15}$ $\frac{2}{15}$ $-\frac{1}{15}$	$\frac{1}{3}$	$\frac{1}{3}$						
2	$ \begin{array}{c ccccc}  & \frac{4}{15} & \frac{2}{15} & -\frac{1}{15} \\  & \frac{2}{15} & \frac{16}{15} & \frac{1}{15} \end{array} $	$\left \begin{array}{c} \frac{4}{3} \end{array}\right $	$\left \begin{array}{c} \frac{4}{3} \end{array}\right $						
	$\begin{bmatrix} \frac{2}{15} & \frac{16}{15} & \frac{1}{15} \\ -\frac{1}{15} & \frac{2}{15} & \frac{4}{15} \end{bmatrix}$ $\begin{bmatrix} \frac{16}{105} & \frac{38}{280} & -\frac{3}{70} & \frac{19}{840} \\ \frac{33}{280} & \frac{27}{35} & -\frac{27}{280} & -\frac{3}{70} \end{bmatrix}$	$\begin{bmatrix} \frac{4}{3} \\ \frac{1}{3} \end{bmatrix}$	$\left[\begin{array}{c} \frac{1}{3} \end{array}\right]$						
	$ \begin{bmatrix} 15 & 15 & 15 \\ \hline 16 & 38 & -3 & 19 \\ \hline 840 \end{bmatrix} $		_ 1 _						
	$\begin{array}{ c c c c c c c c c c c c c c c c c c c$	$\begin{bmatrix} \overline{4} \\ 3 \end{bmatrix}$	$\begin{bmatrix} \frac{1}{4} \\ \frac{1}{3} \end{bmatrix}$						
3	$\frac{35}{280}$ $\frac{27}{35}$ $-\frac{27}{280}$ $-\frac{3}{70}$		$\begin{bmatrix} \frac{3}{4} \end{bmatrix}$						
	$\begin{bmatrix} \frac{33}{280} & \frac{27}{35} & -\frac{27}{280} & \frac{3}{70} \\ -\frac{3}{70} & -\frac{27}{280} & \frac{27}{35} & \frac{33}{280} \\ \frac{19}{840} & -\frac{3}{70} & \frac{38}{280} & \frac{16}{105} \end{bmatrix}$	$\begin{bmatrix} \frac{1}{4} \\ \frac{3}{4} \\ \frac{3}{4} \end{bmatrix}$	$\left \begin{array}{c} \frac{3}{4} \end{array}\right $						
	$\left[\begin{array}{ccc} \frac{19}{840} & -\frac{3}{70} & \frac{38}{280} & \frac{16}{105} \end{array}\right]$	$\left[\begin{array}{c} \frac{1}{4} \end{array}\right]$	$\left[\begin{array}{c} \frac{1}{4} \end{array}\right]$						
	$ \begin{array}{ c c c c c c c c c c c c c c c c c c c$	7 7	$\begin{bmatrix} \frac{4}{7} \\ \frac{7}{45} \end{bmatrix}$						
	2835 2835 945 405 2835	45	45						
	$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	$\frac{32}{45}$	$\frac{32}{45}$						
$\mid _{4}\mid$	$\begin{bmatrix} -\frac{58}{945} & -\frac{128}{945} & \frac{208}{315} & -\frac{128}{945} & -\frac{58}{945} \end{bmatrix}$	4	4						
4	$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	$\overline{15}$	15						
	$\begin{array}{c ccccccccccccccccccccccccccccccccccc$	$     \begin{bmatrix}       7 \\       45 \\       32 \\       45 \\       4 \\       \hline       15 \\       32 \\       \hline       45 \\       \hline       45 \\       \hline       7 \\       \hline       45     $	$\begin{bmatrix} \frac{4}{15} \\ \frac{32}{45} \end{bmatrix}$						
	$\begin{bmatrix} -\frac{29}{2835} & \frac{8}{405} & -\frac{58}{945} & \frac{296}{2835} & \frac{292}{2835} \end{bmatrix}$	7	$\begin{bmatrix} \frac{40}{7} \\ \frac{7}{45} \end{bmatrix}$						
		45	45						

For linear and quadratic trial spaces, the 2-point and 3-point Newton-Cotes quadrature formulae exactly integrate the gradient operator, as shown in Table 2.2. Thus, for linear and quadratic trial spaces, schemes that use (i) equally-spaced interpolation points and traditional lumping, or (ii) equally-spaced interpolation points and self-lumping numerical integration, or (iii) Lobatto quadrature points as interpolation points and self-lumping numerical integration will yield identical solutions.

#### 2.5 Numerical Results

In this Section, we present numerical results for two 1-D slab problems. For the first problem, we consider a source-free pure absorber with vacuum boundary conditions on the right, a known flux  $\psi_{in,d}$  incident on the left face, and a spatially constant total cross section  $\sigma_t$ . The second problem consists of a slab with vacuum boundary conditions on both sides, no scattering, constant  $\sigma_t$ , and a fixed  $\delta$ -source.

For  $\mu_d > 0$ , the numerical approximations to the angular flux near the cell inflow and outflow are as follows:

$$\widetilde{\psi}_{in,d} = \sum_{j=1}^{N_P} \psi_{j,d} \mathbf{B}_{\mathbf{j}}(-1)$$
(2.30)

$$\widetilde{\psi}_{out,d} = \sum_{j=1}^{N_P} \psi_{j,d} \mathbf{B}_{\mathbf{j}}(1). \qquad (2.31)$$

Regardless of the sign of  $\mu_d$ , the numerical approximation to the cell average angular flux is defined as:

$$\widetilde{\psi}_{A,d} = \frac{1}{2} \sum_{j=1}^{N_P} w_j \psi_{j,d} \,.$$
 (2.32)

We used the following quadrature weight normalization:  $\sum_{j=1}^{N_P} w_j = 2$ . In Eq. (2.30), Eq. (2.31), and Eq. (2.32),  $\psi_{j,d}$  are the components of  $\vec{\psi}_d$ , the numerical solution obtained by solving Eq. (2.11). Hence, the numerical angular flux solution of any

of the previously discussed DFEM schemes can be obtained as a function of h, the number of mean free paths divided by  $\mu_d$ ,

$$h = \frac{\sigma_t \Delta x}{\mu_d} \,. \tag{2.33}$$

## 2.5.1 Incident Flux Single-Cell Outflow Comparison

For the incident-flux problem, the analytical solution of Eq. (2.1) is:

$$\psi(x, \mu_d) = \begin{cases} \psi_{in,d} \exp\left[-\frac{\sigma_t(x - x_L)}{\mu_d}\right] & \text{for } \mu_d > 0\\ 0 & \text{for } \mu_d < 0 \end{cases}$$
 (2.34)

The analytic angular flux outflow,  $\psi_{out,d} = \psi(x_R, \mu_d)$ , is given by:

$$\psi_{out,d} = \psi_{in,d} \exp[-h]. \tag{2.35}$$

Similarly, the analytic average angular flux within the cell,  $\psi_{A,d}$ , is:

$$\psi_{A,d} = \frac{1}{\Delta x} \int_{x_L}^{x_R} \psi(x, \mu_d) \ dx = \frac{\psi_{in,d}}{h} \left( 1 - \exp[-h] \right) \ . \tag{2.36}$$

The solution components are given by

$$\vec{\psi}_d = \psi_{in,d} \left( \mathbf{G} + \frac{h}{2} \mathbf{M} \right)^{-1} \vec{f}, \qquad (2.37)$$

which allows us to compare the various choices of interpolatory points and numerical integration strategies solely as a function of h.

Figures 2.1-2.4 shows the numerically calculated cell outflow,  $\widetilde{\psi}_{out,d}$ , as a function of h for all methods considered. All methods converge to the analytical solution

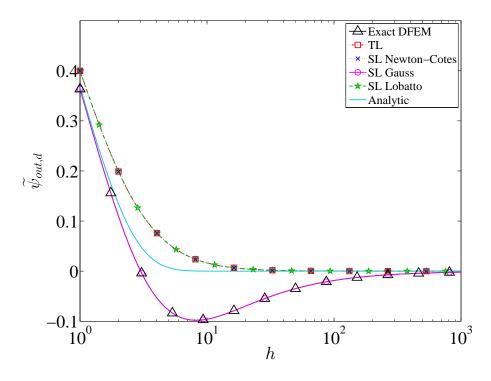


Figure 2.1: Numerical outflow values as a function of h, for a single cell homogeneous absorber problem with a linear DFEM trial space.

as  $h \to 0$ , thus we have zoomed in the range where the methods visually differ (i.e.,  $h \ge 1$ ). We observe that:

- SL Gauss yields strictly positive outflows for even degree polynomial trial spaces,
- SL Lobatto and SL Newton-Cotes yield strictly positive outflows for odd degree polynomial trial spaces, and
- TL yields strictly positive outflows only for a linear trial space.

We also numerical verify the remarks made in Section 2.4, that is:

• SL Gauss is equivalent to Exact DFEM,

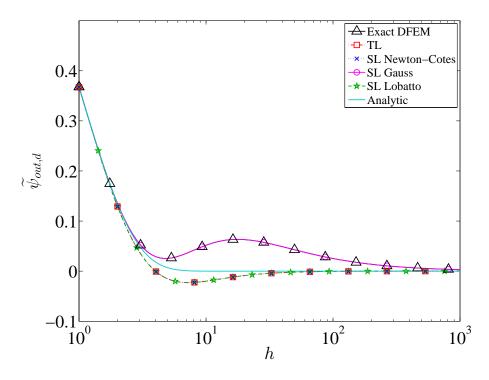


Figure 2.2: Numerical outflow values as a function of h, for a single cell homogeneous absorber problem with a quadratic DFEM trial space.

- SL Lobatto, SL Newton-Cotes, and TL are equivalent for linear and quadratic trial spaces, and
- for even degree trial spaces, the outflow value computed by SL Gauss is not monotonically decreasing as a function of h for cells of intermediate optical thickness (the same was noted in [28] for Exact DFEM).

# 2.5.2 Fixed Source Single-Cell Inflow Comparison

As noted in [15], it is possible for LDFEM to yield negative solutions near cell inflows for source driven problems. In this second problem, we use a  $\delta$ -source:

$$Q_d(x) = \begin{cases} \delta(x - x_o) & \text{for } \mu_d > 0 \\ 0 & \text{for } \mu_d < 0 \end{cases}, \qquad (2.38)$$

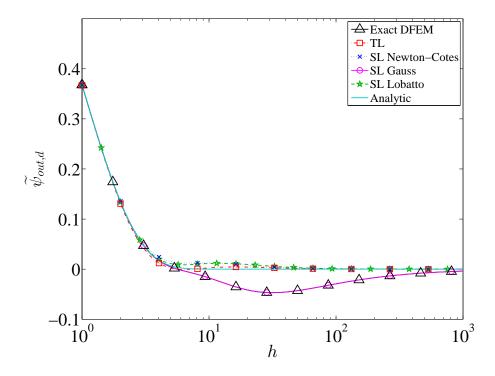


Figure 2.3: Numerical outflow values as a function of h, for a single cell homogeneous absorber problem with a cubic DFEM trial space.

 $x \in [-1, 1]$ , and  $-1 \le x_o \le 1$ . The analytic solution to this problem for  $\mu_d > 0$  is:

$$\psi(x, \mu_d) = \begin{cases} \exp\left[-\frac{\sigma_t(x - x_o)}{\mu_d}\right] & x \ge x_o \\ 0 & x < x_o \end{cases}$$
 (2.39)

(For  $\mu_d < 0$ ,  $\psi(x, \mu_d) = 0$ .) We now examine the numerical approximation to the angular flux near the cell inflow,  $\widetilde{\psi}_{in,d}$ , for various integration schemes, trial space degrees, and as a function of the ratio of the first Legendre moment of the source,  $S_1$ , to the zero-th Legendre moment of the source,  $S_0$ . Note that the physical range of that ratio,  $\frac{S_1}{S_0}$ , is [-3,3], corresponding to a  $\delta$ -source at the left cell edge ( $\frac{S_1}{S_0} = -3$ ) or at the right edge ( $\frac{S_1}{S_0} = 3$ ).

We first consider the case of a vacuum ( $\sigma_t = 0$ ), thus only testing the effect of

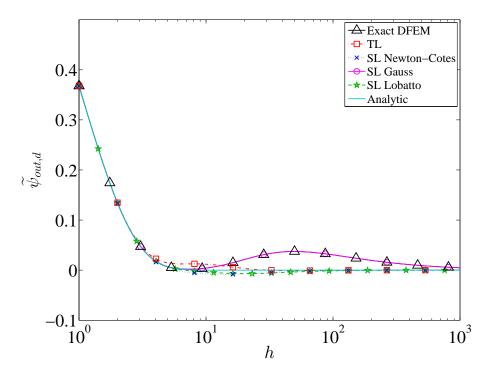


Figure 2.4: Numerical outflow values as a function of h, for a single cell homogeneous absorber problem with a quartic DFEM trial space.

quadrature accuracy in evaluating  $\vec{Q}_d$  and  $\bf{G}$ . In Figs. 2.5-2.8, we plot  $\widetilde{\psi}_{in,d}$  for three schemes:

- 1. Lobatto quadrature, which is exact for G and approximate for the source moments, Eq. (2.24),
- 2. Gauss quadrature: which is exact for both **G** and the source moments, and
- 3. Newton-Cotes quadrature: which is approximate for both **G** and the source moments.

The dotted vertical lines in Figs. 2.5-2.8 correspond to the extrema values of  $\frac{S_1}{S_0}$  that yield a strictly positive polynomial source representation of degree P (indeed, the degree-P Legendre expansion of the  $\delta$ -source is not everywhere positive for a

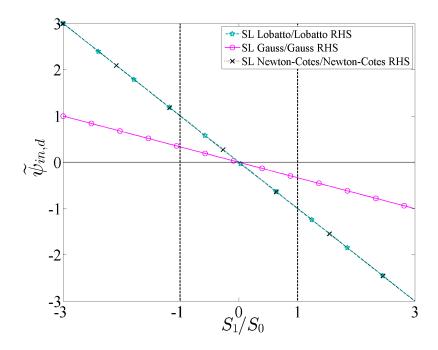


Figure 2.5: Numerical inflow values as a function of  $\frac{S_1}{S_0}$  for a single cell (vacuum case) with a  $\delta$ -shaped source, using polynomial orders P=1 through P=4.

wide range of possible  $\frac{S_1}{S_0}$  that are physically realizable). For all trial space degrees, the Gauss scheme exhibits less negativity than either of the other two schemes. The dramatic difference between the Gauss scheme and the Lobatto scheme is solely due to the quadrature formula used to evaluate  $\vec{Q}_d$  since both schemes exactly integrate  $\mathbf{G}$ . The Newton-Cotes scheme exhibits less severe negativities than the Lobatto scheme but is less robust than the Gauss scheme. Given the results shown in Figs. 2.5-2.8, we conclude that the most robust schemes exactly integrate the source moments, Eq. (2.24).

In Figs. 2.9-2.12, we again examine the positivity of  $\widetilde{\psi}_{in,d}$ , but for a non-vacuum case. The total cell optical thickness was chosen to be 5 mean free paths because this value led to the clearest plots. The relative behaviors observed do not change with cell optical thickness, but using a thicker domain reduces the magnitude for the

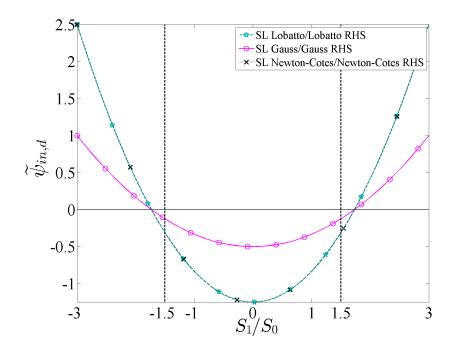


Figure 2.6: Numerical inflow values as a function of  $\frac{S_1}{S_0}$  for a single cell (vacuum case) with a  $\delta$ -shaped source, using polynomial orders P=1 through P=4.

values of  $\widetilde{\psi}_{in,d}$ . All methods in Figs. 2.9-2.12 exactly integrate Eq. (2.24). Regardless of trial space chosen, all schemes exhibit some negativities, but the SL Gauss scheme exhibits the greatest negativities and oscillations. The SL Newton-Cotes scheme presents the least severe negativities.

### 2.5.3 Single-Cell Taylor Series Analysis

Next, we perform a local truncation error analysis by comparing the Taylor series expansions for the exact and numerical angular fluxes as a function of powers of h for the source-free, incident flux pure absorber problem. Matlab [16] has been employed to perform the symbolic Taylor series expansions about h = 0. We denote the Taylor-expanded quantities using the subscript T. The expansions for the analytical inflow,

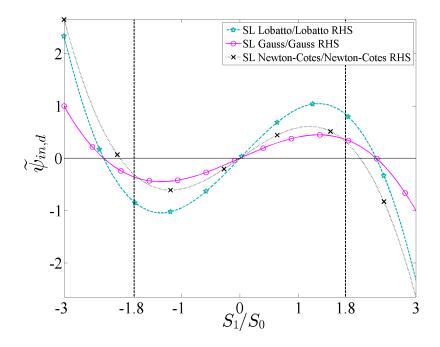


Figure 2.7: Numerical inflow values as a function of  $\frac{S_1}{S_0}$  for a single cell (vacuum case) with a  $\delta$ -shaped source, using polynomial orders P=1 through P=4.

cell average, and outflow are given below:

$$\psi_{in,d,T} = \psi_{in,d} \tag{2.40a}$$

$$\psi_{A,d,T} = \psi_{in,d} \left( 1 - \frac{h}{2} + \frac{h^2}{6} - \frac{h^3}{24} + \frac{h^4}{120} - \frac{h^5}{720} \dots \right)$$
 (2.40b)

$$\psi_{out,d,T} = \psi_{in,d} \left( 1 - h + \frac{h^2}{2} - \frac{h^3}{6} + \frac{h^4}{24} - \frac{h^5}{120} \dots \right).$$
(2.40c)

The Taylor expansions of the numerical analogues to the quantities in Eqs. (2.40) depend on the trial space polynomial degree, the choice of interpolatory points, and the numerical integration strategy. For brevity, we omit giving these numerical analogues. Table 2.4, Table 2.5, and Table 2.6 give the lowest order h term and the magnitude of its constant (in parenthesis) of the difference between the exact

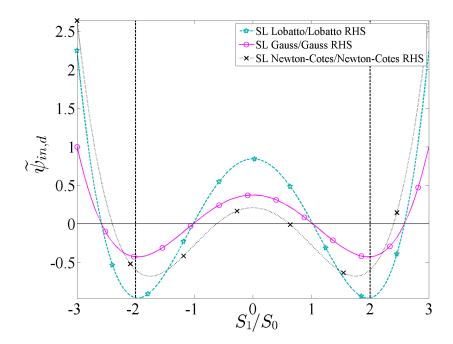


Figure 2.8: Numerical inflow values as a function of  $\frac{S_1}{S_0}$  for a single cell (vacuum case) with a  $\delta$ -shaped source, using polynomial orders P=1 through P=4.

Taylor-expanded quantities and the corresponding Taylor expansions of the numerical approximations to the angular flux near the cell inflow, cell average angular flux, and cell outflow angular flux, respectively.

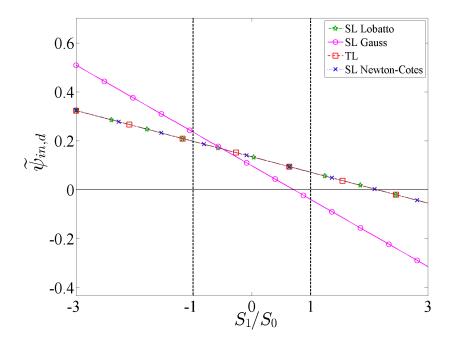


Figure 2.9: Numerical inflow values as a function of  $\frac{S_1}{S_0}$ , for a single cell (absorber case) with a  $\delta$ -shaped source, using polynomial orders P=1 through P=4.

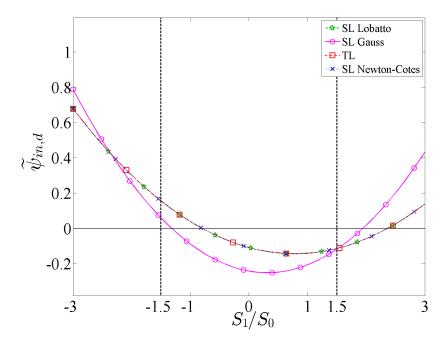


Figure 2.10: Numerical inflow values as a function of  $\frac{S_1}{S_0}$ , for a single cell (absorber case) with a  $\delta$ -shaped source, using polynomial orders P=1 through P=4.

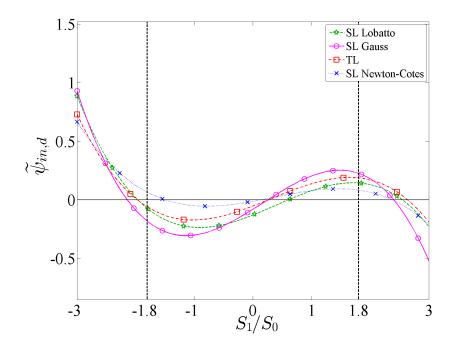


Figure 2.11: Numerical inflow values as a function of  $\frac{S_1}{S_0}$ , for a single cell (absorber case) with a  $\delta$ -shaped source, using polynomial orders P=1 through P=4.

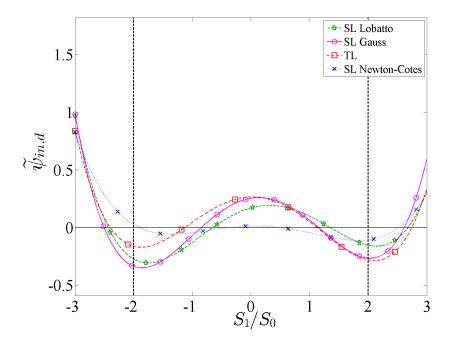


Figure 2.12: Numerical inflow values as a function of  $\frac{S_1}{S_0}$ , for a single cell (absorber case) with a  $\delta$ -shaped source, using polynomial orders P=1 through P=4.

Table 2.4: Local truncation error analysis in  $\widetilde{\psi}_{in,d}$  for a single cell problem with constant cross section. Values given as q(C) are to be read as  $Ch^q$  with  $h = \sigma_t \Delta x / \mu$ .

SL Lobatto		$2(5 \times 10^{-1})$	$3(2 \times 10^{-2}) 3(4 \times 10^{-2})$	$4 (1 \times 10^{-3})   4 (3 \times 10^{-3})$	$5 (1 \times 10^{-4})$	$6 (3 \times 10^{-6})   6 (7 \times 10^{-6})  $	$7 (1 \times 10^{-7}) 7 (3 \times 10^{-7})$	$8 (4 \times 10^{-9}) 8 (8 \times 10^{-9})$
SL Gauss		$2(2 \times 10^{-1})$ $2(5 \times 10^{-1})$	$3(2 \times 10^{-2})$	$4 (1 \times 10^{-3})$	$5 (7 \times 10^{-5})$	$6 (3 \times 10^{-6})$	$7 (1 \times 10^{-7})$	$8 (4 \times 10^{-9})$
SL Newton-Cotes   SL Gauss   SL Lobatto		$2 (5 \times 10^{-1})$	$3 (4 \times 10^{-2})$	$2(1 \times 10^{-1})$	$3 (1 \times 10^{-2})$	$2 (6 \times 10^{-2})$	$3(9 \times 10^{-3})$	$2 (4 \times 10^{-2})$
$ m L\Gamma$		$2(2 \times 10^{-1}) 2(5 \times 10^{-1})$	$3 (2 \times 10^{-2}) 3 (4 \times 10^{-2})$	$2 (7 \times 10^{-2})$	$5 (7 \times 10^{-5}) 3 (1 \times 10^{-2})$	$2 (5 \times 10^{-2})$	$3 (1 \times 10^{-2})$	$2 (5 \times 10^{-2})$
Exact	DFEM	$2(2 \times 10^{-1})$	$3 (2 \times 10^{-2})$	$4 (1 \times 10^{-3}) 2 (7 \times 10^{-2})$	$5 (7 \times 10^{-5})$	$6 (3 \times 10^{-6}) 2 (5 \times 10^{-2})$	$7 (1 \times 10^{-7}) 3 (1 \times 10^{-2})$	$8 (4 \times 10^{-9})   2 (5 \times 10^{-2})$
Polynomial	Degree of $\widetilde{\psi}$		2	3	4	5	9	7

Table 2.5: Local truncation error analysis in  $\widetilde{\psi}_{A,d}$  for a single cell problem with constant cross section. Values given as q(C) are to be read as  $Ch^q$  with  $h = \sigma_t \Delta x/\mu$ . "Machine Precision" entries are meant to indicate that Taylor series analysis was inconclusive due to all coefficients being within machine precision.

	SL Lobatto		$2(2 \times 10^{-1})$	$4 (2 \times 10^{-3})$	$6 (1 \times 10^{-5})$	$8 (5 \times 10^{-8})$	$10 (1 \times 10^{-10})$	$12 (2 \times 10^{-13})$	Machine Precision   Machine Precision
	SL Gauss		$3(1 \times 10^{-2})$	$5(1 \times 10^{-4})$	$7 (7 \times 10^{-7})$	$9(2 \times 10^{-9})$	$11 (5 \times 10^{-12})$	$13 (7 \times 10^{-15})$	Machine Precisio
1	SL Newton-Cotes		$2(2 \times 10^{-1})$	$4 (2 \times 10^{-3})$	$4 (6 \times 10^{-4})$	$6 (8 \times 10^{-6})$	$6 (2 \times 10^{-6})$	$8 (2 \times 10^{-8})$	$8 (3 \times 10^{-9})$
	TL		$2(2 \times 10^{-1})$	$4 (2 \times 10^{-3})$	$3 (3 \times 10^{-3})$	$5 (8 \times 10^{-5})$	$3 (1 \times 10^{-3})$	$5 (7 \times 10^{-5})$	ne Precision $3 (1 \times 10^{-3})$
	Exact	DFEM	$3 (1 \times 10^{-2})$	$5 (1 \times 10^{-4})$	$7 (7 \times 10^{-7})$	$9 (2 \times 10^{-9})$	$11 (5 \times 10^{-12})$	$13 \ (7 \times 10^{-15})$	Machine Precision
	Polynomial	Degree of $\widetilde{\psi}$	-	2	3	4	5	9	2

Table 2.6: Local truncation error analysis in  $\widetilde{\psi}_{out,d}$  for a single cell with constant cross section. Values given as q(C) are to be read as  $Ch^q$  with  $h = \sigma_t \Delta x/\mu$ . "Machine Precision" entries are meant to indicate that Taylor series analysis was inconclusive due to all coefficients being within machine precision.

Exact TL SL Newton-Cotes S	SL Newton-Cotes		$\mathbf{S}$	SL Gauss	SL Lobatto
DFEM					
$4 (1 \times 10^{-2})$ $3 (2 \times 10^{-1})$ $3 (2 \times 10^{-1})$		$3(2 \times 10^{-1})$		$4 (1 \times 10^{-2})$	$3(2 \times 10^{-1})$
$6 (1 \times 10^{-4}) \qquad 5 (2 \times 10^{-3}) \qquad 5 (2 \times 10^{-3})$		$5(2 \times 10^{-3})$		$6 (1 \times 10^{-4})$	$5(2 \times 10^{-3})$
$8 (7 \times 10^{-7})$ $4 (3 \times 10^{-3})$ $5 (6 \times 10^{-4})$		$5 (6 \times 10^{-})$	4)	$8 (7 \times 10^{-7})$	$7 (1 \times 10^{-5})$
$10 (2 \times 10^{-9})   6 (1 \times 10^{-2})   7 (8 \times 10^{-6})$		$7 (8 \times 10^{-})$	$\binom{9}{9}$	$10 (2 \times 10^{-9})$	$9 (5 \times 10^{-8})$
$12 (5 \times 10^{-12})   4 (1 \times 10^{-3})   7 (2 \times 10^{-6})$		$7(2 \times 10^{-})$	(9-	$12 (5 \times 10^{-12})$	$11 (1 \times 10^{-10})$
$14 (7 \times 10^{-15})   6 (7 \times 10^{-5})   9 (2 \times 10^{-8})$		$9 (2 \times 10^{-})$	(8-8)	$14 \ (7 \times 10^{-15})$	$13 (2 \times 10^{-13})$
[achine Precision $  4 (1 \times 10^{-3})   9 (3 \times 10^{-9})  $		$9 (3 \times 10^{-})$	(6-	Machine Precision   Machine Precision	Machine Precision

This local truncation error analysis illustrates the following.

- 1. Exact DFEM and SL Gauss, which are equivalent, exactly integrate the mass matrix, and are the most accurate,
- 2. TL does not guarantee increasing order of accuracy by using higher degree polynomial trial spaces,
- 3. TL converges at most third or fifth order for  $\widetilde{\psi}_{A,d}$  and fourth or sixth order for  $\widetilde{\psi}_{out,d}$  for odd or even polynomial trial spaces, respectively,
- 4. SL Newton-Cotes increases in accuracy with higher degree polynomial trial spaces, but only for  $\widetilde{\psi}_{out,d}$  and  $\widetilde{\psi}_{A,d}$ ,
- 5. TL and SL Newton-Cotes are at most second order or third order accurate for  $\widetilde{\psi}_{in,d}$  for odd or even polynomial trial spaces, respectively,
- 6. SL Gauss is order 2P+1 accurate in calculating  $\widetilde{\psi}_{A,d}$  and order 2P+2 accurate in calculating  $\widetilde{\psi}_{out,d}$ ,
- 7. SL Lobatto is order 2P accurate in calculating  $\widetilde{\psi}_{A,d}$  and order 2P+1 in calculating  $\widetilde{\psi}_{out,d}$ ,
- 8. SL Gauss, SL Lobatto, and Exact DFEM are accurate to order P+1 in calculating  $\widetilde{\psi}_{in,d}$ , and
- 9. SL Gauss is more accurate than SL Lobatto (smaller error constant) in computing  $\widetilde{\psi}_{in,d}$ , but not an order of h.

### 2.5.4 Convergence Rates for Spatially Discretized 1-D Domains

Here, we consider a homogeneous pure absorber material placed in a 1-D slab configuration and uniformly mesh the domain using  $N_{cells}$  cells. We use:  $x \in [0, 10 \ cm]$ ,

 $\sigma_t = 1 \ [cm^{-1}]$ , no external sources, vacuum conditions on the right face of the slab, and a normally incident unit beam on the left face. The analytical solution to this problem is trivial to obtain:

$$\psi(x, \mu_d) = \begin{cases} \exp\left[-\sigma_t x\right] & \mu_d = 1\\ 0 & \text{otherwise} \end{cases}$$
 (2.41)

The  $L_2$  norm of the error is:

$$E_{\psi} = \sqrt{\sum_{i=1}^{N_{cells}} \int_{x_{i-1/2}}^{x_{i+1/2}} \left( \psi(x, \mu_d) - \widetilde{\psi}_{d,i}(x) \right)^2 dx}, \qquad (2.42)$$

where we recall that  $\widetilde{\psi}_{d,i}(x)$  is the DFEM approximation of the angular flux in cell *i*. To evaluate the above integral, we use a high-order Gauss quadrature set  $(x_{f,q}, w_{f,q})$  that employs a large number of quadrature points:

$$E_{\psi} \approx \sqrt{\sum_{i=1}^{N_{cells}} \frac{\Delta x_i}{2} \sum_{q=1}^{N_{qf}} w_{f,q} \left( \psi(x_{f,q}, \mu_d) - \widetilde{\psi}_d(x_{f,q}) \right)^2}$$
 (2.43)

Values of  $E_{\psi}$  shown here are calculated using  $N_{qf} = 10$ . In addition to the  $L_2$  error, we also present the cell average angular flux error,  $E_{\psi_A}$ , defined as

$$E_{\psi_A} = \sqrt{\sum_{i=1}^{N_{cells}} \Delta x_i \left(\psi_{A,d,i} - \widetilde{\psi}_{A,d,i}\right)^2},$$
(2.44)

and the cell outflow error,  $E_{\psi_{out}}$ , given by:

$$E_{\psi_{out}} = \sqrt{\sum_{i=1}^{N_{cells}} \Delta x_i \left( \psi(x_{i+1/2}, \mu_d) - \widetilde{\psi}_{out,d,i} \right)^2}.$$
 (2.45)

In Eq. (2.43), Eq. (2.44), and Eq. (2.45),  $\Delta x_i$  is the cell width of cell i and  $\psi_{A,d,i}$  is the exact cell-averaged angular flux in cell i, which, for  $\mu_d = 1$ , is simply:

$$\psi_{A,d,i} = \exp[-\sigma_t x_{i-1/2}] \frac{1}{\Delta x_i} \left(1 - \exp[-\sigma_t \Delta x_i]\right). \tag{2.46}$$

In the plots that follow, we omit plotting the errors of Exact DFEM since the Exact DFEM solution is identical to that of SL Gauss. For linear and quadratic polynomials, we plot only SL Lobatto and omit plotting TL and SL Newton-Cotes since these methods yield identical solutions for linear and quadratic trial spaces. Figures

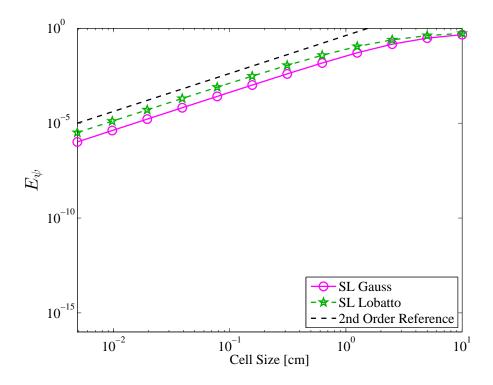


Figure 2.13: Convergence rate of the  $L_2$  norm of the error,  $E_{\psi}$ , as a function of the mesh cell size for a pure absorber  $(\sigma_t(x) = 1 \ [cm^{-1}] \ and \ x \in [0, 10 \ [cm]])$ .

2.13-2.16 mirror the results of Table 2.4, which is expected since the convergence

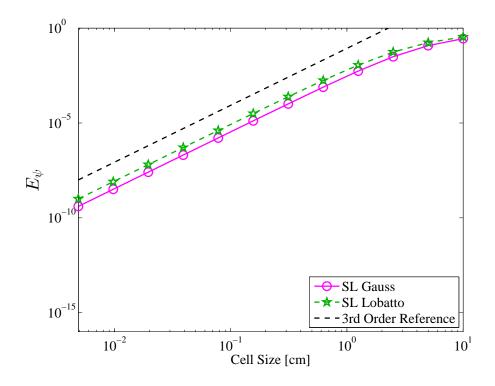


Figure 2.14: Convergence rate of the  $L_2$  norm of the error,  $E_{\psi}$ , as a function of the mesh cell size for a pure absorber  $(\sigma_t(x) = 1 \ [cm^{-1}] \ and \ x \in [0, 10 \ [cm]])$ .

rate of  $E_{\psi}$  will be limited by the slowest converging local approximation which is  $\widetilde{\psi}_{in,d}$ . Similarly, Figs. 2.17-2.20 are the multiple-cell analogue of the local truncation error analysis of  $\widetilde{\psi}_{A,d}$  given in Table 2.5.  $E_{\psi_{out}}$ , as shown in Figs. 2.21-2.24, does not converge at the local truncation error rates of Table 2.6. The accumulation of errors in multiple-cell problems causes  $E_{\psi_{out}}$  to globally converge one order of accuracy lower than the local truncation orders given in Table 2.6. It should be noted that the plateauing of errors  $E_{\psi}$ ,  $E_{\psi_A}$ , and  $E_{\psi_{out}}$  to values  $\approx 10^{-14}$  in Figs. 2.13-2.16, Figs. 2.17-2.20, and Figs. 2.21-2.24, respectively, is simply a result of our numerical solutions being limited by machine precision (double precision).

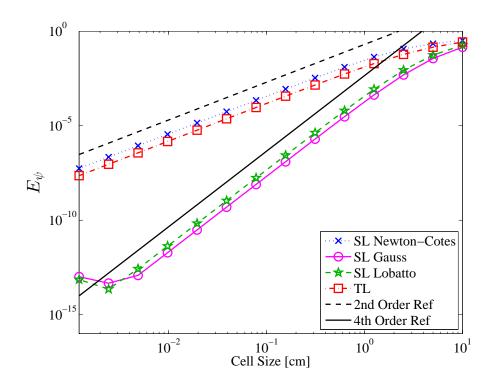


Figure 2.15: Convergence rate of the  $L_2$  norm of the error,  $E_{\psi}$ , as a function of the mesh cell size for a pure absorber  $(\sigma_t(x) = 1 \ [cm^{-1}] \ and \ x \in [0, 10 \ [cm]])$ .

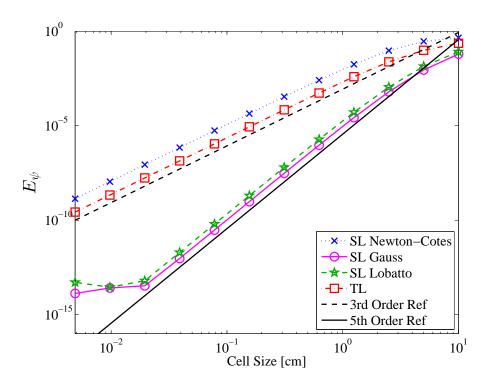


Figure 2.16: Convergence rate of the  $L_2$  norm of the error,  $E_{\psi}$ , as a function of the mesh cell size for a pure absorber  $(\sigma_t(x) = 1 \ [cm^{-1}] \ and \ x \in [0, 10 \ [cm]])$ .

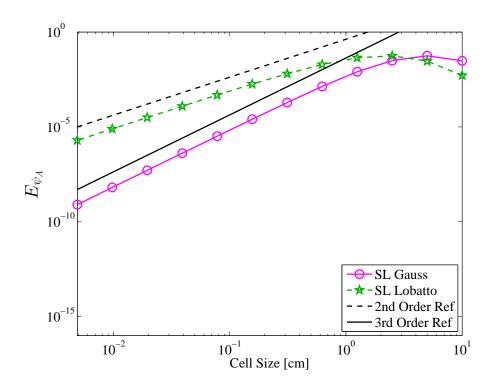


Figure 2.17: Convergence rate for  $E_{\psi,A}$  as a function of the mesh cell size for a homogeneous pure absorber and linear DFEM.

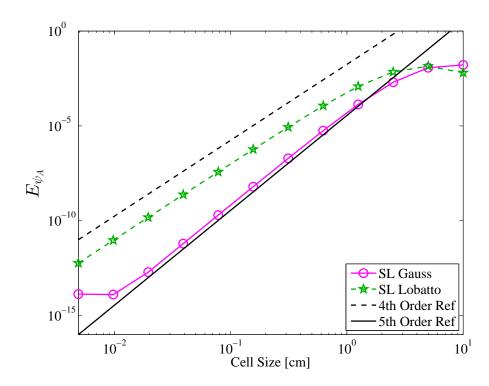


Figure 2.18: Convergence rate for  $E_{\psi,A}$  as a function of the mesh cell size for a homogeneous pure absorber and quadratic DFEM.

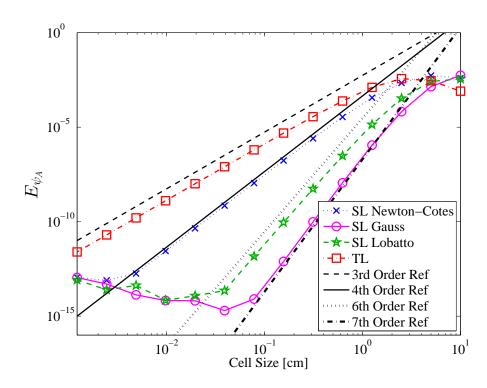


Figure 2.19: Convergence rate for  $E_{\psi,A}$  as a function of the mesh cell size for a homogeneous pure absorber and cubic DFEM.

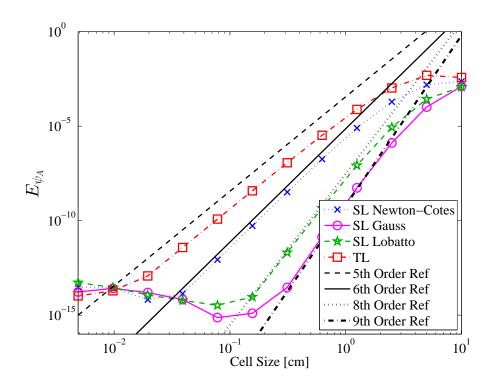


Figure 2.20: Convergence rate for  $E_{\psi,A}$  as a function of the mesh cell size for a homogeneous pure absorber and quartic DFEM.

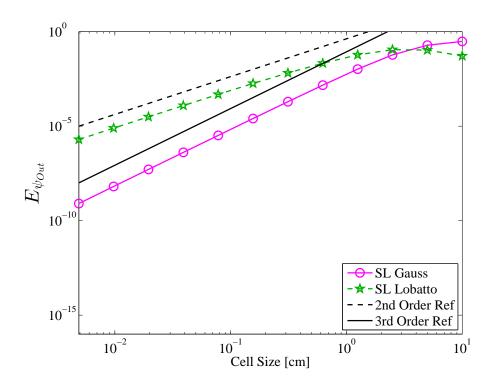


Figure 2.21: Convergence rate of  $E_{\psi,out}$  as a function of the mesh cell size for a homogeneous pure absorber for linear DFEM.

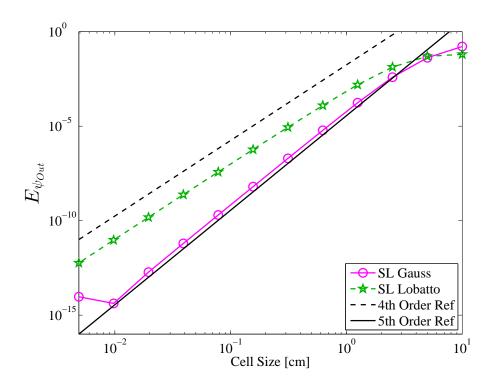


Figure 2.22: Convergence rate of  $E_{\psi,out}$  as a function of the mesh cell size for a homogeneous pure absorber for quadratic DFEM.

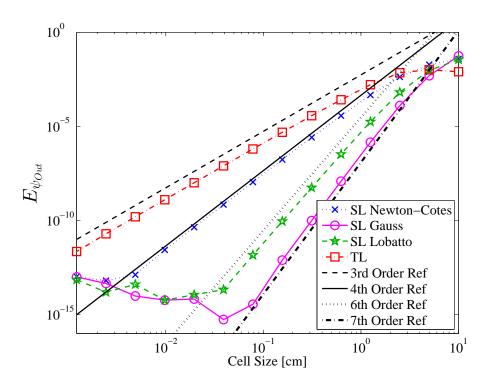


Figure 2.23: Convergence rate of  $E_{\psi,out}$  as a function of the mesh cell size for a homogeneous pure absorber for cubic DFEM.

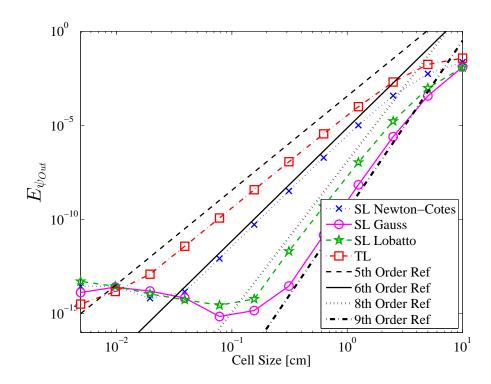


Figure 2.24: Convergence rate of  $E_{\psi,out}$  as a function of the mesh cell size for a pure absorber for quartic DFEM.

#### 3. LAST CHAPTER: THE IMPORTANCE OF RESEARCH

Thermal radiative transfer interaction opacities can be rapidly varying functions of temperature. For example, consider Marshak wave problems and the canonical  $T^{-3}$  dependence [19] of absorption opacity. Opacity variations of several orders of magnitude near the heated/cold material interface are easily possible. Historically, the neutron transport and thermal radiative transfer communities assumed interaction cross section and opacities, respectively, were cell-wise constant [3, 14, 17]. Adams first described [2] and then presented computational results [4] for a "simple" corner balance (SCB) spatial discretization method that explicitly accounted for the spatial variation of opacity within individual spatial cells. The SCB scheme (which can be shown to be related to a LDFEM for certain geometries) accounts for opacity spatial variation within each cell via vertex-based quadrature evaluation. Similar strategies have been adapted to LDFEM radiative diffusion [19] and LDFEM TRT [18] calculations. For accurate TRT solutions, use of higher order DFEM will requires the development of corresponding higher order strategies for treating the within cell spatial variation of opacities.

#### 3.1 New Section

#### 3.2 Another Section

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- 3.2.1 Subsection
- 3.2.2 Subsection

A table example is going to follow.

- 3.2.2.1 This is a subsubsection
  - 3.3 Another Section



Figure 3.1: TAMU figure

Table 3.1: This is a table template

Product	1	2	3	4	5
Price	124	136	85	156	23
Guarantee [years]	1	2	_	3	1
Rating	89%	84%	51%		45%
Recommended	yes	yes	no	no	no

- 4. LAST CHAPTER: THE IMPORTANCE OF RESEARCH
  - 4.1 New Section

# 5. LAST CHAPTER: THE IMPORTANCE OF RESEARCH

5.1 New Section

# 6. LAST CHAPTER: THE IMPORTANCE OF RESEARCH

6.1 New Section

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# APPENDIX A

### FIRST APPENDIX

Text for the Appendix follows.



Figure A.1: TAMU figure

### APPENDIX B

### SECOND APPENDIX WITH A LONGER TITLE - MUCH LONGER IN FACT

Text for the Appendix follows.

B.1 Appendix Section



Figure B.1: TAMU figure