

A NON-NEGATIVE, NON-LINEAR, PETROV-GALERKIN METHOD FOR BILINEAR DISCONTINUOUS DIFFERENCING OF THE S_N EQUATIONS

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ABSTRACT

We have developed a new, non-negative, non-linear, Petrov-Galerkin discontinuous finite element method (NNPGDFEM), for use in conjunction with Galerkin bilinear discontinuous (BLD) finite element differencing of the 2-D Cartesian geometry S_N equations for quadrilaterals on an unstructured mesh. This work is an extension of the idea that drove our previous development of a NNPGDFEM for use with linear discontinuous (LD) differencing of the 2-D Cartesian geometry S_N equations for rectangular mesh cells. We present the theory and equations that describe the new method. Additionally, we numerically compare the accuracy of our proposed method to the accuracy of the BLD scheme (without lumping) and the subcell corner balance method (equivalent to a “fully” lumped bilinear discontinuous scheme) for a test problem in which the BLD solution contains negative angular flux solutions

Key Words: Radiation transport, DFEM, non-negative, bilinear, quadrilaterals

1 INTRODUCTION

Discontinuous finite element method (DFEM) spatial discretizations of the S_N neutron transport equation and S_N thermal radiative transfer equations can result in negative angular flux and negative angular intensity solutions. These negative solutions are non-physical, but inherent to the mathematics that define the radiation spatial differencing scheme. Several researchers have examined several different methods (matrix lumping [1], fix-ups [2], and strictly non-negative solution representations [3]) that inhibit or eliminate the negativities of the linear discontinuous (LD) finite element scheme on a variety of spatial mesh cell types (slab, rectangular, triangular, ...), for the S_N neutron transport equation. However, Adams showed that LD does not maintain the neutronics thick diffusion limit on quadrilaterals [1]. We are interested in accurate methods for radiative transfer on quadrilaterals, therefore we seek methods that can maintain the radiative transfer equilibrium diffusion limit on quadrilaterals. If a radiative transfer spatial discretization is to maintain the equilibrium diffusion limit, its neutron transport analog must preserve the thick diffusion limit. As a first step towards accurate methods for radiative transfer on quadrilaterals, we thus seek non-negative, bilinear discontinuous (BLD) finite element spatial discretizations of the neutron transport equation on quadrilaterals.

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The Galerkin BLD spatial discretization for quadrilaterals, more commonly referred to as unlumped bilinear discontinuous (UBLD) yields negative angular flux solutions for spatial cells with glancing radiation incidence and/or large optical thickness [1]. To our knowledge, only matrix lumping has been considered in an attempt to inhibit negative angular flux solutions of BLD spatial discretizations. While more common forms of matrix lumping, such as mass matrix or combination mass and surface matrix lumping, inhibit negative angular flux solutions, they do not guarantee a strictly non-negative BLD angular flux solution [1]. Wareing, et. al, derived the fully lumped BLD (FLBLD) scheme [4], that uses additional manipulations of the UBLD equations to yield angular flux solutions that are strictly non-negative. Unfortunately, Adams demonstrated that FLBLD, which is equivalent to the subcell balance method on rectangles, is less accurate than the unlumped BLD (UBLD) scheme for spatial mesh cells of thin and intermediate thicknesses [5].

In [3], we developed a non-negative, non-linear Petrov-Galerkin DFEM for use in conjunction with LD spatial differencing of the S_N equations in slab and rectangular Cartesian geometry. In this paper, will extend the main idea of [3] to create a non-negative, non-linear Petrov-Galerkin DFEM to be used with UBLD spatial differencing on unstructured quadrilaterals. The remainder of this paper is divided as follows: a brief derivation common to all bilinear DFEM in Section 2, description and derivation of our new, bilinear consistent set-to-zero (BCSZ) Petrov-Galerkin scheme is given in Section 3, computational results demonstrating the strictly positive nature of BCSZ and its improved accuracy relative to UBLD and FLBLD are given in Section 4, and conclusions are given in Section 5.

2 MOMENT EQUATIONS

We begin by first considering the 2-D Cartesian discrete ordinates transport equation:

$$\vec{\Omega}_d \cdot \nabla \psi(x, y, \vec{\Omega}_d) + \sigma_t(x, y) \psi(x, y, \vec{\Omega}_d) = S_d(x, y), \quad (1)$$

where $\vec{\Omega}_d$ is the neutron direction, $\psi(x, y, \vec{\Omega}_d)$ is the angular flux [$n/(cm^s \text{ sec ster})$], $\sigma_t(x, y)$ is the total interaction cross section [cm^{-1}], and $S_d(x, y)$ is the total source (scattering + fixed sources) in direction $\vec{\Omega}_d$. Following the standard Galerkin procedure, we take the spatial moment of Eq. (1) with respect to basis function $B_i(x, y)$ by first multiplying by basis function $B_i(x, y)$ and then integrating over the spatial cell K . Assuming cell-wise constant σ_t , the i -th spatial moment equation is:

$$\int_K B_i(x, y) \left[\vec{\Omega}_d \cdot \nabla \psi(x, y, \vec{\Omega}_d) + \sigma_t \psi(x, y, \vec{\Omega}_d) \right] dx dy = \int_K B_i(x, y) S(x, y) dx dy. \quad (2)$$

Using integration by parts Eq. (2) becomes:

$$\begin{aligned} (\vec{\Omega}_d \cdot \vec{n}) \oint_R B_i(x, y) \psi(x, y, \vec{\Omega}_d) dS - \int_R \psi(x, y, \vec{\Omega}_d) \left[\vec{\Omega}_d \cdot (\nabla_{xy} B_i(x, y)) \right] dx dy \\ + \sigma_t \int_R B_i(x, y) \psi(x, y, \vec{\Omega}_d) dx dy. \end{aligned} \quad (3)$$

Defining a reference element mapping as in Fig. 1: a reference point (s, t) , $s \in [-1, 1]$ $t \in [-1, 1]$,

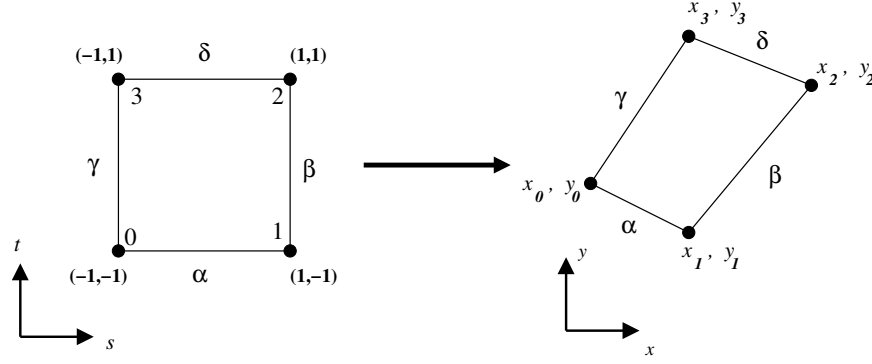


Figure 1. Reference element mapping.

is transformed to a physical point (x, y) such that:

$$x = x_0 B_0(s, t) + x_1 B_1(s, t) + x_2 B_2(s, t) + x_3 B_3(s, t) \quad (4)$$

$$y = y_0 B_0(s, t) + y_1 B_1(s, t) + y_2 B_2(s, t) + y_3 B_3(s, t). \quad (5)$$

In this work, we use mapped, bilinear Lagrange interpolatory functions as our basis functions:

$$B_0(s, t) = \frac{1-s}{2} \frac{1-t}{2} \quad (6a)$$

$$B_1(s, t) = \frac{s+1}{2} \frac{1-t}{2} \quad (6b)$$

$$B_2(s, t) = \frac{s+1}{2} \frac{t+1}{2} \quad (6c)$$

$$B_3(s, t) = \frac{1-s}{2} \frac{t+1}{2}. \quad (6d)$$

As a result, following the Galerkin procedure creates four equations with many more unknowns than equations. To solve the exact moment equations, one must assume a solution representation, $\tilde{\psi}(s, t, \vec{\Omega}_d)$, to approximate the true angular flux, $\psi(s, t, \vec{\Omega}_d)$.

The UBLD scheme assumes a solution trial space equal to the weight/basis space,

$$\tilde{\psi}_{UBLD} = \sum_{i=0}^3 \psi_{i,UBLD} B_i(s, t). \quad (7)$$

Under this assumption, the spatial moments of the transport equation become a 4×4 linear system of equations. Interested readers are directed to [1] or one of the many other papers that have derived and used UBLD on rectangles and quadrilaterals for a more complete derivation.

The FLBLD [1, 4] alternatively derived as the subcell balance method on quadrilaterals [5] begins with the UBLD equations then lumps (diagonalizes) the UBLD mass and surface matrices. The FLBLD equations are then further manipulated to result in a strictly non-negative solution representation that is second order convergent in space, and is found by solving a 4×4 linear system of equations. Again, the interested reader is directed to [1, 4, 5] for a more detailed derivation.

The BCSZ scheme is defined as being a bilinear function, $\widehat{\psi}_{BCSZ}$,

$$\widehat{\psi}_{BCSZ}(s, t) = \sum_{i=0}^3 \psi_{i,BCSZ} B_i(s, t), \quad (8)$$

everywhere $\widehat{\psi}_{BCSZ}$, is positive and zero otherwise:

$$\widetilde{\psi}_{BCSZ}(s, t) = \begin{cases} \widehat{\psi}_{BCSZ}(s, t) & \widehat{\psi}_{BCSZ}(s, t) > 0 \\ 0 & \text{otherwise} \end{cases}. \quad (9)$$

The initial iterate of $\widehat{\psi}_{BCSZ}$ is $\widetilde{\psi}_{UBLD}$. If, and only if, $\widetilde{\psi}_{UBLD} \geq 0$ everywhere within a cell, $\widetilde{\psi}_{BCSZ} = \widetilde{\psi}_{UBLD}$. Using the definition of $\widetilde{\psi}_{BCSZ}$ given in Eq. (9) turns the four spatial moments of the transport equation into four non-linear equations with four fundamental unknowns, $\psi_{i,BCSZ}$ that describe the bilinear function $\widehat{\psi}_{BCSZ}$.

3 BCSZ SCHEME

For brevity, we have omitted completely deriving the four spatial moment equations. Rather, we choose to focus on defining the important characteristics of the BCSZ scheme, namely how the BCSZ scheme defines the following moments equation quantities:

1. edge leakage, $\psi_{i,edge}$,
2. cell volume gradients, $\psi_{i,\mu}$ and $\psi_{i,\eta}$, and
3. cell volume moments, $\psi_{i,M}$.

The $\psi_{i,edge}$ terms come from the moment equation integration by parts:

$$\begin{aligned} (\vec{\Omega}_d \cdot \vec{n}) \oint_R B_i(x, y) \psi(x, y, \vec{\Omega}_d) dS &= (\vec{\Omega}_d \cdot \vec{n}_\alpha) \frac{|J_\alpha|}{2} \int_{-1}^1 B_i(s, -1) \psi(s, -1) ds \\ &+ (\vec{\Omega}_d \cdot \vec{n}_\beta) \frac{|J_\beta|}{2} \int_{-1}^1 B_i(1, t) \psi(1, t) dt + (\vec{\Omega}_d \cdot \vec{n}_\delta) \frac{|J_\delta|}{2} \int_{-1}^1 B_i(s, 1) \psi(s, 1) ds \\ &+ (\vec{\Omega}_d \cdot \vec{n}_\gamma) \frac{|J_\gamma|}{2} \int_{-1}^1 B_i(-1, t) \psi(-1, t) dt, \quad (10a) \end{aligned}$$

$$(\vec{\Omega}_d \cdot \vec{n}) \oint_R B_i(x, y) \psi(x, y, \vec{\Omega}_d) dS = (\vec{\Omega}_d \cdot \vec{n}_\alpha) \frac{|J_\alpha|}{2} \psi_{i,\alpha} + (\vec{\Omega}_d \cdot \vec{n}_\beta) \frac{|J_\beta|}{2} \psi_{i,\beta} + (\vec{\Omega}_d \cdot \vec{n}_\delta) \frac{|J_\delta|}{2} \psi_{i,\delta} + (\vec{\Omega}_d \cdot \vec{n}_\gamma) \frac{|J_\gamma|}{2} \psi_{i,\gamma}, \quad (10b)$$

where $|J|_z$ is the length of side z and \vec{n}_z is the outward directed unit normal of side z . The cell volume gradients, $\psi_{i,\mu}$ and $\psi_{i,\eta}$ come from:

$$\int_R \psi(x, y, \vec{\Omega}_d) \left[\vec{\Omega} \cdot (\nabla_{xy} B_i(x, y)) \right] dx dy = \vec{\Omega}_x \int_{-1}^1 \int_{-1}^1 \psi(s, t) \left(\frac{\partial y}{\partial t} \frac{\partial B_i}{\partial s} - \frac{\partial y}{\partial s} \frac{\partial B_i}{\partial t} \right) ds dt \\ + \vec{\Omega}_y \int_{-1}^1 \int_{-1}^1 \psi(s, t) \left(\frac{\partial x}{\partial s} \frac{\partial B_i}{\partial t} - \frac{\partial x}{\partial t} \frac{\partial B_i}{\partial s} \right) ds dt \quad (11a)$$

$$\int_R \psi(x, y, \vec{\Omega}_d) \left[\vec{\Omega} \cdot (\nabla_{xy} B_i(x, y)) \right] dx dy = \mu \psi_{i,\mu} + \eta \psi_{i,\eta}. \quad (11b)$$

The $\psi_{i,M}$ term comes from the reaction term:

$$\sigma_t \int_R B_i(x, y) \psi(x, y, \vec{\Omega}_d) dx dy = \sigma_t \int_{-1}^1 \int_{-1}^1 B_i(s, t) \psi |J| ds dt = \sigma_t \psi_{i,M}. \quad (12)$$

In Eq. (11), all $\frac{\partial}{\partial s}$ terms are linear functions in t , all $\frac{\partial}{\partial t}$ terms are linear functions in s , J is the Jacobian matrix of the coordinate transformation:

$$J = \begin{bmatrix} \frac{\partial x}{\partial s} & \frac{\partial y}{\partial s} \\ \frac{\partial x}{\partial t} & \frac{\partial y}{\partial t} \end{bmatrix}. \quad (13)$$

3.1 BCSZ Cell Integration

Given the definition of $\hat{\psi}_{BCSZ}$ in Eq. (9), the integral contributions to $\psi_{i,\mu}$, $\psi_{i,\eta}$, and $\psi_{i,M}$ are non-trivial only over a portion of the cell where $\hat{\psi}_{BCSZ}(s, t) > 0$. There are seven possible geometric integration cases to be considered for all values of $\hat{\psi}_{BCSZ}$. Six are shown in Fig. 2. The other case is when $\hat{\psi}_{BCSZ} > 0$ everywhere in the cell, in which case the integration of $\psi_{i,\mu}$, $\psi_{i,\eta}$, and $\psi_{i,M}$ is straight forward, and identical to that required by the definition of the UBLD scheme. Though other cases are possible, all can be transformed into one of the cases in Fig. 2 via rotation. By definition, along each solid line in Fig. 2, $\hat{\psi}_{BCSZ} = 0$. To evaluate $\psi_{i,\mu}$, $\psi_{i,\eta}$, and $\psi_{i,M}$ over some region, R , in Fig. 2 where $\hat{\psi}_{BCSZ} > 0$ and one edge is bounded by a curve, we use a variable limit of integration in t . To do this, we first transform $\hat{\psi}_{BCSZ}$ from an interpolatory polynomial to a moment based polynomial, $f(s, t)$:

$$f(s, t) = f_c + s f_s + t f_t + st f_{st}. \quad (14)$$

We find the coefficients of this formula using the interpolatory definition of the basis functions:

$$\begin{bmatrix} 1 & -1 & -1 & 1 \\ 1 & 1 & -1 & -1 \\ 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \end{bmatrix} \begin{bmatrix} f_c \\ f_s \\ f_t \\ f_{st} \end{bmatrix} = \vec{\psi}_{BCSZ}, \quad (15)$$

with

$$\vec{\psi}_{BCSZ} = [\psi_{0,BCSZ}, \psi_{1,BCSZ}, \psi_{2,BCSZ}, \psi_{3,BCSZ}]^T. \quad (16)$$

Since $f(s, t) = 0$ along each solid line in Fig. 2, Eq. (14) can be manipulated to find a variable limit of integration with respect to t , \hat{l}_t , that is a function of s :

$$\hat{l}_t = -\frac{f_c + f_s s}{f_t + f_{st} s}. \quad (17)$$

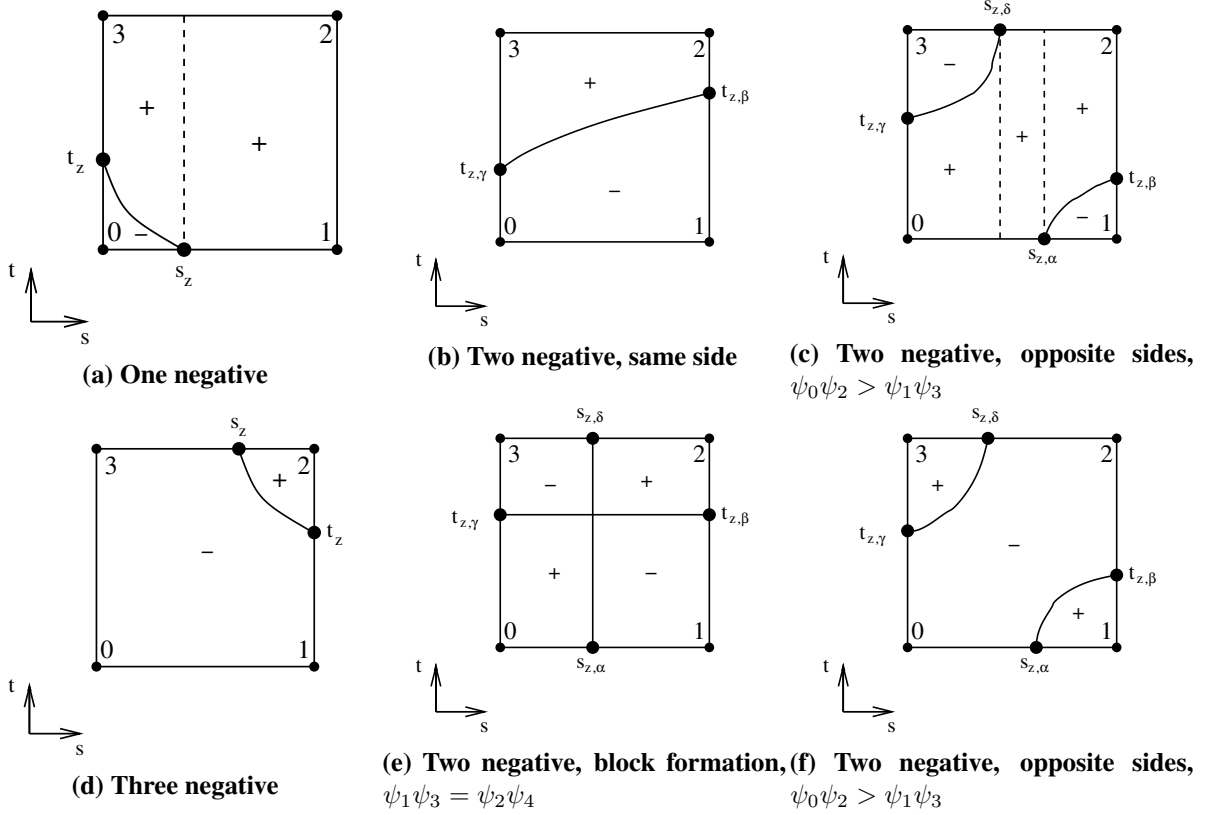


Figure 2. BCSZ cell integration cases requiring special treatment.

Rather than evaluate each $\psi_{i,\mu}$, $\psi_{i,\eta}$, and $\psi_{i,M}$ integral, we seek a single, generic integrand that is only a function of s and t . We find this generic integrand by first expanding the specific $\tilde{\psi}_{BCSZ}$ integrand definitions of $\psi_{i,\mu}$, $\psi_{i,\eta}$, and $\psi_{i,M}$ over R . Starting with the integrand of $\psi_{i,\mu}$,

$$\widehat{\psi}_{BCSZ}(s, t) \left(\frac{\partial y}{\partial t} \frac{\partial B_i}{\partial s} - \frac{\partial y}{\partial s} \frac{\partial B_i}{\partial t} \right) = [f_c + sf_s + tf_t + stf_{st}] \dots$$

$$([y_{t,c} + sy_{t,s}][b_{i,s,c} + tb_{i,s,t}] - [y_{s,c} + ty_{s,t}][b_{i,t,c} + sb_{i,t,s}]) , \quad (18a)$$

then the $\psi_{i,\eta}$ integrand:

$$\widehat{\psi}_{BCSZ}(s, t) \left(\frac{\partial x}{\partial s} \frac{\partial B_i}{\partial t} - \frac{\partial x}{\partial t} \frac{\partial B_i}{\partial s} \right) = [f_c + sf_s + tf_t + stf_{st}] \dots$$

$$([x_{s,c} + tx_{s,t}][b_{i,t,c} + sb_{i,t,s}] - [x_{t,c} + sx_{t,s}][b_{i,s,c} + tb_{i,s,t}]) , \quad (18b)$$

and finally the $\psi_{i,M}$ integrand:

$$B_i(s, t) \widehat{\psi}_{BCSZ}(s, t) |J(s, t)| = [b_{i,c} + sb_{i,s} + tb_{i,t} + stb_{i,st}] [f_c + sf_s + tf_t + stf_{st}] [g_c + sg_s + tg_t] . \quad (18c)$$

In Eqs. (18) we have defined the following:

$$B_i(s, t) = b_{i,c} + sb_{i,s} + tb_{i,t} + stb_{i,st} \quad (19a)$$

$$\frac{\partial B_i}{\partial s} = b_{i,s,c} + tb_{i,s,t} \quad (19b)$$

$$\frac{\partial B_i}{\partial t} = b_{i,t,c} + sb_{i,t,s} \quad (19c)$$

$$|\mathbf{J}(s, t)| = g_c + sg_s + tg_t \quad (19d)$$

$$\frac{\partial x}{\partial s} = x_{s,c} + tx_{s,t} \quad (19e)$$

$$\frac{\partial x}{\partial t} = x_{t,c} + sx_{t,s} \quad (19f)$$

$$\frac{\partial y}{\partial s} = y_{s,c} + ty_{s,t} \quad (19g)$$

$$\frac{\partial y}{\partial t} = y_{t,c} + sy_{t,s} . \quad (19h)$$

Using MATLAB [6], each integrand in Eqs. (18) is further expanded, then terms of equal degree bivariate polynomials, $s^m t^n$, with $0 \leq m \leq 3, 0 \leq n \leq 3$, are collected. This allows us to calculate the twelve separate integrations of $\psi_{i,\mu}$, $\psi_{i,\eta}$, and $\psi_{i,M}$, as the multiplication of twelve unique sets of constants, $\mathbf{C}_{i,\mu}$, $\mathbf{C}_{i,\eta}$, and $\mathbf{C}_{i,M}$, multiplied by the integrations of a single set of bivariate polynomials, over R .

3.1.1 Symbolic integration versus numerical integration

Initially, MATLAB [6] symbolic algebra generated expressions for the integrations of the generic bivariate polynomials over R were used to evaluate $\psi_{i,\mu}$, $\psi_{i,\eta}$, and $\psi_{i,M}$. This worked well at low cell counts, but caused the $\tilde{\psi}_{BCSZ}$ non-linear iteration to fail at higher cell counts. To verify the MATLAB generated expressions, we compared the “exact” symbolic algebra generated results for calculating $\psi_{i,M}$ for $\tilde{\psi}_{BCSZ} = [-2 \ 0.1 \ 200 \ 10]^T$ to the value obtained using N_s Gauss quadrature points in s along the curved boundary. A two-point Gauss quadrature in t was used for each corresponding Gauss point in s (tensor product quadrature). An example of the quadrature layout is given in Fig. 3 for $N_s = 4$. In Fig. 4a, we plot $E_{i,quad}$, where:

$$E_i = \frac{|\psi_{i,sym} - \psi_{i,num}|}{|\psi_{i,sym}|}, \quad (20)$$

$\psi_{i,sym}$ is the evaluation of $\psi_{i,M}$ using the symbolic algebra generated expressions, and $\psi_{i,num}$ is the quadrature evaluation of $\psi_{i,M}$ using $2N_s + 4$ quadrature points. Compare the result of Fig. 4a to Fig. 4b, which plots \hat{E}_i :

$$\hat{E}_i = \frac{|\psi_{i,MAX} - \psi_{i,num}|}{|\psi_{i,MAX}|}, \quad (21)$$

where $\psi_{i,MAX}$ is the quadrature approximation of $\psi_{i,M}$ using Gauss quadrature and $N_s = 40$. It is clear that the “exact” symbolic evaluated expressions suffer from numerical round-off caused by taking the small difference of large numbers. As such, we prefer quadrature integration to evaluate cell integral quantities for the BCSZ scheme. However, for a fixed number of Gauss points in s , we cannot apriori estimate the error in our quadrature approximation of bivariate polynomial integrals over the region with a curved boundary. Gauss-Kronrod quadrature [7] allows for an estimate of the

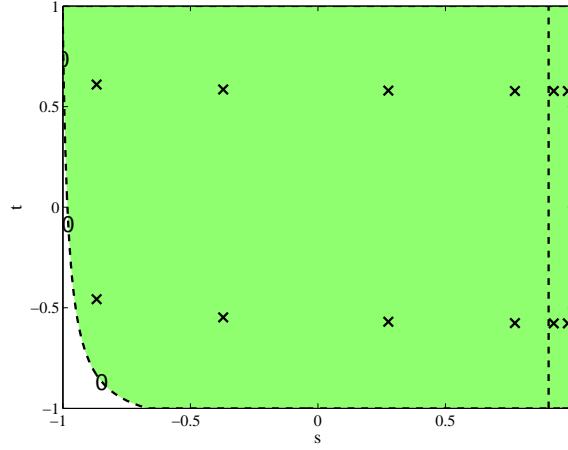
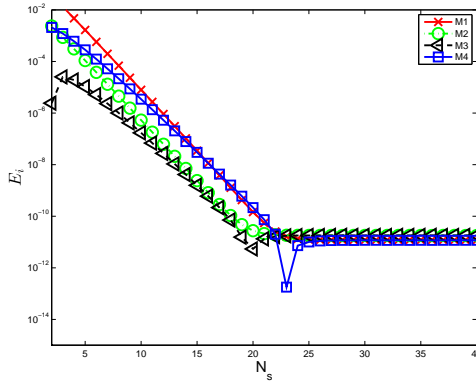
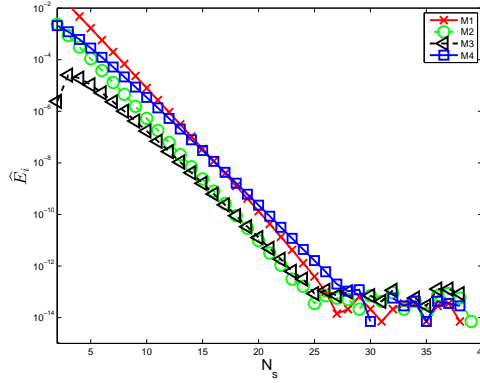


Figure 3. Quadrature point locations for $N_s = 4$ for quadrature integration test.



(a) E_i for quadrature test.



(b) \hat{E}_i for quadrature test.

Figure 4. Comparison of quadrature vs. exact integration errors.

quadrature error to the approximation of an integration. In practice, we now use the 7-point Gauss / 15-point Kronrod quadrature set in s with a 2-point Gauss quadrature in t to integrate all BCSZ quantities. Along with sub-interval refinement, this integration strategy, and the decompositions shown in Fig. 2 allow for the computation of all BCSZ cell integral quantities to a tolerance less than our non-linear iteration tolerance.

3.2 BCSZ Edge Integration

Along any edge, there are four possible cases. Assuming that we are looking at edge α , but with easy translation to any other edge:

1. $\hat{\psi}_{BCSZ} > 0$ along whole edge,

2. $\hat{\psi}_{BCSZ} < 0$ along whole edge,
3. $\psi_{0,BCSZ} < 0, \psi_{1,BCSZ} > 0$, and
4. $\psi_{0,BCSZ} > 0, \psi_{1,BCSZ} < 0$.

Case one is straightforward and identical to the integration used by the UBLD scheme. Case two is by definition, zero along the integral. Cases three and four are handled by first determining s_z , such that $\hat{\psi}_{BCSZ}(s_z, -1) = 0$:

$$s_z = \frac{\psi_{0,BCSZ} + \psi_{1,BCSZ}}{\psi_{0,BCSZ} - \psi_{1,BCSZ}} \quad (22)$$

Then a two point Gauss quadrature is mapped to the interval $[s_z, 1]$ for case 3 and $[-1, s_z]$ for case 4, and the integral of $\psi_{i,\alpha}$ is approximated (exactly) using function evaluations at the mapped quadrature points.

4 NUMERICAL RESULTS

Some text

5 CONCLUSIONS

Thoughts

6 ACKNOWLEDGMENTS

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7 REFERENCES

- [1] M. L. Adams, “Discontinuous Finite Element Transport Solutions in Thick Diffusive Problems,” *Nuclear Science and Engineering*, **137**, pp. 298–333 (2001).
- [2] E. D. Fichtl, J. S. Warsa, and J. D. Densmore, “The Newton-Krylov Method Applied to Negative-Flux Fixup in S_N Transport Calculations,” *Nuclear Science and Engineering*, **165**, pp. 331–341 (2010).
- [3] P. G. Maginot, J. E. Morel, and J. C. Ragusa, “A Non-negative Moment Preserving Spatial Discretization Scheme for the Linearized Boltzmann Transport Equation in 1-D and 2-D Cartesian Geometries,” *Journal of Computational Physics*, **231**, pp. 6801–6826 (2012).
- [4] T. A. Wareing, E. W. Larsen, and M. L. Adams, “Diffusion Accelerated Discontinuous Finite Element Schemes for the S_N Equations in Slab and X,Y Geometries,” *Proc. International Topical Mtg. on Advances in Mathematics, Computations and Reactor Physics*, Pittsburgh, PA, April 28-May 2, 1991.

- [5] M. L. Adams, “Subcell Balance Methods for Radiative Transfer of Arbitrary Grids,” *Transport Theory and Statistical Physics*, **26**, pp. 385–431 (1997).
- [6] Mathworks, “MATLAB R-2011a,” 2011.
- [7] T. N. L. Patterson, “The Optimum Addition of Points to Quadrature Formulae,” *Mathematics of Computation*, **22**, pp. 847–856 (1968).