A Non-Negative Bilinear DFEM Scheme for S_N Transport

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Outline

1. Goal/Motivation
2. BCSZ Method
3. Initial Results

Goal

- Long term goal: Accurate methods for multi-dimensional radiative transfer
- Near term goal: Non-negative bilinear DFEM for neutron transport
  - Bilinear DFEM required on quads to maintain thick diffusion limit
  - Radiative transfer cells will almost certainly be optically thick
- History: Extension of non-negative linear $(1, x, y)$ scheme developed on rectangles

BCSZ Definition

Solution representation, $\widetilde{\psi}_{BCSZ}(s,t)$:

$$\widetilde{\psi}_{BCSZ}(s,t) = \begin{cases} \widehat{\psi}_{BCSZ}(s,t) & \widehat{\psi}_{BCSZ}(s,t) > 0 \\ 0 & \text{otherwise} \end{cases} . \tag{1}$$

Bilinear function, $\widehat{\psi}_{BCSZ}$, to search for,

$$\widehat{\psi}_{BCSZ}(s,t) = \sum_{i=0}^{3} \psi_{i,BCSZ} B_i(s,t) , \tag{2}$$

Moment Equation Edge Integration

DFEM moment equations will need to integrate quantities like this on cell edges:

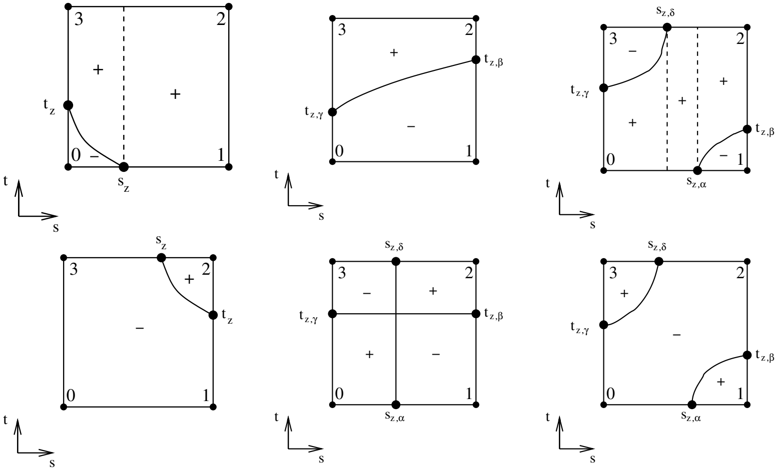
$$(\vec{\Omega}_d \cdot \vec{n}_\alpha) \int_\alpha B_i(s,-1)\widetilde{\psi}_{BCSZ}\ ds$$

1. Check vertices for negativity
2. By definition of $\widetilde{\psi}_{BCSZ}$, integrate $\widehat{\psi}_{BCSZ}$ only over portion of the interval where $\widehat{\psi}_{BCSZ} \geq 0$
3. If $\psi_L < 0$ or $\psi_R < 0$:

$$s_z = \frac{\psi_L + \psi_R}{\psi_L - \psi_R}$$

Cell Interior Integration

Must integrate terms like, $B_i \widetilde{\psi}_{BCSZ} |J|$, over areas like these:



Enabling Idea

Along every integration area curve:

$$\widehat{\psi}_{BCSZ}(s,t) = 0$$

Transform interpolatory $\widehat{\psi}_{BCSZ}$ to moment based $f(s,t)$:

$$f(s,t) = f_c + sf_s + tf_t + stf_{st} \tag{3}$$

$$\begin{bmatrix} 1 & -1 & -1 & 1 \\ 1 & 1 & -1 & -1 \\ 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \end{bmatrix} \begin{bmatrix} f_c \\ f_s \\ f_t \\ f_{st} \end{bmatrix} = \vec{\psi}_{BCSZ} \tag{4}$$

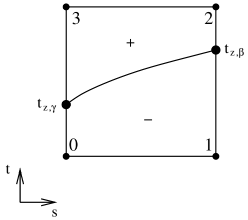
Enabling Idea- 2

Along each integration area defined by a curve, $f(s,t)=0$, and

$$\hat{l}_t = -\frac{f_c + f_s s}{f_t + f_{st} s}\,, \tag{5}$$

enabling the use of variable limits of integration.

Consider integration over the domain, R_+, where $\widehat{\psi}_{BCSZ} > 0$:



$$\int\int_{R_+} M(s,t) = \int_{-1}^{1} ds \int_{\hat{l}_t}^{1} dt\; M(s,t)$$

Isn't MATLAB Right?

Initial thinking:

- Must respect curved boundary of integration regions
  - Only possible with analytic integration via variable limits of integration.
- MATLAB gives a solution, that solution must be right
  - Boldly [blindly] assumes we live in an analytic, not finite precision world

This results in:

- Occasional trouble with non-linear iteration
  - Predominantly with nearly zero solutions
- Maybe blindly trusting MATLAB is bad?

Quadrature Test

Quadrature integrate $\psi_{i,M}$

$$\int\int_{R^+} |\mathbf{J}|\, B_i \widehat{\psi}_{BCSZ}\ dsdt$$

$$E_i = \frac{|\psi_{i,sym} - \psi_{i,num}|}{|\psi_{i,sym}|}$$

$$\widehat{E}_i = \frac{|\psi_{i,MAX} - \psi_{i,num}|}{|\psi_{i,MAX}|}$$

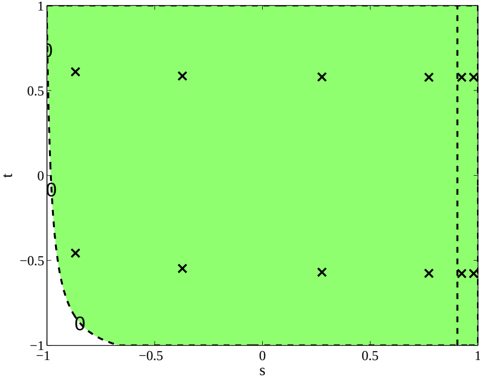


Figure: Quadrature layout with $i = 4$

Evidence of Numerical Precision Issues

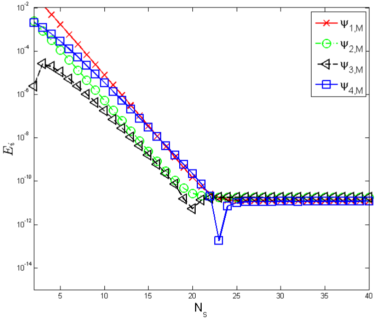


Figure: E_i for quadrature test.

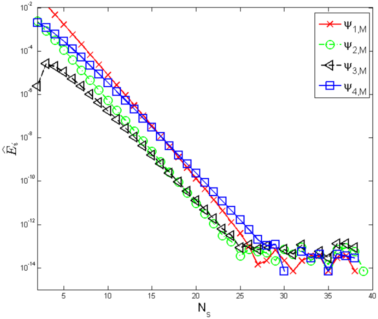


Figure: $\widehat{E}_i$ for quadrature test.

Modification: Adaptive Gauss-Kronrod quadrature to evaluate cell integrals

Non-linear Iteration

- Newton iteration with finite difference formed Jacobian
- $\widehat{\psi}^{(0)}_{BCSZ} = \widetilde{\psi}_{UBLD}$
- Damping with restart based on iteration count
- Solve for local unknowns (1 solve per cell, direction, group [if needed])
- Search for scaled $\widehat{\psi}_{BCSZ}$. Scale using $\widehat{\psi}^{(0)}_{BCSZ}$
- $\epsilon = \epsilon_{rel} R^{(0)} + \epsilon_{abs} \left\| \text{RHS} \right\|_{L_2}$
- $\epsilon_{rel} = 10^{-10}$, $\epsilon_{abs} = 10^{-12}$
- Usually 7-10 Newton iterations per solve

Implementation in PDT

- PDT assumes unknowns live at cell vertices, and all methods are linear (not non-linear)
    - But, BCSZ is obviously non-linear
- Work around required
    1. Add if statement in sweep. Affects all methods
    2. Multiply $\psi_{i,M}$ of converged $\widetilde{\psi}_{BCSZ}$ by inverse mass matrix
        - Gives a bilinear function with same cell $\psi_{i,M}$ moments as $\widetilde{\psi}_{BCSZ}$
    3. Prepare outflow for downwind cells
        - Calculate linear/nodal values necessary to yield BCSZ edge moments
- Exact BCSZ solution representation cannot be recreated without sweeping again
    - Cell average BCSZ flux retained with work around
    - Spatial moments preserved, does not affect physics coupling

Methods to Compare

1. UBLD: Unlumped Bilinear DFEM- Galerkin DFEM, no explanation necessary
2. SCB/FLBLD: Subcell Corner Balance- On rectangles, Equivalent to UBLD with mass matrix lumping, surface matrix lumping, and other manipulations
3. BCSZ: Bilinear consistent set-to-zero- Non-linear, Petrov-Galerkin DFEM, satisfies all bilinear spatial moments of the transport equation

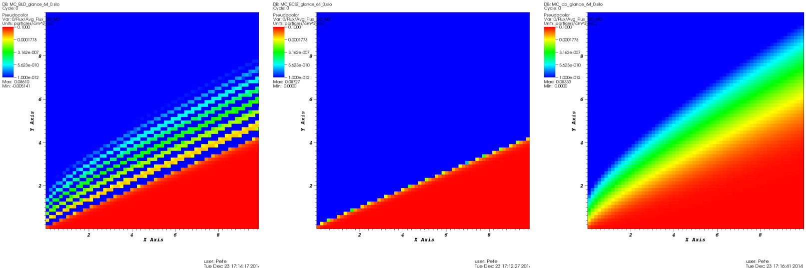
Test Problem

- $10[cm] \times 10[cm]$ square void
- Vacuum BC on left, top, right edges
- Incident flux of 1 $[n/(cm^2 - sec - ster)]$ in one direction on bottom edge
  - $\mu = 0.868890300722, \ \eta = 0.35002117452$
- L^2 like norm of cell average scalar flux

$$E_{\phi_A} = \sqrt{\sum_{c=1}^{N_{cells}} \Delta x_c \Delta y_c (\widetilde{\phi}_A - \phi_{A,exact})^2} \,,$$

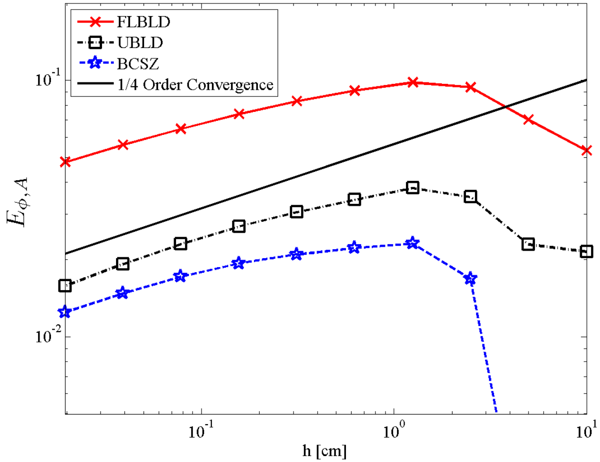
Orthogonal Mesh

625 square mesh cells



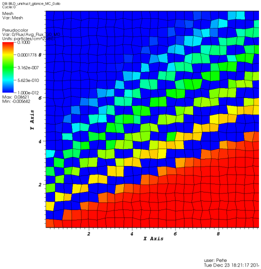
(a) UBLD (b) BCSZ (c) SCB/FLBLD

Convergence

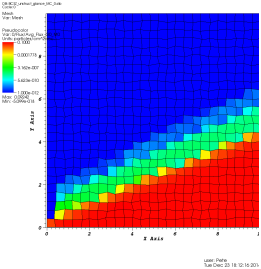


Distorted Mesh

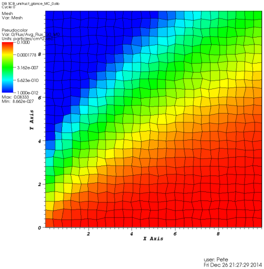
25 $\times$ 25 cells, with distorted interior vertices



(a) UBLD



(b) BCSZ



(c) SCB

Conclusions and Future Work

Conclusions

- BCSZ is strictly non-negative
- BCSZ is more accurate than UBLD or SCB for a glancing void
- BCSZ can be applied to non-orthogonal meshes
- BCSZ requires significant local computation, but is computationally feasible

Future Work

- Develop a problem large/complex enough that timing can be performed
- Move non-linear iteration out of individual cells to enable preconditioning / DSA
- Consider removing case selection statement in favor of apply GK quad to entire cell

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DOE CSGF

CERT
Center for Exascale Radiation Transport