Error Estimates for Discrete Ordinates Methods Used in Solving the Neutron Transport Equation

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0. Outline

0. Nuclear Computational Science Group at PSU
1. The Transport Equation
2. Local Error Analysis
3. Global Error Analysis
4. High Order Methods
5. Conclusion

0. Nuclear Computational Science Group at PSU

Josh Hykes: Schreyer Honors Scholar, DOE-CSG Fellow

Honors Thesis: *Verification of a Computational Model for the Determination of Dose Due to CT Scan*

Andy Bielen: MS Student, DOE-NE Fellow

Thesis: *Spherical Harmonic Solutions to the Self-Adjoint Angular Flux Equations for Charged Particle Transport*

Joe Zerr: MS Student, PSU-University Graduate Fellow

Thesis: *Effect of Direction-Dependent Diffusion Coefficients on the Accuracy of the Diffusion Model for LWR Cores*

0. Nuclear Computational Science Group at PSU

Dan Gill: MS Student, DOE-NPP Fellow

Thesis: ***Behavior of the Diamond Difference and Low-order Nodal Numerical Transport Methods in the Thick Diffusion Limit for Slab Geometry***

Kursat Bekar: PhD Student

Thesis: ***Developing a Modular Optimization Package to Design New Beam Ports for the PSBR***

Max Rosa: PhD Student

Thesis: ***Properties of the Discrete Ordinates Equivalent Integral Transport Operator***

0. Nuclear Computational Science Group at PSU

Jose Duo: PhD Student

Thesis: ***Error Estimates for Spatial Approximations of the Discrete Ordinates Method in Two Dimensional Transport Problems***

Mike Ferrer: PhD Student – INL Staff

Thesis: ***Arbitrarily High Order Transport (AHOT) Method of the Characteristic Type for Unstructured Grids***

Jesse Klingensmith: PhD Student – Areva Staff

Thesis: ***TBD***

1. Neutron Transport Equation

- **Special case of Boltzmann equation: First-order integrodifferential**
  - Neutral particles ⇨ no electro-magnetic forces
  - Low particle densities ⇨ ignore neutron-neutron collisions ⇨ linear
- **Balance over infinitesimal element in phase space:** $(\vec{\mathbf{r}}, \hat{\mathbf{\Omega}}, E)$
- **Dependent variable: Angular flux** $\psi(\vec{\mathbf{r}}, \hat{\mathbf{\Omega}}, E, t)$

$$\overbrace{\frac{1}{v}\frac{\partial \psi(\vec{\mathbf{r}}, E, \hat{\mathbf{\Omega}}, t)}{\partial t}}^{\text{Transient}} + \overbrace{\hat{\mathbf{\Omega}} \cdot \nabla \psi(\vec{\mathbf{r}}, E, \hat{\mathbf{\Omega}}, t)}^{\text{Streaming}} + \overbrace{\Sigma_t(\vec{\mathbf{r}}, E)\psi(\vec{\mathbf{r}}, E, \hat{\mathbf{\Omega}}, t)}^{\text{Total collision}}$$

$$\text{Scattering}\left\{ = \int_{4\pi} d\hat{\mathbf{\Omega}}' \int_0^\infty dE' \Sigma_s(E', \hat{\mathbf{\Omega}}' \to E, \hat{\mathbf{\Omega}}) \psi(\vec{\mathbf{r}}, E', \hat{\mathbf{\Omega}}', t) \right.$$

$$\text{Fission}\left\{ + \frac{\chi(E)}{4\pi}\left[\int_0^\infty dE' \nu(E') \Sigma_f(\vec{\mathbf{r}}, E') \int_{4\pi} d\hat{\mathbf{\Omega}}' \psi(\vec{\mathbf{r}}, E', \hat{\mathbf{\Omega}}', t) \right] \right. + \underbrace{s(\vec{\mathbf{r}}, E, \hat{\mathbf{\Omega}}, t)}_{\text{Fixed source}}$$

1. Interface & Boundary Conditions

- **Steady state: Time derivative vanishes**
- **Interface condition: Angular flux continuous along direction of motion, $\hat{\Omega}$, across material boundaries**
- **Physical intuition: Can specify what goes into a system**
  - What comes out is a consequence of the transport process inside
  - Example: shining light into crystal
    - Can choose color/intensity of incoming light
    - Can't choose color/intensity of outgoing light: depends on what happens inside
- **Typical Boundary Condition (BC):**
  - Set ***incoming*** flux $\psi(\vec{\mathbf{r}}_s, E, \hat{\mathbf{\Omega}}) = \psi_{in}(\vec{\mathbf{r}}_s, E, \hat{\mathbf{\Omega}})$ for:
    - All energies: $E \in [0, \infty]$
    - Each $\vec{\mathbf{r}}_s$ on the boundary S
    - Each incoming angle: $\hat{\mathbf{\Omega}} \cdot \hat{\mathbf{e}}_s < 0$; $\hat{\mathbf{e}}_s$ is the normal unit vector at $\vec{\mathbf{r}}_s$ pointing out of the volume enclosed by S
  - The function $\psi_{in}(\vec{\mathbf{r}}_s, E, \hat{\mathbf{\Omega}})$ can be specified explicitly or implicitly
    - Vacuum BC: $\psi_{in}(\vec{\mathbf{r}}_s, E, \hat{\mathbf{\Omega}}) = 0$

1. Discretization of Transport Equation

- **Implementation on digital computer ⇨ discretize independent variables & consequently dependent variables**
- **Energy: Multigroup ⇨ discretization into *bins* E_g**
  - Victory, 1985: Total & scattering cross section fluctuations diminish with refinement of energy group structure

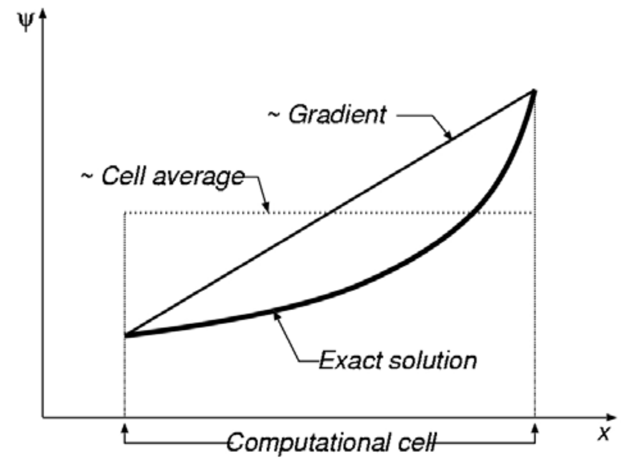
    ⇨ Multigroup solution → exact solution
- **Angle: Discrete-ordinates ⇨ discretization along discrete $\hat{\Omega}_n$**
  - Madsen, 1971: Quadrature formula converges with increasing order

    ⇨ Discrete Ordinates solution → exact one-speed solution
- **Space: Multitude of methods to discretize $\nabla\psi$ on spatial mesh**
  - Madsen, 1972: Exact solution has bounded 3rd derivatives

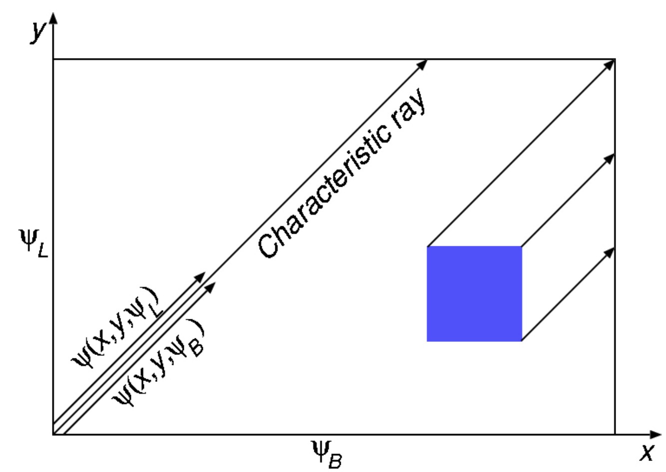
    ⇨ Diamond Difference solution → exact Discrete Ordinates solution
  - Smoothness hypothesis unrealistic for most applications

1. Spatial Approximation Methods

- **Diamond Difference (DD) method**
  - Originally derived in slab geometry ⇨ ψ continuous over thin cells justifies:
    - Central differencing of streaming derivative
    - Cell-averaged flux = simple average edge fluxes (aux)



- **Arbitrarily High Order Transport (AHOT)**
  - Nodal (AHOT-N): Transverse-averaging then exact solution of resulting ODEs
  - Characteristic (AHOT-C): Integration of streaming operator along *characteristics* (or particle path)



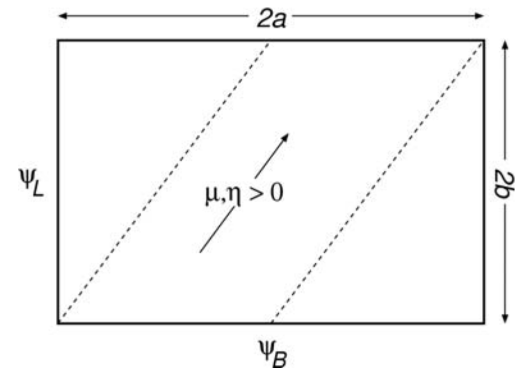
- **Difficulties with extension to multi-dimensions:**
  - Potential for flux discontinuity: If specified incoming boundary flux discontinuous at corner
  - Potential for derivative discontinuity: Across characteristic rays emanating from corners

5. Conclusion

- **Local error analysis of WDD methods ⇨ solutions do not converge with diminishing cell size if incoming face-averaged fluxes unequal**
- **WDD solution converges with mesh refinement away from the singular characteristic because flux inequality diminishes**
- **AHOT-C locally exact, but large global error ⇨ dominance of outgoing face flux smearing effect**
- **High-order methods: higher accuracy, but almost same rate of convergence**
- **The case against smearing of the outgoing face flux:**
  - Only approximation in AHOT-C0: locally exact
  - Maximum error (fine meshes) located near characteristic where smearing worst
  - ξ=1 case with no smearing across discontinuity ⇨ cell-wise convergence
  - New ***Singular Characteristic Tracking*** algorithm avoids smearing ⇨ convergence
- **Error estimation with scattering: Method of Manufactured Solutions**
- **Rigorous *a posteriori* error estimator ⇨ Adaptive Mesh Refinement, AMR**

2. Local Error Analysis

- **Configuration: Rectangular region**
  - σ = total cross section, non-scattering
  - $\mu,\eta > 0$, without any loss of generality
  - ε_x , ε_y = cell optical dimensions, e.g. $\varepsilon_x = 2\sigma a/\mu$
  - ξ = cell optical aspect ratio = $\varepsilon_y/\varepsilon_x$



- ***Local* analysis ⇨ Assume exact:**
  - ❖ Incoming face-averaged fluxes: ψ_B , ψ_L (constant approximation)
  - ❖ Cell-averaged distributed source: S (constant approximation)

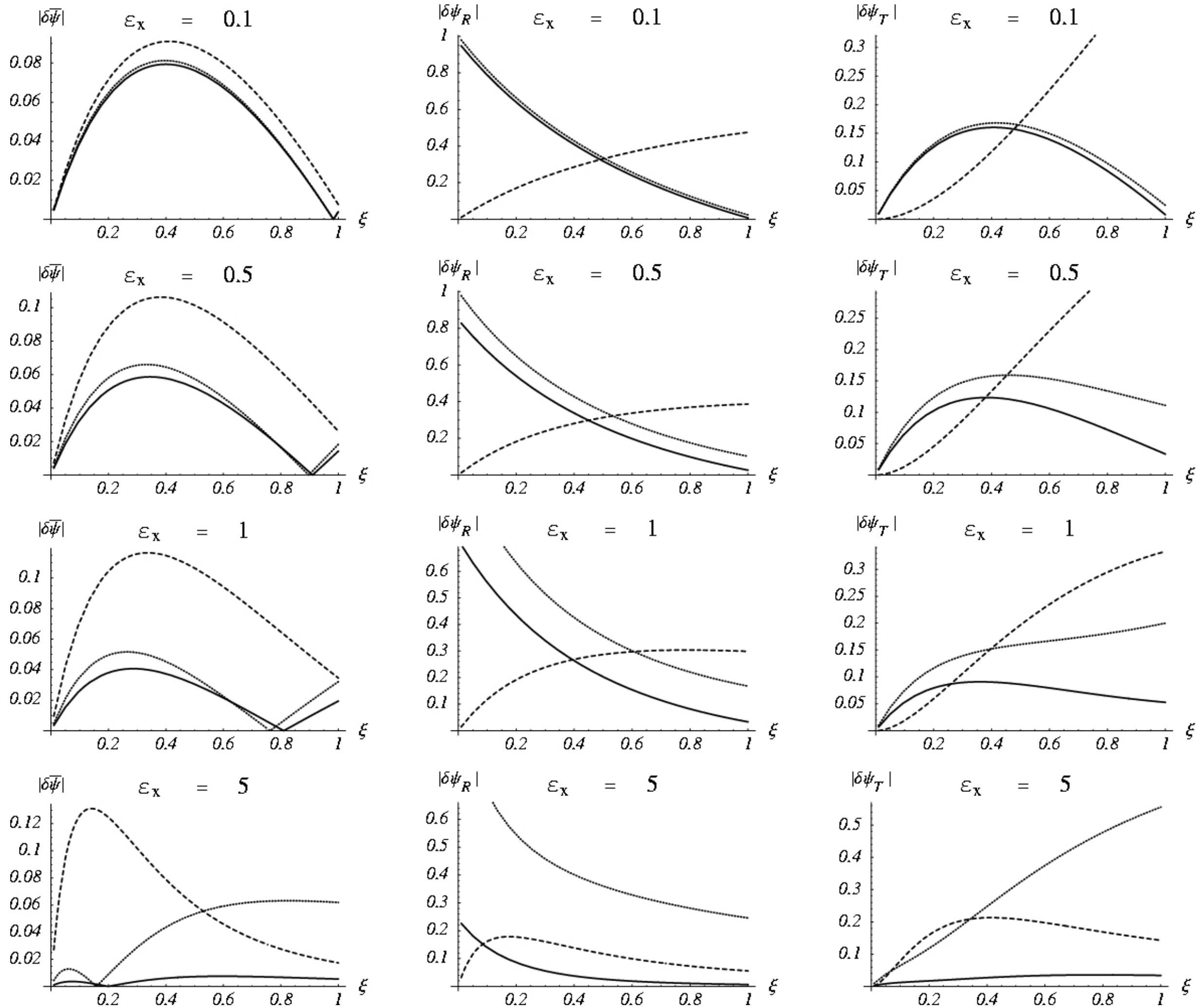
- **Characteristic method: Exactly solve transport equation over cell**
  - ❖ Determine $\psi(x,y)$ in three cell regions defined by characteristics
  - ❖ Compute cell-averaged flux: Ψ
  - ❖ Compute outgoing face-averaged (top & right) fluxes: Ψ_T & Ψ_R

2. WDD Local Solution

- **The generic WDD set of equations:**
  - Balance: $(\psi_R - \psi_L)/\,\varepsilon_x + (\psi_T - \psi_B)/\,\varepsilon_y + \psi = S/\sigma$
  - WDD: $2\ \psi = (1+\alpha_x)\ \psi_R + (1-\alpha_x)\ \psi_L = (1+\alpha_y)\ \psi_T + (1-\alpha_y)\ \psi_B$
  - Spatial weights, $\alpha_u \in [0,1]$, $u = x$ or y, selects solution method:
    - $\alpha_u = 0$ ⇨ DD
    - $\alpha_u = 1$ ⇨ Step Method (SM)
    - $\alpha_u = \coth(\varepsilon_u/2) - 2/\,\varepsilon_u$ ⇨ AHOT-N0
- **Solve 3 WDD equations**
  - For: Cell-averaged flux: ψ and outgoing face-averaged fluxes: ψ_T & ψ_R
  - In terms of incoming face-averaged fluxes ψ_B, ψ_L and cell-averaged source S
- **Reduce parameter space dimensionality by 1:**
  - Solution proportional to sources: Normalize $\psi_B + \psi_L + S/\sigma = 1$
  - Require $\psi_B + \psi_L \leq 1$ ⇨ eliminate $S/\sigma \geq 0$ from parameter space
- **Compute error $\delta q = q - Q$, $q = \psi, \psi_T, \psi_R$, for DD, AHOT-N0, SM as function of ε_x, $\xi \in (0,1]$ & various $\{\psi_B, \psi_L\}$ combinations**

2. Local Error for ψ_L=0, ψ_B=1

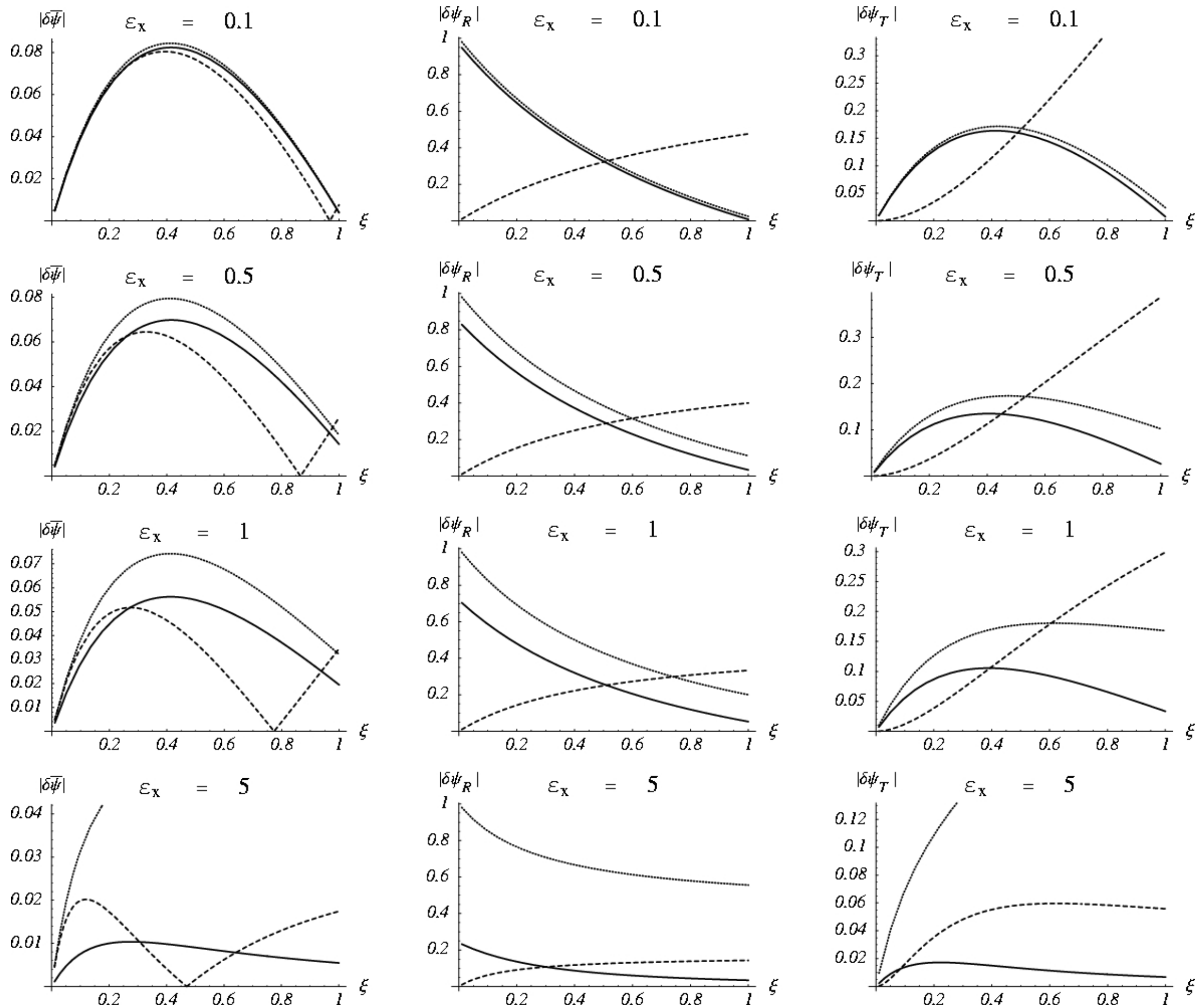
- **AHOT-N0 error → DD error as $\varepsilon_x \to 0$, ξ = *const.***
- **Errors do not vanish for most ξ as $\varepsilon_x \to 0$**



Legend	
··············	DD
- - - - -	SM
————	AHOT-N0

2. Local Error for $\psi_L=1$, $\psi_B=0$

- Same as previous case



DD

SM

AHOT-N0

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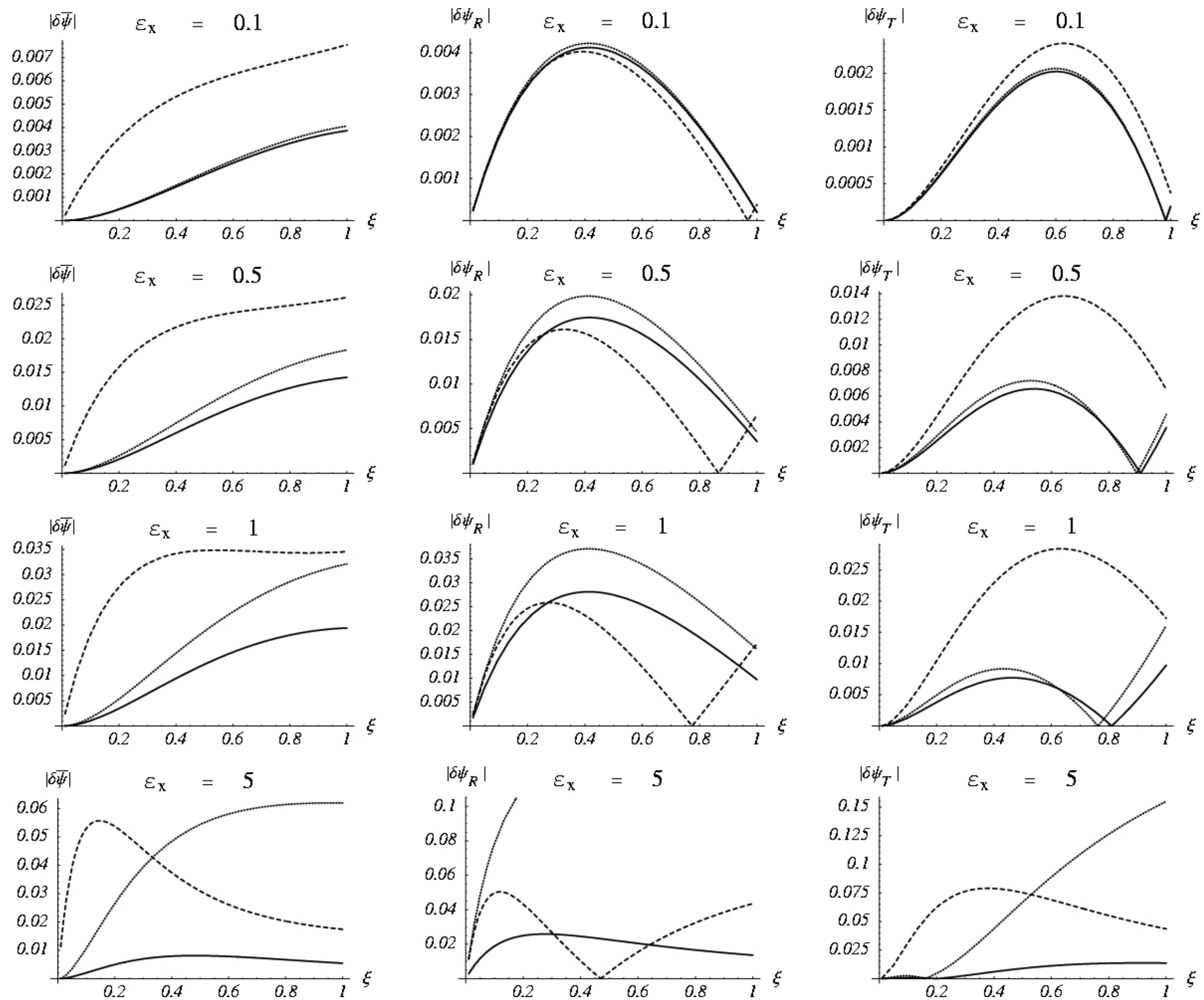
2. Local Error for ψ_L=0.5, ψ_B=0.5

- Solution is continuous across characteristic
- Errors vanish as $\varepsilon_x \rightarrow 0$



···········	**DD**
- - - - -	**SM**
———	**AHOT-N0**

2. Results of Local Analysis

- **If $\psi_B = \psi_L$:**
  - Solution continuous across characteristic line; first derivative discontinuous
  - WDD solutions converge like $O(\varepsilon_x)$
- **Otherwise:**
  - Solution discontinuous across characteristic line
  - WDD solutions do not converge as $\varepsilon_x \to 0$, $\xi = const.$
- **Asymptotic behavior of exact solution:**

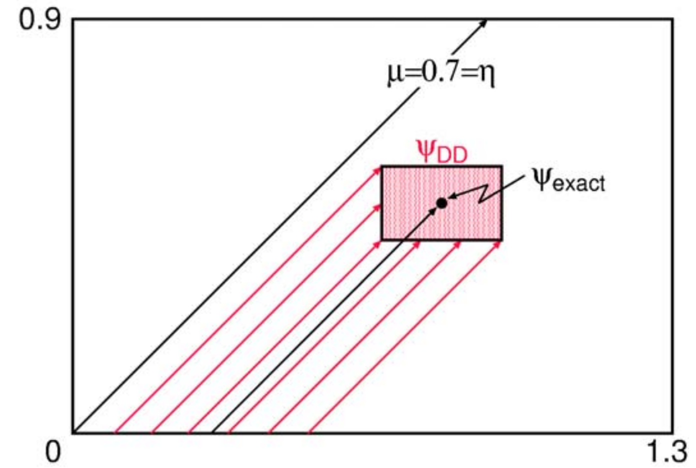
$$\Psi \to (1 - \xi/2)\ \psi_B + (\xi/2)\ \psi_L + O(\varepsilon_x)$$

- **Asymptotic behavior of WDD (with fixed α_x & α_y) solution:**

$$\psi \to [1+\xi(1+\alpha_y)/(1+\alpha_x)]^{-1}\ \psi_B + [1+\xi^{-1}(1+\alpha_x)/(1+\alpha_y)]^{-1}\ \psi_L + O(\varepsilon_x)$$

- **Observations on asymptotic formulas:**
  - Dependence on S is $O(\varepsilon_x)$, on incoming face-averaged fluxes is $O(1)$
  - In general the exact & numerical formulas do not approach the same limit as $\varepsilon_x \to 0$
  - For DD ($\alpha_u = 0$) & AHOT-N0 ($\alpha_u \to 0$ as $\varepsilon_u \to 0$):
    - If $\psi_B = \psi_L$
    - Local error: $\delta\psi \to 0$ as $O(\varepsilon_x)$

3. Larsen’s Benchmark Problem



- **Original configuration:**
  - Rectangle: $X \times Y = 1.3 \times 0.9$ *mfp*
  - Uniform $2^n \times 2^n$ mesh, $n = 0,1,2, \ldots$
  - Single discrete ordinate: $\mu = 0.7 = \eta$
  - Nonscattering material, source-free : $S = 0$
  - ***Equal*** constant incoming fluxes: $\psi_B = 1 = \psi_L$
- **Larsen’s analysis:**
  - Determined exact point solution using the characteristic formula
  - Computed local error as difference between DD solution in a cell and exact point value of flux at cell center
  - Error order of convergence same if exact cell-averaged flux used instead
- **Larsen’s conclusion:**
  - DD error → 0 as a fractional power of cell optical size

3. Global Error Norm Definitions

- **Global error analysis: Accumulate numerical errors in edge fluxes**

- **Absolute difference between exact and numerical cell-averaged angular flux:** $\varepsilon_{i,j} = \left| \overline{\Psi}_{i,j} - \overline{\psi}_{i,j} \right|$
  - $\overline{\psi}_{i,j}$: ***Exact*** cell-averaged flux evaluated from characteristic solution
  - $\overline{\Psi}_{i,j}$: Approximate cell-averaged flux computed via mesh sweep

- **Error norms:**
  - L_1: $\|\varepsilon\|_1 = \sum_{i,j} \varepsilon_{i,j} \Delta x_i \Delta y_j$
  - L_2: $\|\varepsilon\|_2 = \left(\sum_{i,j} \varepsilon_{i,j}^2 \Delta x_i \Delta y_j \right)^{1/2}$
  - L_∞ : $\|\varepsilon\|_\infty = \max_{i,j} \varepsilon_{i,j}$

Convergence in integral sense

Cell-wise Convergence

3. Variations on Larsen's Benchmark

- **Numerical method:**
  - DD: lowest order spatial approximation
  - AHOT-N0/1/2: AHOT-N0 same behavior as DD as cell size → 0
  - AHOT-C0/1/2: locally exact

- **Incoming boundaries fluxes:**
  - Determines degree of smoothness of exact solution

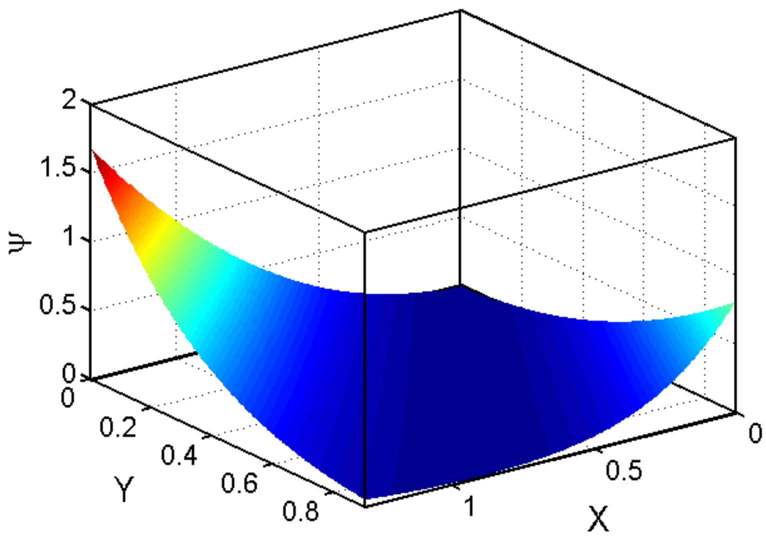
- **For meshes n = 0,…,15, compute in 64-bit arithmetic:**
  - Exact cell-averaged flux for each cell
  - Numerical method cell-averaged flux for each cell
  - Error distribution by cell
  - L_1 , L_2 & L_∞ norms of the error

3. Bounded 3rd Derivative

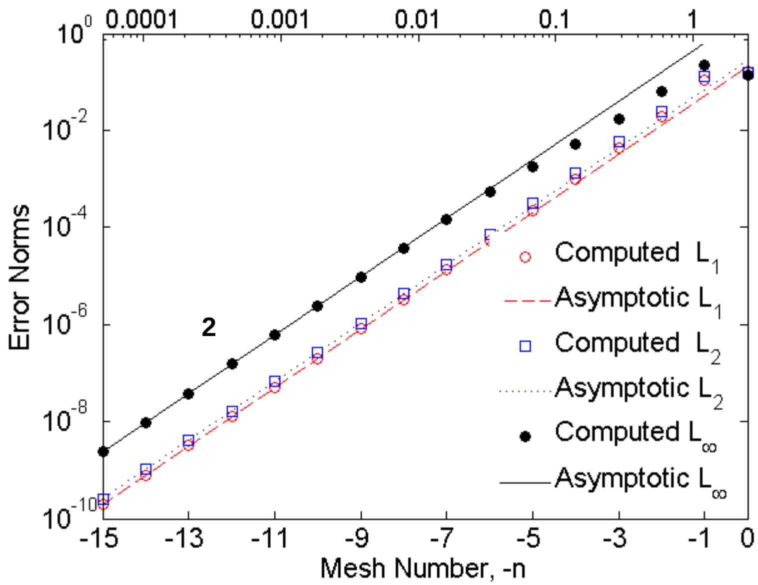
- **BCs: Bounded 2nd derivatives &**

$$\sigma[\eta\psi'_L(0) - \mu\psi'_B(0)] = \mu^2\psi''_B(0) - \eta^2\psi''_L(0)$$

- **Consistent with Madsen's proof: DD solution is $O(h^2)$ accurate under this stringent smoothness condition**



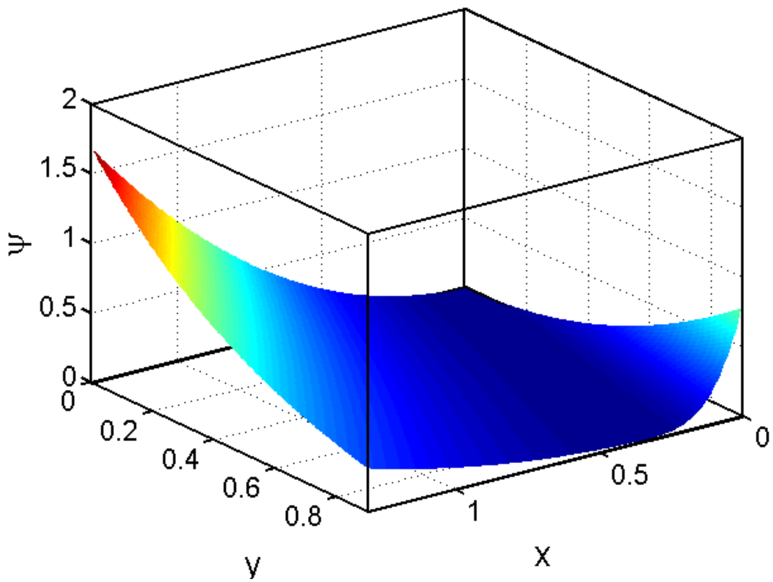
Angular Flux (exact solution)



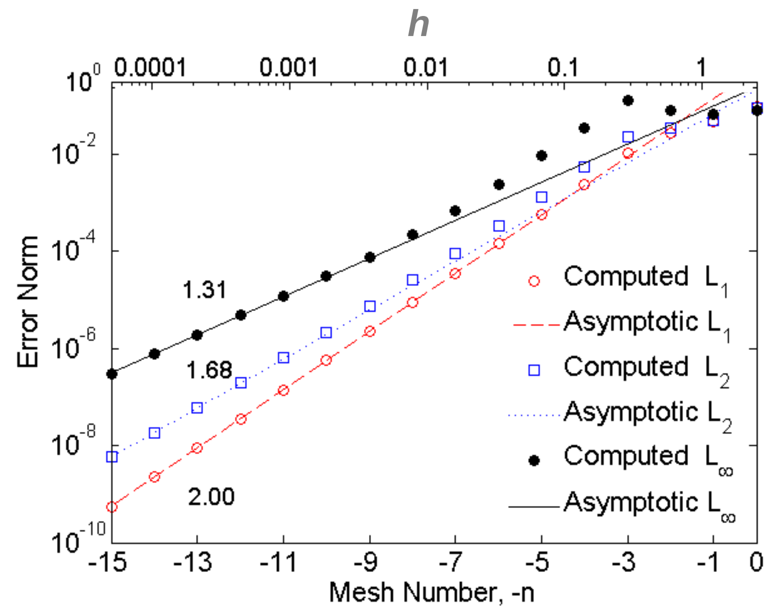
Error Norms vs. *h* (mesh size)

3. Bounded 2nd Derivative

- BCs: Bounded 1st derivatives & $\sigma \psi_L(0) = -\eta \psi'_L(0) - \mu \psi'_B(0)$
- DD has different convergence orders depending on L_l norm



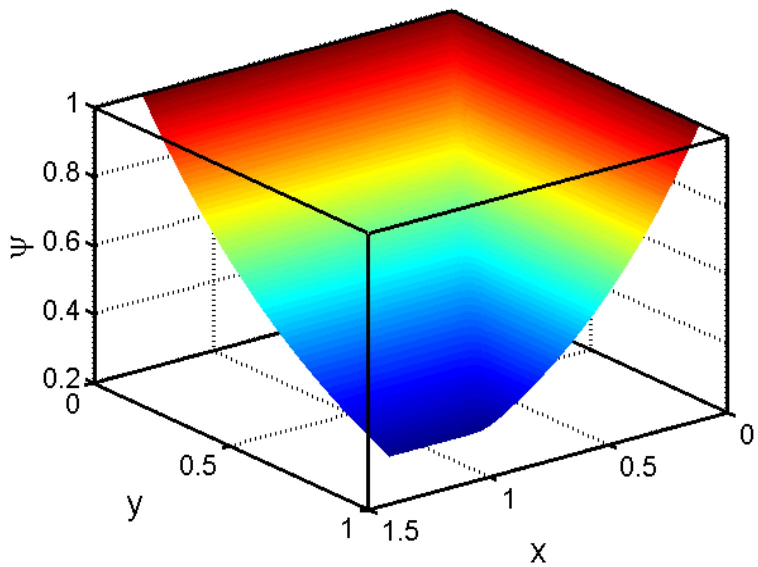
Angular Flux (exact solution)



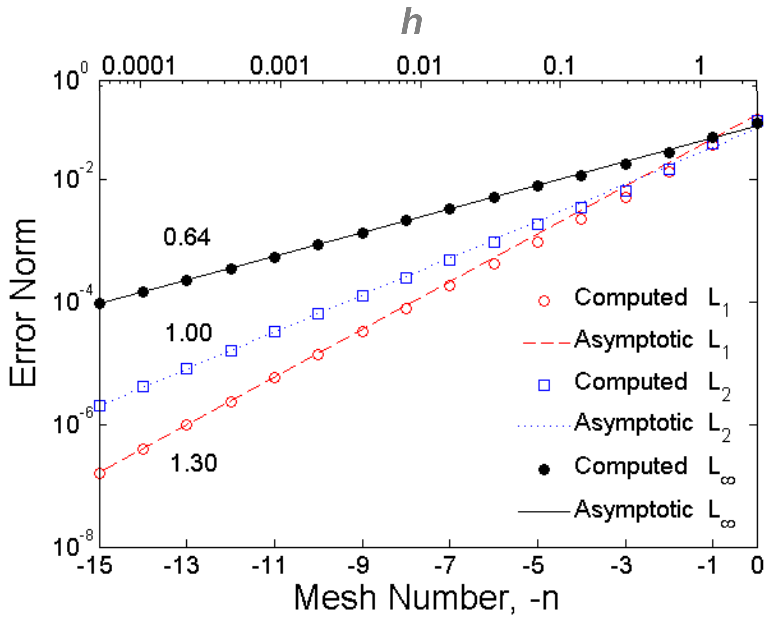
Error Norms vs. *h* (mesh size)

3. Bounded 1st Derivative

- BCs: $\psi_B(0) = \psi_L(0)$ ⇨ continuous flux
- DD convergence order falls below 1 for L_∞ norm



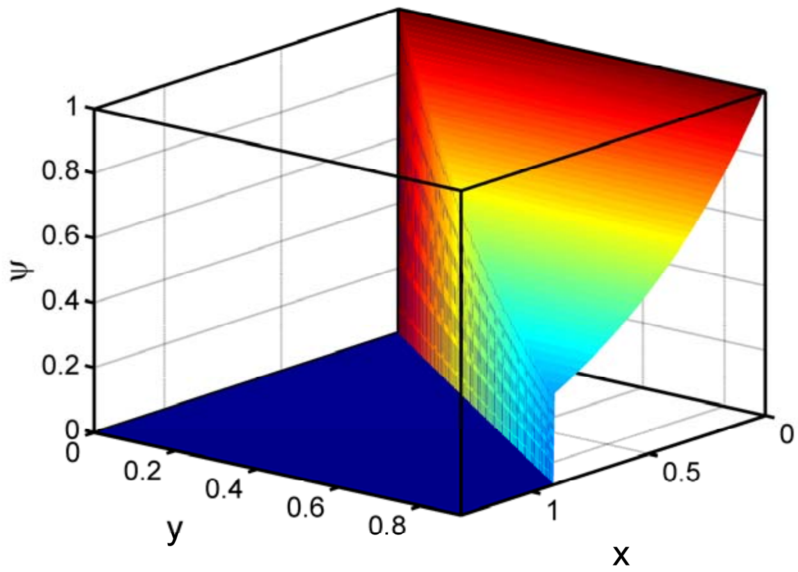
Angular Flux (exact solution)



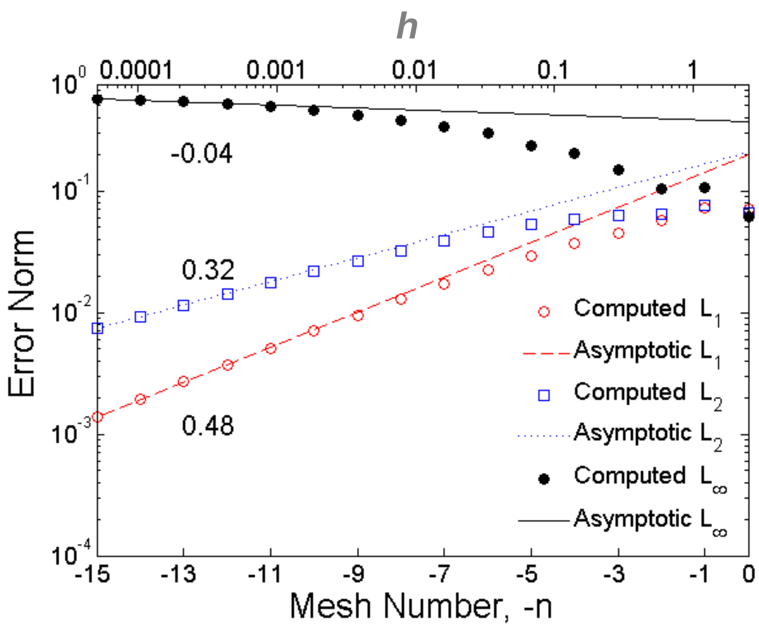
Error Norms vs. *h* (mesh size)

3. Discontinuous Angular Flux

- BCs: $\psi_B(0) \neq \psi_L(0)$
- DD does *not* converge in L_∞ norm (cell-wise) to the exact solution
- Similar general behavior by AHOT-N0 & AHOT-C0



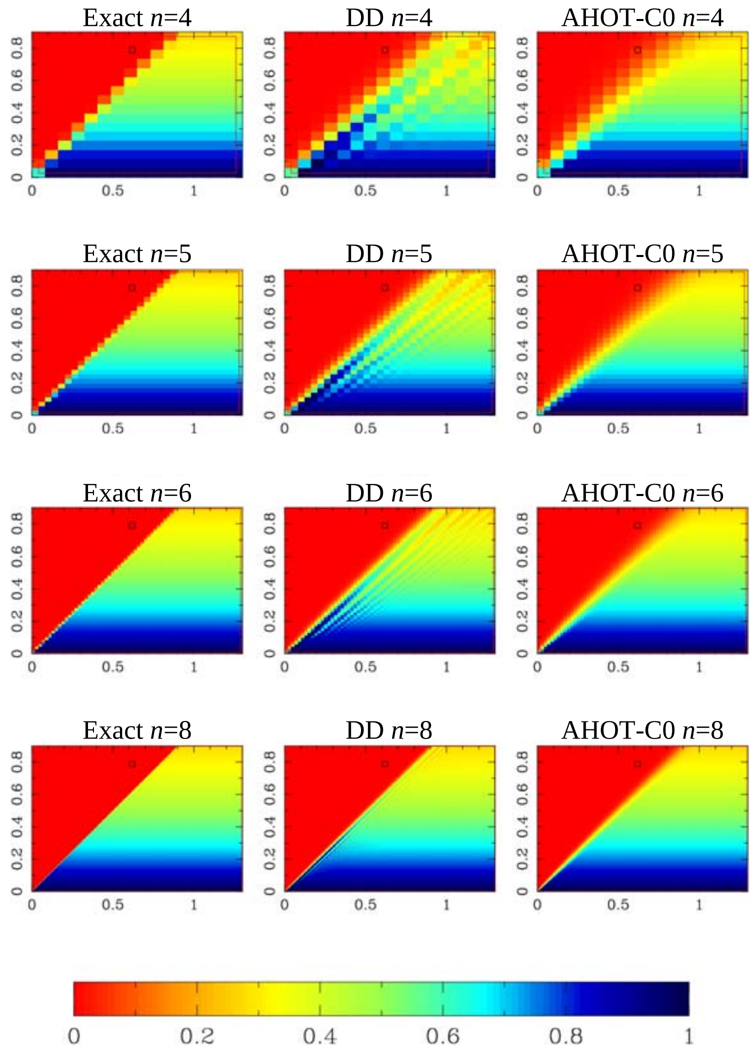
Angular Flux (exact solution)



Error Norms vs. *h* (mesh size)

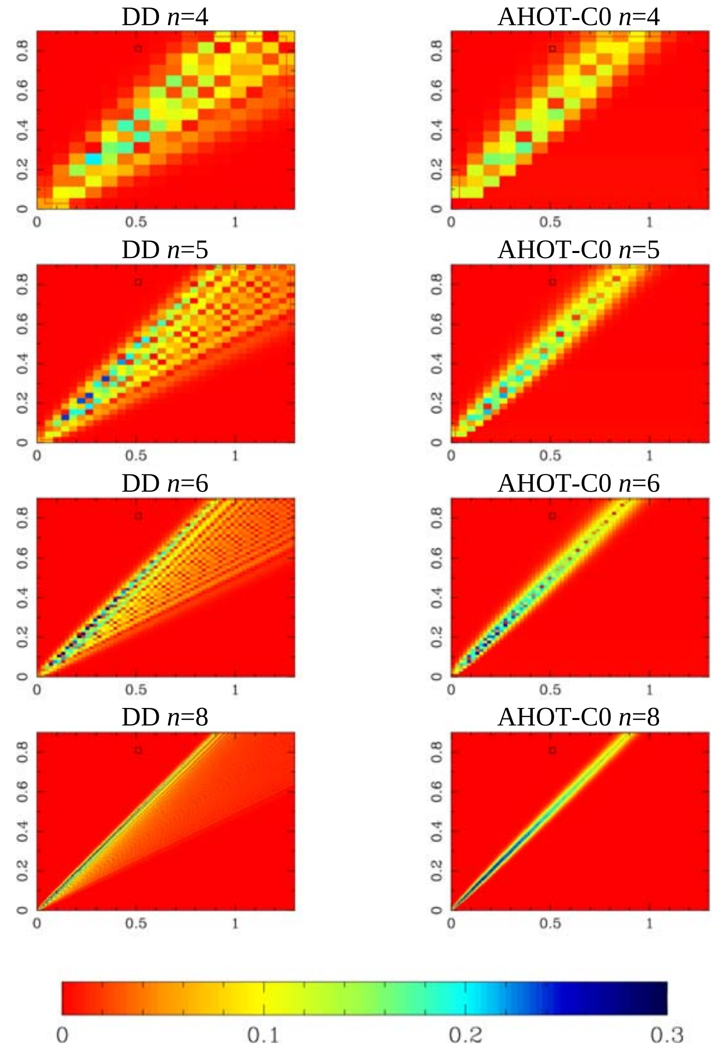
3. Perspective on Discontinuity Effect

- **Detrimental effect of discontinuity evident from L_∞ norm of error**
- **Convergence of L_1 & L_2 error norms:**
  - Adverse effect of discontinuity is local
  - Mesh refinement *squeezes* extent of error narrower
- **Plots of cell-wise flux:**
  - Ripples in DD solution below singular characteristic line
  - Width of ripple band diminishes with mesh refinement
  - No ripples in AHOT-C0 solution but wider transition region



3. Cell-wise Error Distribution

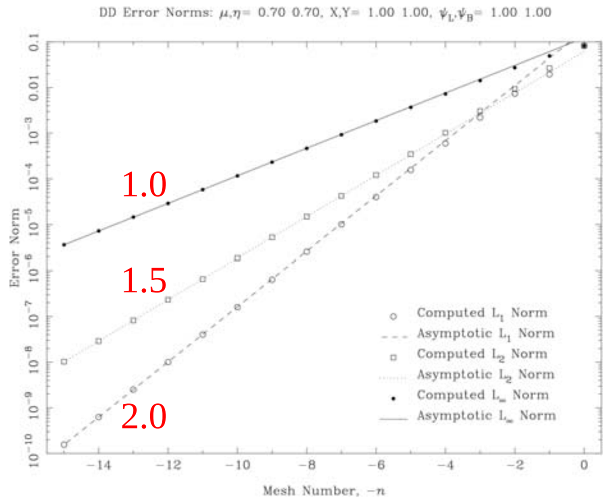
- AHOT-N0 plots visually similar to DD
- AHOT-C0 solution highly accurate below diagonal
- AHOT-C0 worst error in tight band around singular characteristic:
  - Results from smearing effect of flux discontinuity
  - Recall: AHOT-C0 locally exact for constant incoming fluxes & source
- AHOT-C0 cell-wise values more trustworthy?

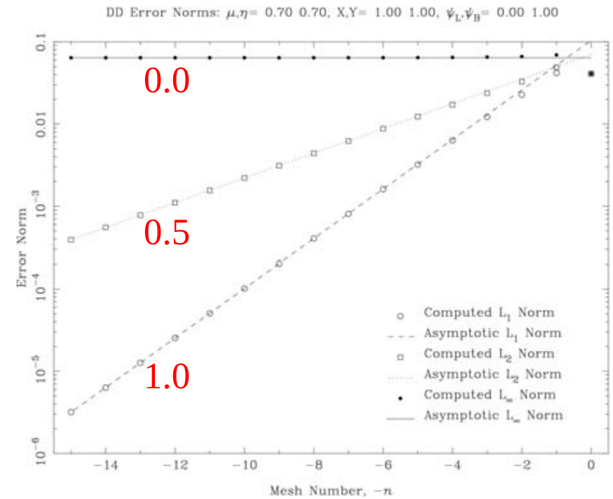


3. Special Case $\xi = 1$

$\psi_L = 1, \;\; \psi_B = 1$ | $\psi_L = 0, \;\; \psi_B = 1$

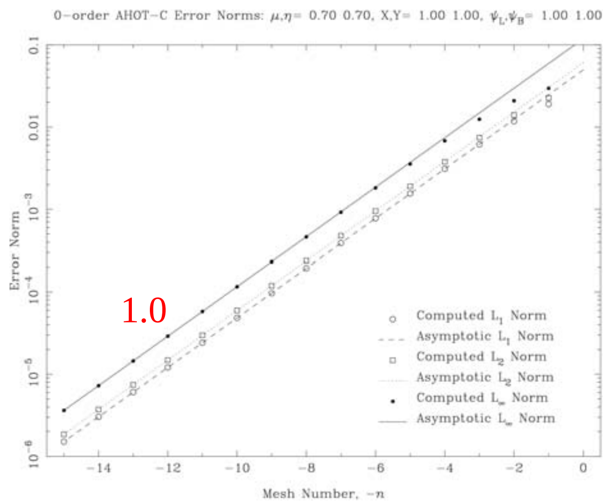
DD

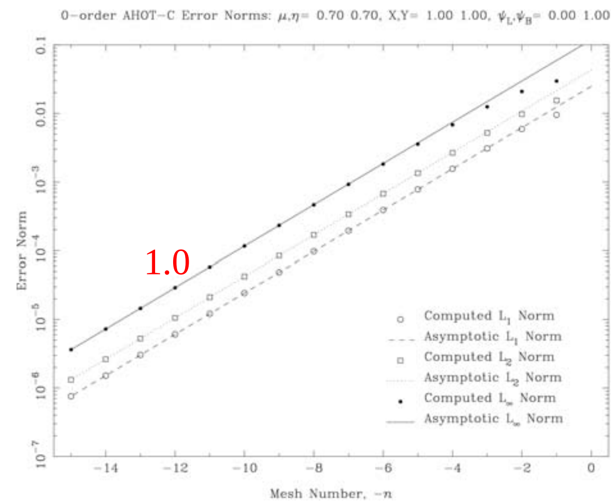




Asymptotic Convergence Rate

AHOT-C0





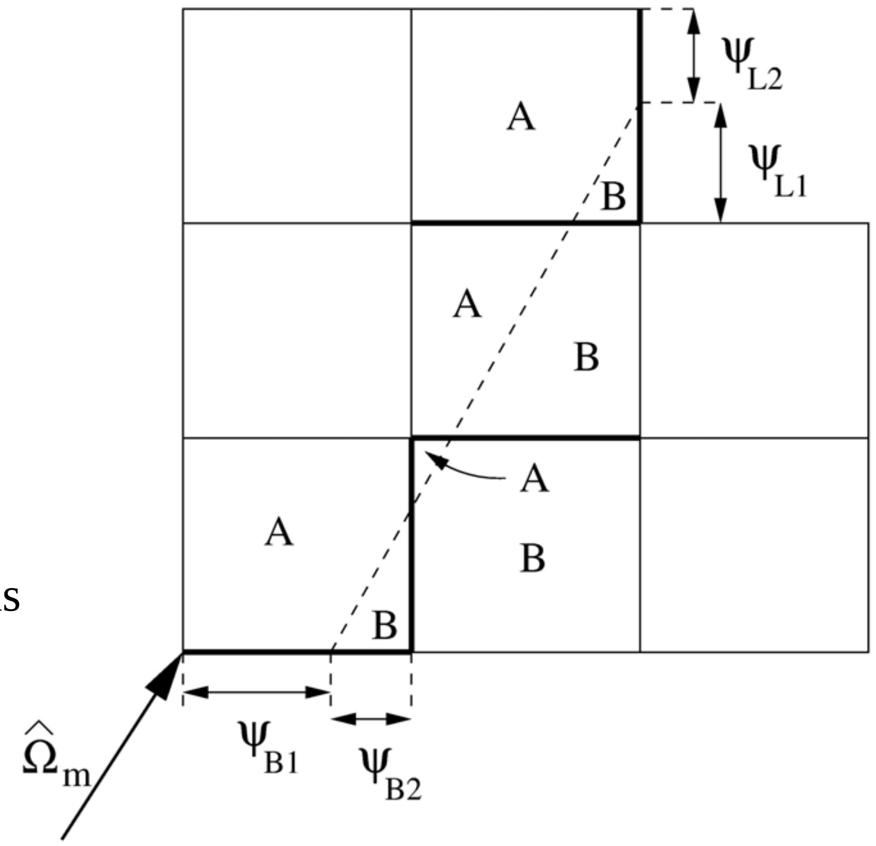
3. Dependence on Optical Aspect Ratio

- **Effect of decreasing ξ on solution accuracy:**
  - Generally better accuracy on finer meshes
  - Accuracy deteriorates on coarse meshes: Slower approach to asymptotic convergence
  - Asymptotic convergence rates almost unchanged

- **$\xi = 1$ Case: Substantial improvement in convergence rates**
  - WDD cell-wise flux:
    - Converges like $O(\varepsilon_x)$ with mesh refinement if solution continuous
    - Does not converge with mesh refinement if solution discontinuous
  - AHOT-C0 cell-wise flux converges like $O(\varepsilon_x)$ regardless of solution continuity:
    - Face-averaged flux ***not*** smeared across discontinuity
    - Only remaining approximation: Averaging outgoing face flux
    - Expanding ***continuous*** face flux in Taylor series ⇨ $O(\varepsilon_x)$ approximation

3. Singular Characteristic Tracking (STC)

- **STC Algorithm based on:**
  - Separate *Step Characteristic* stencil in each cell intersected by singular characteristic
  - Standard DD stencil in all other cells
- **Error computation for cases with scattering:**
  - Method of Manufactured solutions
  - Construct solution at will
  - Substitute into Transport Eq
  - Determine exact source & BCs
  - Use these ⇨ numerical solution

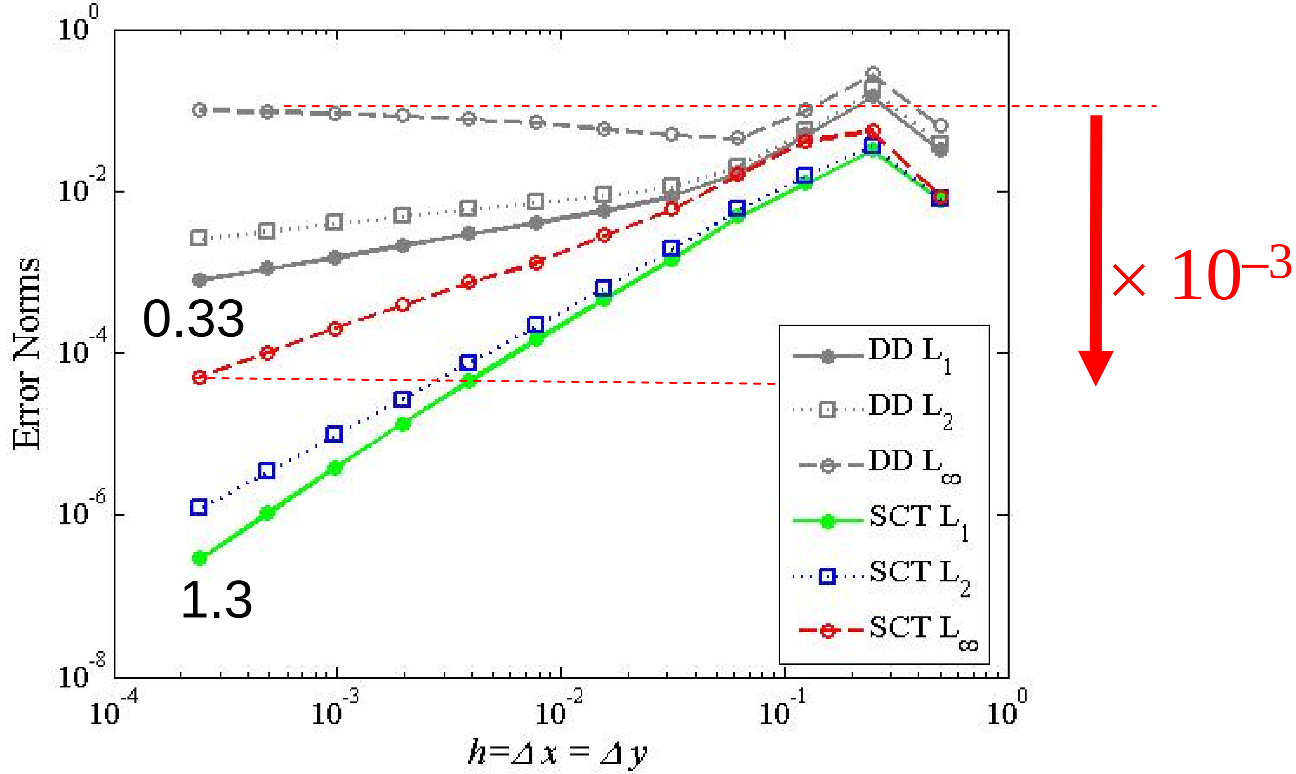


3. Accuracy of SCT *vs* DD

- **Discontinuous flux ($\psi_L = 1$, $\psi_B = 0$); S_8; $\sigma_s/\sigma = ½$**

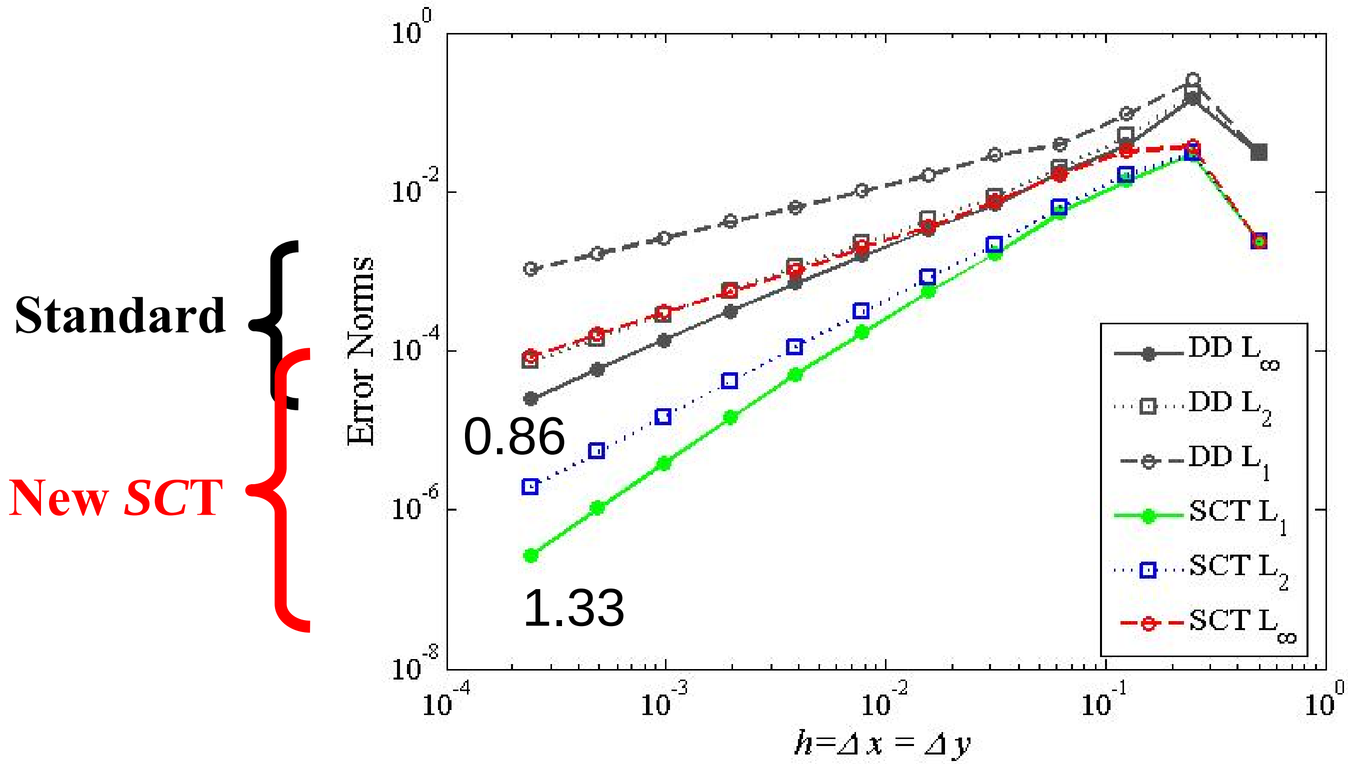
Standard

New *SCT*



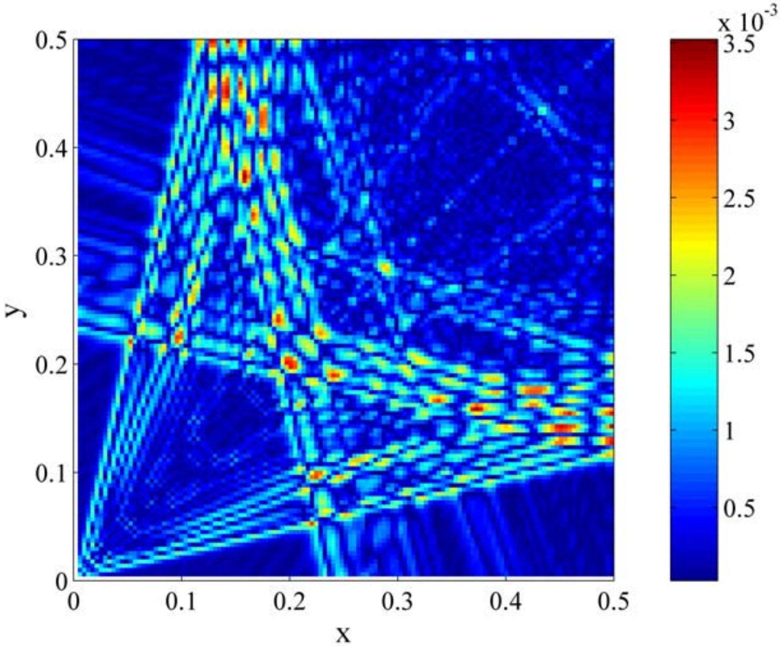
3. Accuracy of SCT *vs* DD

- **Discontinuous 1st derivative ($\psi_L = 0$, $\psi_B = 0$); S_4; $\sigma_s/\sigma = ½$**

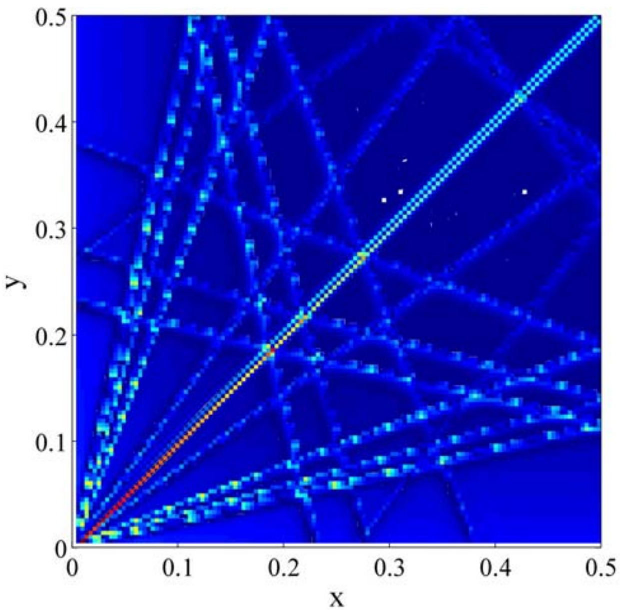


3. Error Patterns

- Discontinuous 1st derivative ($\psi_L = 0$, $\psi_B = 0$); S_4; $\sigma_s/\sigma = ½$



DD



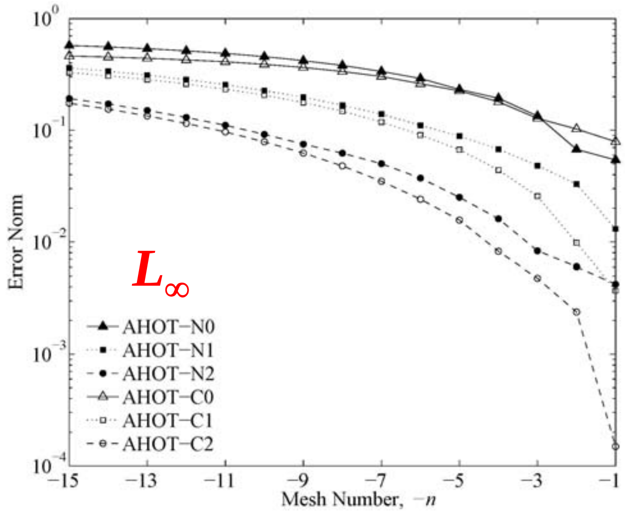
SCT (× 5)

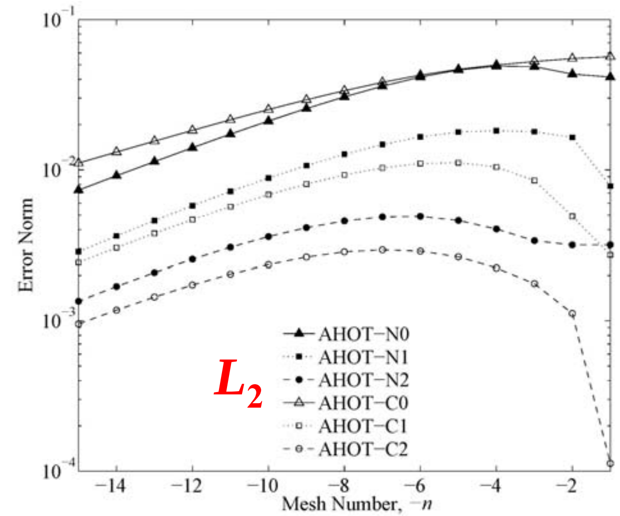
4. High Order Methods

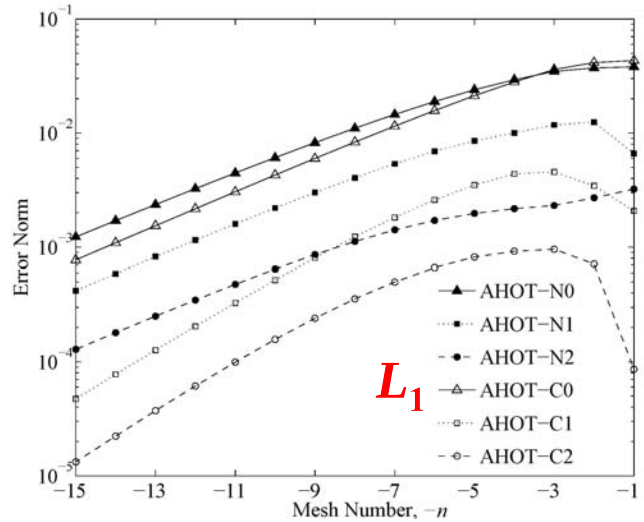
- **Spatial approximation of angular flux & source truncated at order higher than constant:**
  - AHOT ⇨ provides expressions for discretized transport equation at arbitrary truncation order Λ
  - AHOT-N: Solve transverse-averaged transport equation ⇨ coupled ODEs
  - AHOT-C: Integrate full transport equation along characteristics then take spatial moments of flux
  - Here we consider only $\Lambda = 0, 1, 2$

- **Case of $\psi_L = 1$, $\psi_B = 0$ ⇨ discontinuous exact solution:**
  - Accuracy improves significantly with increasing spatial approximation order
  - Still fails to converge cell-wise fluxes
  - AHOT-C generally more accurate than AHOT-N of same order
  - Convergence rates approximately same for all methods/orders
    - Except L_1 for AHOT-C1/2 higher order

4. Error Norms

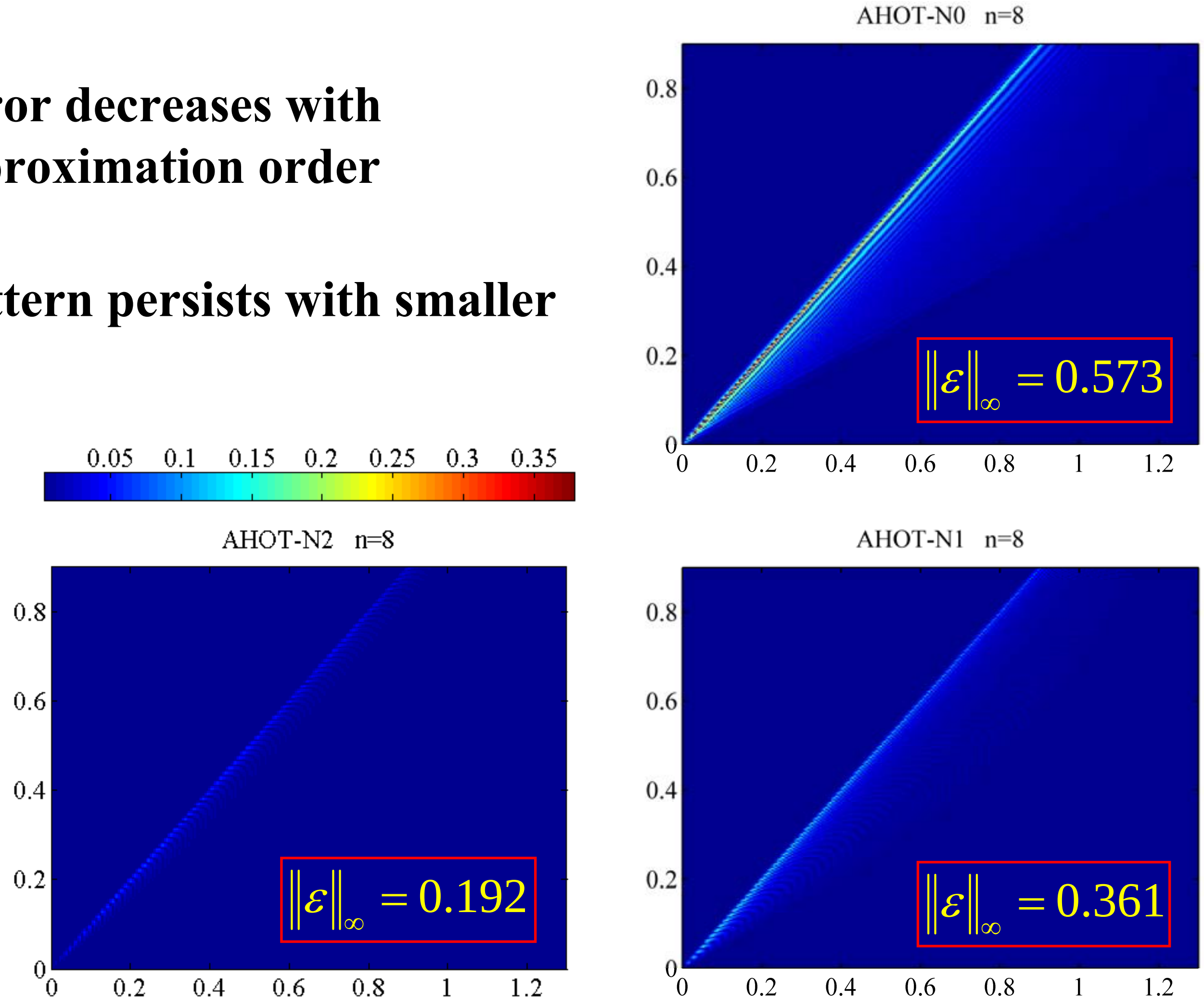






4. AHOT-N Error Distribution

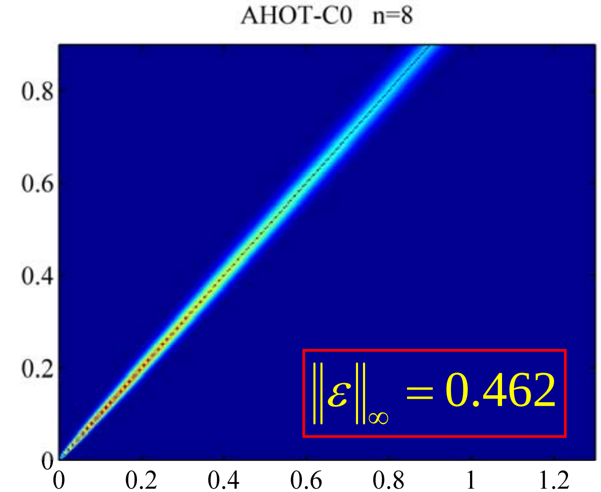
- Maximum Error decreases with increasing approximation order
- Oscillation pattern persists with smaller amplitude

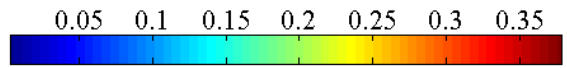


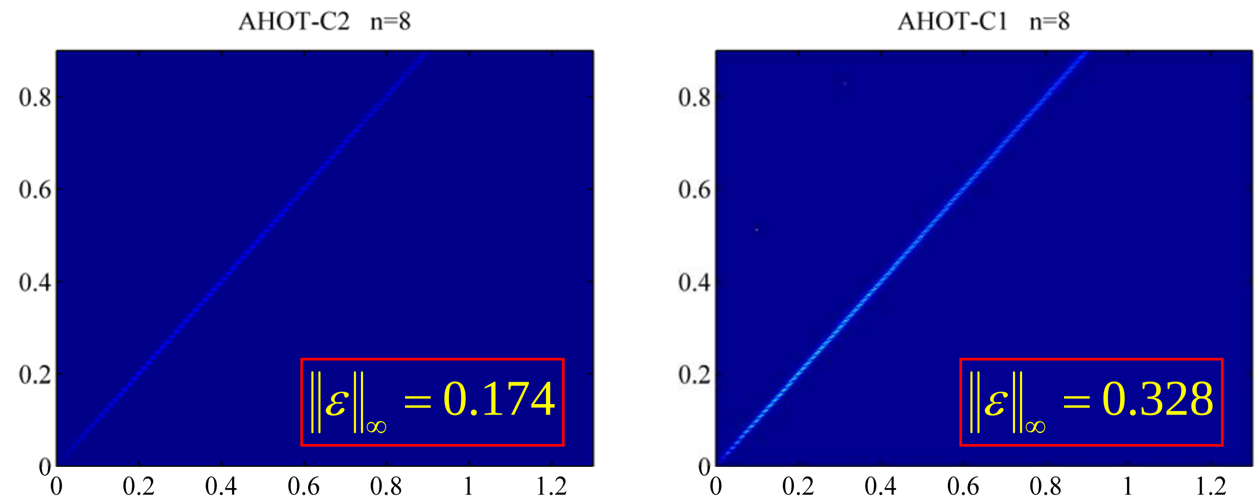
4. AHOT-C Error Distribution

- Maximum Error decreases with increasing approximation order

- Band where error is largest narrows with increasing order





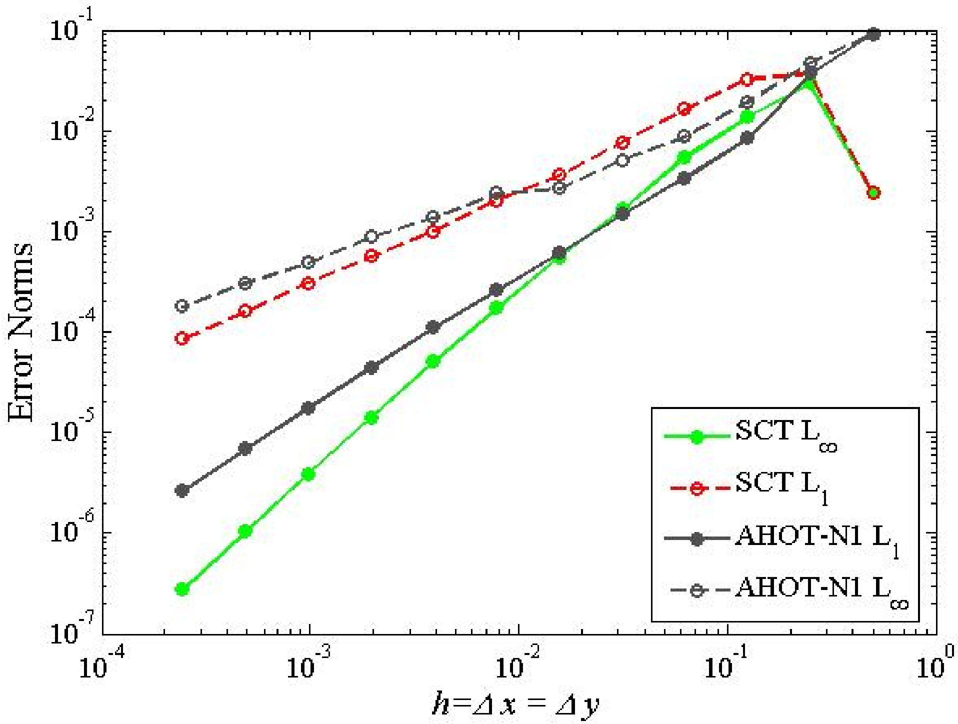


5. Conclusion

- **Local error analysis of WDD methods ⇨ solutions do not converge with diminishing cell size if incoming face-averaged fluxes unequal**
- **WDD solution converges with mesh refinement away from the singular characteristic because flux inequality diminishes**
- **AHOT-C locally exact, but large global error ⇨ dominance of outgoing face flux smearing effect**
- **Case ξ=1: AHOT-C0 converges cell-wise, WDD does not**
- **High-order methods: higher accuracy, but almost same rate of convergence**
- **The case against smearing of the outgoing face flux:**
  - Only approximation in AHOT-C0: locally exact
  - Maximum error (fine meshes) located near characteristic where smearing worst
  - ξ=1 case with no smearing across discontinuity ⇨ cell-wise convergence
  - New ***Singular Characteristic Tracking*** algorithm avoids smearing ⇨ convergence
- **Error estimation with scattering: Method of Manufactured Solutions**
- **Rigorous *a posteriori* error estimator ⇨ Adaptive Mesh Refinement, AMR**

SCT vs AHOT-N1 (Nodal Linear)

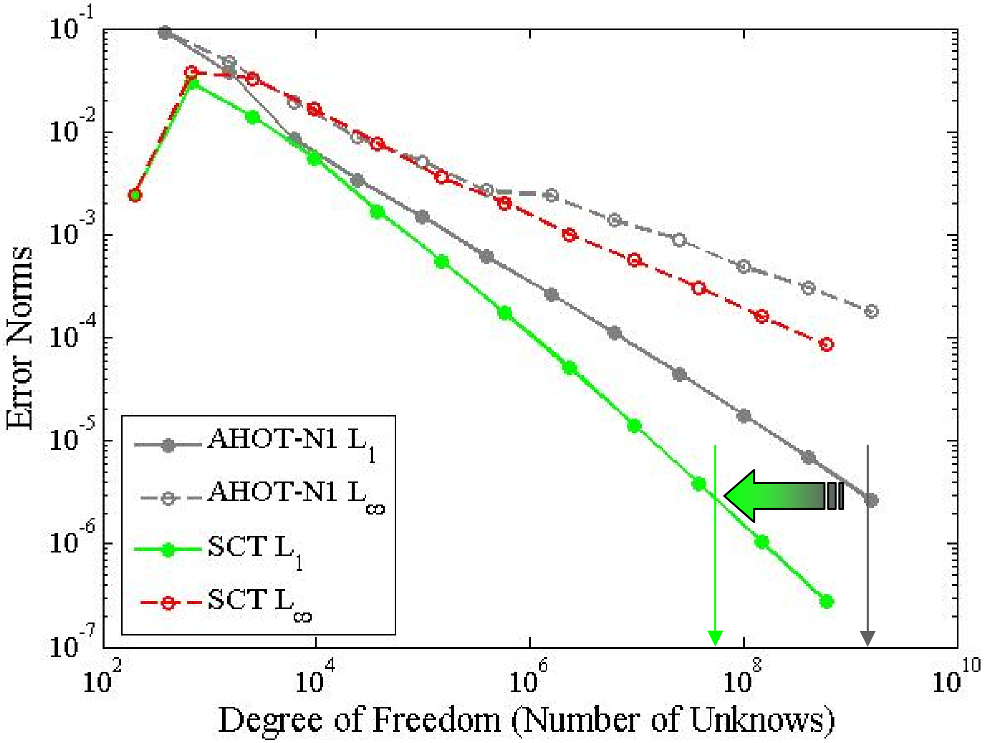
- Discontinuous 1st Partial Derivative: $\sigma_s/\sigma = ½$



- L_1, L_2 and L_∞ error norms for AHOT-N1 and SCT for the case *with zero boundary conditions*. S_4 Quadrature.

SCT vs AHOT-N1 (Nodal Linear)

- Discontinuous 1st Partial Derivative: $\sigma_s/\sigma = ½$



- *SCT* gives the same level of error that AHOT-N1 for fewer number of unknowns <u>saving computational time</u>.

Conclusions

- Convergence properties of the 2D Discrete Ordinates Method have been numerically characterized.

- Using the rate of convergence and error pattern as guiding parameters, a new algorithm has been devised.

- The SCT algorithm has been tested successfully in two dimensional problems with isotropic scattering.

- The SCT algorithm yields comparable accuracy to a linear nodal method at a much lower (number of unknowns) cost.