A Multigrid Iterative Method for Solving Two-Dimensional Discrete-Ordinates ($S_N$) Transport Problems

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Four Problem “Classes”

<table>
<thead>
<tr>
<th>Homogeneous Material; Uniform Grid</th>
<th>Heterogeneous Material; Uniform Grid</th>
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<tr>
<td>Homogeneous Material; Non-Uniform Grid</td>
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Fourier Analysis of a Three-Level Multigrid Iteration Matrix

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Motivation (Manteuffel, et al.)

The Boltzmann Transport Equation

Multigrid Iterative Schemes

Conceptual Framework
The continuous Boltzmann equation is reduced to a nested set of discrete equations.

\[ \frac{1}{v(E)} \frac{\partial \Psi(\mathbf{r}, E, \Omega, t)}{\partial t} + \Omega \cdot \nabla \Psi(\mathbf{r}, E, \Omega, t) + \sigma_t(\mathbf{r}, E, t) \Psi(\mathbf{r}, E, \Omega, t) = \int_{0}^{4\pi} \int \sigma_s(\mathbf{r}, E' \rightarrow E, \Omega' \rightarrow \Omega, t) \Psi(\mathbf{r}, E', \Omega', t) d\Omega' dE' + Q(\mathbf{r}, E, \Omega, t) \]

Examine a single time step

Discretize the energy domain (multigroup)

\[ \Omega \cdot \nabla \Psi(\mathbf{r}, E, \Omega) + \sigma_t(\mathbf{r}, E) \Psi(\mathbf{r}, E, \Omega) = \int_{0}^{4\pi} \int \sigma_s(\mathbf{r}, E' \rightarrow E, \Omega' \rightarrow \Omega) \Psi(\mathbf{r}, E', \Omega', \Omega) d\Omega' dE' + \tilde{Q}(\mathbf{r}, E, \Omega) \]

Discrete-ordinates \((S_N)\) approximation

\[ \Omega'_k \cdot \nabla \Psi_{k,g}(\mathbf{r}) + \sigma_t(\mathbf{r}) \Psi_{k,g}(\mathbf{r}) = \frac{\sigma_s(\mathbf{r})}{4\pi} \sum_{k'=1}^{N} w_{k'} \Psi_{k',g}(\mathbf{r}) + \tilde{Q}_{k,g}(\mathbf{r}) \]

This work summarizes the development of a multigrid iterative method for solving this equation – spatially discretized with existing 1D & 2D DFEMs.
Multigrid methods attempt to attenuate a wide range of error-mode frequencies.

Before convergence a solution will have error modes of varying frequencies.

Source Iteration

Simple source-iteration ineffectively damps low-frequency error modes.

Diffusion Synthetic Acceleration (DSA)

DSA powerfully attenuates low-frequency error modes, but requires the consistent spatial discretization of the transport and diffusion equations.

Transport Synthetic Acceleration (TSA)

TSA eliminates the consistency issue (partly), but requires more iterations than DSA.

Error modes that are low-frequency on the fine grid can be represented as high-frequency error modes on a suitably coarse grid.

Tremendous success has been achieved with multigrid solution-methods applied to elliptic problems.
The Multigrid Philosophy

- Nested set of grids describing the same physical domain
  \[ G^\ell, G^{2\ell}, G^{4\ell}, \ldots, G^{(2^N)\ell} \]
- Relaxation step (smoothing) attenuates error modes that are high-frequency on a given grid
- Characterize the error’s spatial shape following relaxation
- Construct coarse-grid operators
- The process continues until the coarsest grid is reached
  - Solve the coarsest grid exactly, or
  - Perform further error relaxation steps if it is not computationally efficient to solve exactly
- Multigrid algorithms are summarized by “cycles”
  - \( V(\nu_1, \nu_2) \) Cycle

**History**: U. Trottenberg, *et al.*; *Multigrid*; Academic Press; 2001; §1.5.5, pp. 23-24

**Efficiency**: A. Brandt; *Multi-Level Adaptive Solutions to Boundary Value Problems*; Mathematics of Computation, Volume 31, Issue 138; April 1977; pp. 33-390
The result of a multigrid cycle is a fine-grid correction

\[ r^{\ell}_{(n)} = Q - \left( L^{\ell} - R^{\ell} \right) \Psi^{\ell}_{(n)} \]

\[ \Psi^{\ell}_{(n+1)} = \Psi^{\ell}_{(n)} + \gamma^{\ell}_{(n+1)} \]

Coarse-grid operators *may* not be standard transport discretizations.

8-Cell Problem

\[ L^{\ell} \psi^{\ell}_{(n+1/3,m+1)} - R^{\ell} \psi^{\ell}_{(n+1/3,m)} = r^{\ell}_{(n)} \]

\[ r^{\ell}_{(n+1/2)} = r^{\ell}_{(n)} - \left( L^{\ell} - R^{\ell} \right) \psi^{\ell}_{(n+1/3)} \]

4-Cell Problem

\[ L^{2\ell} \psi^{2\ell}_{(n+1/3,m+1)} - R^{2\ell} \psi^{2\ell}_{(n+1/3,m)} = r^{2\ell}_{(n)} \]

\[ r^{2\ell}_{(n+1/2)} = r^{2\ell}_{(n)} - \left( L^{2\ell} - R^{2\ell} \right) \psi^{2\ell}_{(n+1/3)} \]

The multigrid algorithm does not assume a method for constructing coarse-grid operators.

The transport problem *up* the V-cycle is the same as *down* the V-cycle, but it has a better estimate of the grid-level correction.

8-Cell Problem

\[ L^{\ell} \psi^{\ell}_{(n+2/3,m+1)} - R^{\ell} \psi^{\ell}_{(n+2/3,m)} = r^{\ell}_{(n)} \]

\[ \psi^{\ell}_{(n+2/3)} \leftarrow \psi^{\ell}_{(n+1/3)} + I^{\ell} \gamma^{\ell}_{(n+1)} \]

4-Cell Problem

\[ L^{2\ell} \psi^{2\ell}_{(n+2/3,m+1)} - R^{2\ell} \psi^{2\ell}_{(n+2/3,m)} = r^{2\ell}_{(n)} \]

\[ \psi^{2\ell}_{(n+2/3)} \leftarrow \psi^{2\ell}_{(n+1/3)} + I^{2\ell} \gamma^{2\ell}_{(n+1)} \]

2-Cell Problem

\[ (L^{4\ell} - R^{4\ell}) \psi^{4\ell}_{(n+1)} = r^{4\ell}_{(n)} \]
Manteuffel, et al., report excellent convergence performance with a 1D multigrid solver

- Fastest transport solver in the literature
  - Computationally less expensive than previous efforts
    - No transport “sweeps”
  - Error convergence ratio approaches zero in the thick-diffusive limit
  - Thin limit $O(\sigma h)^3$; Thick limit $O(\sigma h)^{-2}$
  - Maximum convergence ratio – 0.078
    - Non-uniform grid
    - Random cells sizes $10^{-2} \leq \sigma h \leq 10^2$

“While any generalization to higher dimensions is fraught with peril, we feel that the multigrid algorithm presented here can be successfully extended.” – T. Manteuffel, et al.
Manteuffel shows that error following relaxation is approximately kinked-linear

- For $S_2$ purely scattering problems, the error following relaxation across a two-cell pair can be exactly interpolated from one coarse-cell’s information.
- For problems with absorption, this shape can be approximated by a “kinked-linear” function.
- Deviation from linearity is computed and is used to interpolate fine-grid information.
- We use a different definition for the kink-factor than Manteuffel.
- One-dimensional interpolation is done with respect to mean-free path space.
Our goal in 1D was to learn, not necessarily to use the computers efficiently

- **S\textsubscript{N}APPER\textsubscript{-}1D**
  - Serial Code
  - FORTRAN90
  - PC
    - IMSL Libraries
    - Memory Intensive
- **Fourier Analyses**
  - Serial Code
  - FORTRAN90
  - PC
    - IMSL Libraries
A V-cycle can be mathematically described by an iteration matrix

- Perform a Fourier analysis representing a multigrid solution to an infinite medium problem
- Mimic an infinite medium with an eight-cell (S$_2$) problem with periodic boundary conditions
  - Analysis allowed for heterogeneous eight-cell repeated patterns
- The analytic result of the Fourier analysis (of the discrete problem) is a V-cycle multigrid iteration matrix for each Fourier mode
  - The largest eigenvalue yields the convergence behavior (spectral radius)

Simple relaxation on the finest grid

Finite-sum approximation to the exact grid-level solution

Coarsest grid is solved exactly
Lesson #1: Kink-factors are intimately linked to the coarse-grid operators

- We explored kink-factors based on a discrete, $S_2$, two-cell problem using standard discretization applied to the given grid.
- The resulting interpolation factors were not consistent with coarse-grid operators.
- This resulted in degraded performance for LLD problems.
- This resulted in disastrous performance for LD problems.
Lesson #2: Negative kink-factors can cause this method to become unstable

- Optically thick problems can produce negative fluxes at a two-cell interface.
- This produces negative kink-factors.
- Coarse-grid operators built with negative kink-factors can cause the smoother to become an error amplifier.
- This problem is easily mitigated by restricting the kink-factors to non-negative values.
- This is not a panacea. It can degrade performance for homogeneous problems with uniform grids.
- This makes it difficult to define a precise necessary condition for stability.

Set of non-uniform-grid test problems

<table>
<thead>
<tr>
<th>$10^1$</th>
<th>$10^2$</th>
<th>$10^3$</th>
<th>$10^4$</th>
<th>$10^5$</th>
<th>$10^6$</th>
</tr>
</thead>
</table>

A single-mfp cell in a group of cells as large as $10^7$ mfp’s

Error Characterization
Cells 7&8 for Problems 1-7

Position (mfp’s) vs. Flux Error
Lesson #3: Multiple kink-factors can help, but do not appear to be worth the effort

- The spatial discretization is discontinuous, yet we use a prolongation operator that assumes a continuous error.
- Angularly dependent variables are interpolated using angularly independent kink-factors.
- Mildly heterogeneous problems will violate these assumptions and result in poor convergence performance.
- Manteuffel attributes discontinuity at two-cell interfaces as the cause of his worst cases in the homogeneous, uniform test suite.
Lesson #4: Poor method performance for difficult problems is not a dead end

• Where this multigrid method does not rapidly converge, Fourier analysis shows that the eigenvalues are well clustered.
• This means the method may be an excellent preconditioner for Krylov solvers.
• Heterogeneous problems with non-uniform grids show distinct differences between Manteuffel's method and our modified method.
• The other three problem classes have smaller differences.
With the 1D experience in hand, we make choices that define the 2D method

- Assume kinked-bilinearity for the error shape across a four-cell quad following relaxation
- Prolongation operator defined by 5 kink-factors
- The iteration matrix in the Fourier analysis has the same form in 1D and 2D
  - The individual operators are more complex, and cell numbering is more complicated in 2D

Our 2D, four-cell interpolation analog to Manteuffel’s 1D, two-cell interpolation
A detailed algebraic analysis of the error following four-cell relaxation is intractable

• Error characterization is easy in 1D
• It is not in 2D
• In 1D, we used finite element weight and “kinked” basis functions to build coarse-grid and prolongation operators
• Can we simply do the same in 2D?
• Sure…but will it work very well?

“fraught with peril”
Fourier analysis allows characterization of the slowest converging error mode

- Determining the spatial shape of the slowest converging error mode replaces an algebraic study of the two-dimensional problem.
- Kink-factors computed from the slowest-converging error mode will produce coarse-grid operators designed to eliminate that mode.
- This is slightly more complex for determining the kink-factors for constructing the coarsest-grid, 16l, operators.
One goal in 2D was to use the computers efficiently

- **S_{N}APP_{E R\_2D}**
  - Serial Code
  - FORTRAN90
  - PC
    - IMLS Libraries
  - QSC
    - LAPACK
    - Memory Conservative
- **Fourier Analysis**
  - Parallel Code (MPI)
  - FORTRAN90 with C routines
  - QSC
    - LAPACK
Given isotropic scattering, a four-cell inverse should involve inverting nothing larger than a 16x16 matrix

- If you know the 16 scalar fluxes it is easy to compute all the angular fluxes.
- The 16 scalar fluxes are all coupled. Thus, we must invert at least a 16x16.
- When we express this physics mathematically we obtain the Sherman-Morrison formula.
- This could be done for any cell shape.

\[
\left( \Pi_0 - VW^T \right)^{-1} = \Pi_0^{-1} + \Pi_0^{-1} V \left( I - W^T \Pi_0^{-1} V \right)^{-1} W^T \Pi_0^{-1}
\]

This matrix is 16x16 when scattering is isotropic.

On coarser grids, this matrix remains 16x16 if the kink-factors are angularly independent.
Multiple kink-factors will complicate the coarse-operator structure and inversion

- The use of angularly-dependent kink-factors causes the solution to depend on more than 16 unknowns.
- This increases the size of the matrix that is left to direct inversion in the Sherman-Morrison decomposition.

\[
\begin{bmatrix}
R & 0 & 0 & 0 \\
0 & R & 0 & 0 \\
0 & 0 & R & 0 \\
0 & 0 & 0 & R
\end{bmatrix}
\begin{bmatrix}
S & S & S & S \\
S & S & S & S \\
S & S & S & S \\
S & S & S & S
\end{bmatrix}
\begin{bmatrix}
T & 0 & 0 & 0 \\
0 & T & 0 & 0 \\
0 & 0 & T & 0 \\
0 & 0 & 0 & T
\end{bmatrix}
= \begin{bmatrix}
\tilde{S} & \tilde{S} & \tilde{S} & \tilde{S} \\
\tilde{S} & \tilde{S} & \tilde{S} & \tilde{S} \\
\tilde{S} & \tilde{S} & \tilde{S} & \tilde{S} \\
\tilde{S} & \tilde{S} & \tilde{S} & \tilde{S}
\end{bmatrix}
\]

\text{Rank\_Before} = \text{Rank\_After}

\[
\begin{bmatrix}
R & 0 & 0 & 0 \\
0 & R & 0 & 0 \\
0 & 0 & R & 0 \\
0 & 0 & 0 & R
\end{bmatrix}
\begin{bmatrix}
S & S & S & S \\
S & S & S & S \\
S & S & S & S \\
S & S & S & S
\end{bmatrix}
\begin{bmatrix}
T & 0 & 0 & 0 \\
0 & T' & 0 & 0 \\
0 & 0 & T'' & 0 \\
0 & 0 & 0 & T'''
\end{bmatrix}
= \begin{bmatrix}
\tilde{S} & \tilde{S}' & \tilde{S}'' & \tilde{S}''' \\
\tilde{S} & \tilde{S}' & \tilde{S}'' & \tilde{S}''' \\
\tilde{S} & \tilde{S}' & \tilde{S}'' & \tilde{S}''' \\
\tilde{S} & \tilde{S}' & \tilde{S}'' & \tilde{S}'''
\end{bmatrix}
\]

\text{Rank\_Before} < \text{Rank\_After}
The 2D method is not as rapidly converging as the 1D method

- The slowest converging error mode in the thin, highly scattering limit is discontinuous everywhere.
- In one-dimension, Manteuffel attributes discontinuous error shapes following relaxation to be the cause of his “worst” cases.
- Discontinuities cause the coarse-to-fine interpolation step to be imprecise. This leads to degraded method performance.
- The degree of degradation can be quantified only by numerical experimentation.
### Fourier analysis spectral radii vs. $S_N$ APPER_1D/2D convergence ratios: $c = 0.9999$, Lumped Equations

<table>
<thead>
<tr>
<th>$\sigma h$</th>
<th>Fourier $S_2$</th>
<th>$S_2$</th>
<th>$S_8$</th>
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<tbody>
<tr>
<td>$10^{-4}$</td>
<td>$8.9 \times 10^{-14}$</td>
<td>$2.9 \times 10^{-14}$</td>
<td>$5.1 \times 10^{-7}$</td>
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<tr>
<td>$10^{2}$</td>
<td>$3.8 \times 10^{-3}$</td>
<td>$4.6 \times 10^{-3}$</td>
<td>$4.6 \times 10^{-3}$</td>
</tr>
<tr>
<td>$10^{3}$</td>
<td>$5.6 \times 10^{-4}$</td>
<td>$6.4 \times 10^{-4}$</td>
<td>$6.1 \times 10^{-4}$</td>
</tr>
<tr>
<td>$10^{4}$</td>
<td>$8.2 \times 10^{-6}$</td>
<td>$8.3 \times 10^{-6}$</td>
<td>$7.6 \times 10^{-6}$</td>
</tr>
</tbody>
</table>

1D, LLD ($\theta = 1$)

<table>
<thead>
<tr>
<th>$\sigma h_x = \sigma h_y$</th>
<th>Fourier $S_2$</th>
<th>$S_2$</th>
<th>$S_8$</th>
</tr>
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<tbody>
<tr>
<td>$10^{-4}$</td>
<td>0.868</td>
<td>0.472</td>
<td>0.463</td>
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<tr>
<td>$10^{-2}$</td>
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<td>$10^{0}$</td>
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<td>0.578</td>
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<tr>
<td>$10^{2}$</td>
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<td>0.922</td>
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<tr>
<td>$10^{3}$</td>
<td>0.801</td>
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<td>0.774</td>
</tr>
<tr>
<td>$10^{4}$</td>
<td>0.222</td>
<td>0.221</td>
<td>0.193</td>
</tr>
</tbody>
</table>

2D, LBLD ($\theta_x=\theta_y=1$)
### Fourier analysis spectral radii vs. \( S_{N}\)APPER_1D/2D convergence ratios: \( c = 0.9999\), Standard Equations

<table>
<thead>
<tr>
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<th>( S_8 )</th>
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<tr>
<td>( 10^{-4} )</td>
<td>( 1.9 \times 10^{-13} )</td>
<td>( 1.3 \times 10^{-14} )</td>
<td>( 5.1 \times 10^{-7} )</td>
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<td>( 2.2 \times 10^{-3} )</td>
</tr>
<tr>
<td>( 10^{0} )</td>
<td>( 1.9 \times 10^{-5} )</td>
<td>( 6.3 \times 10^{-5} )</td>
<td>( 7.8 \times 10^{-3} )</td>
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<td>( 10^{2} )</td>
<td>( 5.9 \times 10^{-3} )</td>
<td>( 6.1 \times 10^{-3} )</td>
<td>( 6.1 \times 10^{-3} )</td>
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<td>( 2.1 \times 10^{-2} )</td>
<td>( 2.1 \times 10^{-2} )</td>
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<th>( S_2 )</th>
<th>( S_8 )</th>
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</thead>
<tbody>
<tr>
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<td>( 0.976 )</td>
<td>( 0.649 )</td>
<td>( 0.638 )</td>
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<td>( 10^{-2} )</td>
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<td>( 10^{2} )</td>
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<td>( 0.924 )</td>
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<tr>
<td>( 10^{3} )</td>
<td>( 0.902 )</td>
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<tr>
<td>( 10^{4} )</td>
<td>( 0.451 )</td>
<td>( 0.449 )</td>
<td>( 0.412 )</td>
</tr>
</tbody>
</table>

1D, LD (\( \theta = 3 \))

2D, BLD (\( \theta_x=\theta_y=3 \))
A three-level Fourier analysis does not accurately predict convergence ratios for cells 1-10 mfp’s thick.

The Fourier analysis code inverts the grid-level 16l operator. This eliminates error modes that are causing higher convergence ratios in the general solver.

For thin problems, the observed convergence ratio approaches the spectral radius from below. Fourier is predictive in the thick limit.
Eigenvector-based kink-factors lead to more rapid convergence in the thick limit.

Eigenkinks: 0.13384190772300
Unity Kinks: 0.222335885364840
Our analysis yields the distribution of the eigenvalues at any stage of a multigrid cycle.

\[ \sigma_h x = \sigma_h y = 1.0 \times 10^{-4}; c = 0.999999 \]
An open question remains regarding this method’s ability to precondition thin problems.

\[
\sigma_{\text{h}_x} = \sigma_{\text{h}_y} = 1.0 \times 10^{-4}; \quad c = 0.999999
\]
Eigenvalue progression maps give a more detailed view of the three-level shortcoming
Homogeneous, non-uniform grid problems behave similarly to the analogous one-dimensional cases.

In 1D, eigenvalues were never observed in this region.

A close look at the distributions of the eigenvalues following a multigrid cycle provides evidence about the method’s preconditioning properties.
Heterogeneous problems can show behavior not observed in any tested one-dimensional problems.

Interestingly, kink-factors generated by the slowest converging error modes cause the method to remain stable.

Unlike the one-dimensional results, two-dimensional heterogeneous problems can exhibit eigenvalues that reflect divergent behavior and are left poorly clustered.
Summary of Results & Conclusions

- Extension of Manteuffel’s methodology to two dimensions has been demonstrated. The four-cell error smoother coupled with kink-flooring always results in a stable iterative method.
  - Although it is not as rapidly converging as the one-dimensional method for simple problems, our two-dimensional multigrid method is a working iterative solver. For simple problems, it always exhibits convergence ratios and spectral radii significantly less than source iteration.

- Manteuffel’s one-dimensional method does not perform well across a wide range of problems. Our extensions to his work also fail to rapidly converge for difficult problems. For a very broad category of problems, eigenvalue distributions are very well clustered.
  - This method is not an ideal stand-alone solver in either one or two dimensions. The distribution of eigenvalues does make this a candidate for preconditioning within a Krylov solver.
Summary of Results & Conclusions

• A three-level Fourier analysis accurately predicted convergence ratios for our general one-dimensional multigrid solver. In 2D, the three-level results were not accurate predictors of multi-level performance. However, three-level analyses can give accurate upper and lower bounds.
  – The Fourier analysis, while difficult, is worth the effort. This analysis provides insight that allows us to propose this multigrid method’s usefulness as a Krylov preconditioner. Without this type of additional analysis, the method might appear to be a failure.

• This multigrid method exhibits different convergence performance for different spatial discretizations. This is true for the one and two-dimensional methods.
  – Great care must be taken when applying multigrid iterative techniques to transport calculations. Good performance for one discretization implies nothing about performance for a different spatial discretization. There is a great deal of literature showing the same effect when DSA is applied to different spatial discretizations. We have shown that the same is true for multigrid.
Summary of Results & Conclusions

• Sherman-Morrison provides an efficient method for inverting the four-cell operator. For isotropic scattering problems using simple kink-factors, the largest matrix requiring direct inversion is 16x16. The dimension of this matrix will increase if higher scattering orders are used.
  – Our one and two-dimensional error smoothing steps are computationally efficient. For problems with anisotropic scattering, greater computational effort will be required.
• Multigrid methods involve storing several pieces of information on different grid levels. Transport solution vectors can be memory intensive for multigroup, time-dependent problems. We have implemented this method storing a minimum amount of information that does not scale with quadrature order.
  – This method does not require much memory storage. Problems that are not already memory-limited will not likely be memory limited with the addition of the necessary multigrid information. This method has reasonable implementation and memory-use demands.
Future Work

• This method should be tested as a preconditioner for a Krylov solver.
• Incorporation of anisotropic scattering would increase the problem domain addressed by this method. Would this method still result in clustered eigenvalues for such problems?
• Multigrid methods should be applied to more complex cell shapes, such as arbitrary polyhedra. In such problems, characterization of the error’s spatial shape may be unreasonably demanding. In that case, algebraic multigrid techniques could be investigated.
• Multigrid transport solvers could be investigated on parallel computing platforms. Pieces of the grid can be distributed as per a domain decomposition. Would it be necessary to go all the way down the V-cycle?
• Since we are using scalar fluxes to generate kink-factors, it may not be necessary to maintain fine angular structure on coarser grids. Angular restriction and prolongation operators could reduce coarse-grid computations.