The Spectral Volume Method as Applied to Transport Problems

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Outline

1. Summary and Motivation

2. Derivation
   - Choice of Sub-Cell Partitioning
   - Properties Of The Spectral Volume Method

3. Numerical Results
   - Reed’s Problem
   - Diffusive Problem

4. Conclusions and Future Work
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To make solutions more accurate:
- p-adaptive mesh refinement methods.
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Not always a bad thing:
In regions with constant cross-sections, the transport solution is often smooth. In such regions high-order reconstructions using large cells can be more efficient. Extra unknowns, if they don't increase the communication burden, might only marginally increase the computational cost.
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- This can be thought of as a generalization of the simple corner balance and other sub-cell balance method previously presented.
- The term spectral is used here to note that the solution in each cell is reconstructed via polynomials in a similar way to a spectral method on a finite domain.
SVM as a sub-grid model for boundary layers

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- This is the topic of ongoing work.
We begin with the steady-state transport equation in slab-geometry, using discrete ordinates:

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- We then further partition each cell \( i \) into \( K \) sub-cells with width \( \Delta x_{i,k} \).
- Averaging over a generic sub-cell \( k \) of cell \( i \) yields

\[ \frac{\mu_l}{\Delta x_{i,k}} \left( \hat{\psi}_{l,k}^{i,k+1/2} - \hat{\psi}_{l,k}^{i,k-1/2} \right) + \sigma_t \psi_{l,k}^i = \frac{\sigma_s}{2} \langle \psi_{l,k}^i \rangle + \frac{Q_{i,k}}{2}, \]
Interfacial values

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- This polynomial is given by

$$p_l(x) = \sum_{k=1}^{K} \varphi_k(x) \psi_{l}^{i,k},$$

where

$$\varphi_k(x) = \prod_{q=1, q\neq k}^{K} \frac{x - x_{iq}}{x_{i,k} - x_{iq}}.$$
We then use this polynomial to give the value of the $\psi_l$ inside of cell $i$. Specifically, this polynomial gives the interfacial values between the sub-cells:

$$\hat{\psi}^{i,k+1/2} = p_l(x_{i,k+1/2}) \quad \text{for } k \in [2, K - 1].$$
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- At the interface between cells we use the principle of upwinding to choose the value. Specifically,

$$\hat{\psi}^i_{l,k-1/2} = \begin{cases} p_l(x_{i-1/2}) & \mu_l < 0 \\ p_{l-1}(x_{i-1/2}) & \mu_l > 0 \end{cases} \quad \text{for } k = 1,$$
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Choice of Sub-Cell Partitioning

- How should one divide the cell into sub-cells?

\[ \Delta x_{i,k} = \frac{\Delta x_i}{K} \]

Unfortunately, this approach leads to non-convergent methods for higher order elements. The polynomials are highly oscillatory near cell edges. This is an example of the Runge phenomenon. Using Gauss-Lobatto quadrature points to define the sub-cell edges has been shown to maintain convergence. For a generic cell this approach leads to:

\[ x_{i,k+\frac{1}{2}} = \frac{\Delta x_i}{2} \left( 1 - \cos \left( \frac{k\pi}{K} \right) \right), \quad k = 0, \ldots, K. \]
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<tbody>
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</tr>
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</tr>
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- Notice how these points are clustered near the edges of the main cell.
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- If we multiply the balance equation for a sub-cell by $\Delta x_{i,k}/\Delta x_i$ and sum over $k = 1 \ldots K$, we get

$$
\frac{\mu_l}{\Delta x_i} \left( \hat{\psi}_{l,K+1/2} - \hat{\psi}_{l,1/2} \right) + \sigma_t \sum_{k=1}^{K} \frac{\Delta x_{i,k}}{\Delta x_i} \psi_{l,k}^i, = \frac{\sigma_s}{2} \left\langle \sum_{k=1}^{K} \frac{\Delta x_{i,k}}{\Delta x_i} \psi_{l,k}^i \right\rangle + \frac{\bar{Q}_i}{2},
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- To show conservation over the entire domain, we multiply this equation by $\Delta x_i$ and sum over all cells to get

$$-\mu_l \left( \hat{\psi}_l^{I,K+1/2} - f_l \right) + \sum_i \Delta x_i \left( \frac{\sigma_s}{2} \langle \bar{\psi}_l^i \rangle - \sigma_t \bar{\psi}_l^i + \frac{\bar{Q}_i^i}{2} \right) = 0, \quad \mu > 0,$$

and

$$-\mu_l \left( g_l - \psi_l^{1,1/2} \right) + \sum_i \Delta x_i \left( \frac{\sigma_s}{2} \langle \bar{\psi}_l^i \rangle - \sigma_t \bar{\psi}_l^i + \frac{\bar{Q}_i^i}{2} \right) = 0, \quad \mu < 0.$$
Accuracy

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- We can see this by writing out the equations for $\mu > 0$ for a generic cell with $K = 2$ and $\Delta x_i = 2\Delta x_{i,k}$:

$$
\frac{\mu_l}{\Delta x_i} \left( (\psi_l^{i,2} + \psi_l^{i,1}) - (3\psi_l^{i-1,2} - \psi_l^{i-1,1}) \right) + \sigma_t \psi_l^{i,1} = \frac{\sigma_s}{2} \langle \psi_l^{i,1} \rangle + \frac{Q_{i,k}^{i}}{2},
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- This gives a corner balance scheme where the value at the cell-center and at the cell edges are linear interpolations from the sub-cell values.
Adaptivity

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- Static adaptivity using the spectral volume method has been shown to be successful in results from multidimensional computational fluid dynamics simulations (Wang, 2004).
- Furthermore, the interpolation inside each cell can be used to deal with dendritic meshes that arise in adaptive mesh refinement calculations.
The communication pattern between cells in the spectral volume method is the same for any number of sub-cells.
High-performance computing

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- Other transport schemes, such as spherical harmonics, could eliminate some of these sub-cell unknowns using Schur complements.
  - This has been demonstrated in recent magnetohydrodynamics methods, possibly making the larger values of $K$ “free”.

McClaren Spectral Volume Method
The spectral volume method is robust in the diffusion limit.
Diffusion Limit

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  - In the limit of optically thick, scattering dominated cells, the discretization limits to a discretization of the diffusion equation.
The spectral volume method is robust in the diffusion limit.

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If we scale the original, discrete transport equation by a small, positive parameter $\epsilon$ as

$$\frac{\epsilon \mu_l}{\Delta x_{i,k}} \left( \hat{\psi}^{i,k+1/2}_l - \hat{\psi}^{i,k-1/2}_l \right) + \sigma_t \psi^{i,k}_l = \frac{1}{2} \left( \sigma_t - \epsilon^2 \sigma_a \right) \langle \psi^{i,k}_l \rangle + \frac{\epsilon^2 Q^{i,k}}{2}.$$

and expand $\psi$ in a power series in $\epsilon$

$$\psi^{i,k}_l = \sum_{j=0}^{\infty} \epsilon^j \psi^{(j),i,k}_l,$$
Diffusion Limit

- We get an angular flux that is isotropic to leading order

\[ \psi_{l}^{(0),i,k} = \frac{1}{2} \langle \psi_{l}^{(0),i,k} \rangle \equiv \frac{\phi^{(0),i,k}}{2}. \]

\[
- \frac{2}{3 \Delta x_i} \left[ \frac{1}{\sigma_{t,i} \Delta x_i} \left( \phi^{(0),i,2} - \phi^{(0),i,1} \right) - \frac{1}{\sigma_{t,i-1} \Delta x_{i-1}} \left( \phi^{(0),i-1,2} - \phi^{(0),i-1,1} \right) \right] \\
+ \sigma_{a,i} \phi^{(0),i,1} + \sigma_{a,i} \phi^{(0),i-1,2} = Q^{i,1} + Q^{i-1,2}.
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\psi^{(0)}_{l,i,k} = \frac{1}{2} \langle \psi^{(0)}_{l,i,k} \rangle \equiv \phi^{(0)}_{l,i,k}.
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And a version of Fick’s law

\[
J^{(1),i,k} = - \frac{1}{6 \sigma_t \Delta x_i, k} \left( \hat{\phi}^{(0),i,k+1/2} - \hat{\phi}^{(0),i,k-1/2} \right),
\]

\[
\frac{-2}{3 \Delta x_i} \left[ \frac{1}{\sigma_{t,i} \Delta x_i} \left( \phi^{(0),i,2} - \phi^{(0),i,1} \right) - \frac{1}{\sigma_{t,i-1} \Delta x_{i-1}} \left( \phi^{(0),i-1,2} - \phi^{(0),i-1,1} \right) \right]
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- For the case of \( K = 2 \), if we turn the crank to get the diffusion equation, we get the consistent, diffusion discretization:

\[
\frac{-2}{3\Delta x_i} \left[ \frac{1}{\sigma_{t,i} \Delta x_i} \left( \phi^{(0),i,2} - \phi^{(0),i,1} \right) - \frac{1}{\sigma_{t,i-1} \Delta x_{i-1}} \left( \phi^{(0),i-1,2} - \phi^{(0),i-1,1} \right) \right] \\
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- We know they have a correct Fick’s law and continuity of $\phi$ at interfaces.
- Numerical results demonstrate the robustness of these methods.
Outline

1. Summary and Motivation

2. Derivation
   - Choice of Sub-Cell Partitioning
   - Properties Of The Spectral Volume Method

3. Numerical Results
   - Reed’s Problem
   - Diffusive Problem

4. Conclusions and Future Work
Reed’s Problem

Reed’s problem has several different material regions

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<tr>
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<td></td>
</tr>
<tr>
<td></td>
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</tr>
<tr>
<td>$Q = 0$</td>
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- The minimum $\Delta x$ that can resolve this material layout is $\Delta x = 1$. 
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  - $K = 2, 3, 4, 5, 6$ as well.
- We’ll use $S_8$ and a sweep-based GMRES scheme to solve the SV equations.
Results with $K = 2, 3$
Results with $K = 2, 3$

$K = 2$

![Graph showing results with $K = 2$ and different $N_x$ values](image-url)
Results with $K = 2, 3$

$K = 2$

$K = 3$

McClarren
Spectral Volume Method
Results with $K = 4, 6$
Results with $K = 4, 6$

$K = 4$

![Graph showing results with $K = 4$]
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- This problem is almost ideal for this method as the scalar flux is only non-smooth at the material interfaces.
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Diffusive Problem (with boundary layer)

- This problem has a strong absorber next to a diffusive region

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- We use $S_8$ and the same sweeping method as before.

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This problem can be described using two cells. For comparison we use a $K = 6$ and $N_x = 512$ solution as a reference ($\max \Delta x_{i,k} = 0.00097656$).
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Results for $K = 2$
Results for $K = 2$
Results for $K = 2$

[Graph showing results for $K = 2$, with different markers for $N_x = 512, 32, 8, 2$.]

McClarren
Spectral Volume Method
For $K = 2$ the transition from the absorber to the scattering region is smoothed out.
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Diffusive Problem Results

- For $K = 2$ the transition from the absorber to the scattering region is smoothed out.
- The $N_x = 32$ solutions under-predicts the maximum value of the scalar flux.
- Away from the boundary layer the solution has the correct slope for $N_x = 8$ and $32$. 
Results for $K = 4$
Results for $K = 4$

Results

\[ \phi(x) \]

- $N_x = 512$ (K=6)
- $N_x = 32$
- $N_x = 8$
- $N_x = 2$
Results for $K = 4$

Results

Detail

Reed's Problem

Diffusive Problem

McClaren

Spectral Volume Method

Summary and Motivation

Derivation

Numerical Results

Conclusions and Future Work
For $K = 4$ does a much better job resolving the solution near the interface, including the maximum scalar flux for $N_x \geq 32$. 
Diffusive Problem Results

- For $K = 4$ does a much better job resolving the solution near the interface, including the maximum scalar flux for $N_x \geq 32$.
- There are small oscillations near the boundary layer.
Diffusive Problem Results

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- There are small oscillations near the boundary layer
  - These are due to interpolating across this sharp change.
Results for $K = 6$
Results for $K = 6$
Results for $K = 6$
For $K = 6$ the solutions are improved over $K = 4$
Diffusive Problem Results

- For $K = 6$ the solutions are improved over $K = 4$
- The $N_x = 32$ solution is beginning to resolve the boundary layer
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- The $N_x = 32$ solution is beginning to resolve the boundary layer
  - Small oscillations remain
What we’ve seen so far

- The spectral volume method seems to be a way to get high order solutions by dividing the problem into sub-cells.
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  - The method is accurate and robust in the diffusion limit.

- One possible benefit of the method is the ability to have a sub-grid means to resolve boundary layers.
  - We saw some evidence of this in a test problem.
  - Still work to be done.

- Might be a good candidate for local parallelism.
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- This might necessitate fancier reconstruction schemes.

![Diagram of subcell divisions](image)
Acknowledgments

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Marshak Wave

- This method also works for time-dependent thermal radiative transfer problems.
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This figure shows the $K = 6$ solution with 5 cells and the analytic diffusion solution at $t = 10, 50, \text{ and } 100$ ns for a problem with a 1 keV incident source and $\sigma = 300/T^3$. 