# The Spectral Volume Method as Applied to Transport Problems

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Image: 1

# Outline



#### 2 Derivation

- Choice of Sub-Cell Partioning
- Properties Of The Spectral Volume Method

#### 3 Numerical Results

- Reed's Problem
- Diffusive Problem



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Motivation

### Background

• Discretization techniques for linear particle transport problems often require several spatial degrees-of-freedom per spatial cell.

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  - 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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- 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.

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- This is the topic of ongoing work.

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Choice of Sub-Cell Partioning Properties Of The Spectral Volume Method

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#### Derivation of the method

$$\mu_l \partial_x \psi_l + \sigma_t \psi_l = \frac{\sigma_s}{2} \langle \psi_l \rangle + \frac{Q}{2}, \qquad l \in [1, L].$$

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# Derivation of the method

• We begin with the steady-state transport equation in slab-geometry, using discrete ordinates:

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• We denote the quadrature sums as  $\langle \psi_l \rangle = \sum_{l=1}^L w_l \, \psi_l \equiv \phi$ .

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  - Cell *i* has a width  $\Delta x_i$
- 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

$$\frac{\mu_l}{\Delta x_{i,k}} \left( \hat{\psi}_l^{i,k+1/2} - \hat{\psi}_l^{i,k-1/2} \right) + \sigma_{\mathbf{t}} \psi_l^{i,k} = \frac{\sigma_{\mathbf{s}}}{2} \langle \psi_l^{i,k} \rangle + \frac{Q^{i,k}}{2},$$

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#### 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

$$\varphi_k(x) = \prod_{q=1, q \neq k}^K \frac{x - x_{iq}}{x_{i,k} - x_{iq}}$$
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## Interfacial values

• 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:

$$\hat{\psi}_l^{i,k+1/2} = p_l(x_{i,k+1/2}) \quad \text{for } k \in [2, K-1].$$

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• At the interface between cells we use the principle of upwinding to choose the value. Specifically,

$$\hat{\psi}_l^{i,k-1/2} = \begin{cases} p_l(x_{i-1/2}) & \mu_l < 0\\ p_l^{i-1}(x_{i-1/2}) & \mu_l > 0 \end{cases} \text{ for } k = 1,$$

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Image: A matrix and a matrix

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### Choice of Sub-Cell Partioning

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McClarren Spectral Volume Method

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- 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

$$x_{i,k+1/2} = \frac{\Delta x_i}{2} \left( 1 - \cos\left(\frac{k\pi}{K}\right) \right), \quad k = 0, \dots, K.$$

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## Sub-cell Edges

• The edges when define with the GL quadrature points are

K	Points
2	0, 0.5, 1
3	0, .25, .75, 1
4	0, 0.146447, 0.5, 0.853553, 1
5	0, 0.0954915, 0.345492, 0.654508, 0.904508, 1
6	0,  0.0669873,  0.25,  0.5,  0.75,  0.933013,  1
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• Notice how these points are clustered near the edges of the main cell.

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### Logarithmically-Spaced Sub-cells

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- This will be the subject of future work.

Choice of Sub-Cell Partioning Properties Of The Spectral Volume Method

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- The spectral volume method can easily be shown to be conservative because we have defined the interfacial values to be continuous between sub-cells.
- If we multiply the balance equation for a sub-cell by  $\Delta x_{i,k}/\Delta x_i$ and sum over  $k = 1 \dots K$ , we get

$$\frac{\mu_l}{\Delta x_i} \left( \hat{\psi}_l^{i,K+1/2} - \hat{\psi}_l^{i,1/2} \right) + \sigma_t \sum_{k=1}^K \frac{\Delta x_{i,k}}{\Delta x_i} \psi_l^{i,k}, = \frac{\sigma_s}{2} \langle \sum_{k=1}^K \frac{\Delta x_{i,k}}{\Delta x_i} \psi_l^{i,k} \rangle + \frac{\bar{Q}^i}{2},$$

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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

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

and

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

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- Also, the case of K = 2 is equivalent to a corner balance method, which are known to be second-order accurate.
- We can see this by writing out the equations for  $\mu > 0$  for a generic cell with K = 2 and  $\Delta x_i = 2\Delta x_{i,k}$ :

$$\frac{\mu_l}{\Delta x_i} \left( (\psi_l^{i,2} + \psi_l^{i,1}) - (3\psi_l^{i-1,2} - \psi_l^{i-1,1}) \right) + \sigma_{\mathsf{t}} \psi_l^{i,1} = \frac{\sigma_{\mathsf{s}}}{2} \langle \psi_l^{i,1} \rangle + \frac{Q^{i,k}}{2},$$

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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.

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# Adaptivity

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# Adaptivity

- The spectral volume method is well-suited to local p-adaptivity where the number of sub-cells varies throughout the problem to resolve features of the solution.
- This is so because cells only communicate through outflow conditions on the main cells and the number of sub-cells only indirectly affects the outflow.

Image: A matrix and a matrix

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# Adaptivity

- The spectral volume method is well-suited to local p-adaptivity where the number of sub-cells varies throughout the problem to resolve features of the solution.
- This is so because cells only communicate through outflow conditions on the main cells and the number of sub-cells only indirectly affects the outflow.
- Also, the sub-cell partitioning can be adaptively selected to resolve mean-free paths where desired, as a form of h-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.

Choice of Sub-Cell Partioning Properties Of The Spectral Volume Method

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### High-performance computing

• The communication pattern between cells in the spectral volume method is the same for any number of sub-cells.

Image: A matrix and a matrix

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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".

Choice of Sub-Cell Partioning Properties Of The Spectral Volume Method

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

$$\frac{\epsilon\mu_l}{\Delta x_{i,k}} \left( \hat{\psi}_l^{i,k+1/2} - \hat{\psi}_l^{i,k-1/2} \right) + \sigma_{\mathrm{t}}\psi_l^{i,k} = \frac{1}{2} \left( \sigma_{\mathrm{t}} - \epsilon^2 \sigma_{\mathrm{a}} \right) \langle \psi_l^{i,k} \rangle + \frac{\epsilon^2 Q^{i,k}}{2}$$

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

$$\psi_l^{i,k} = \sum_{j=0}^\infty \epsilon^j \psi_l^{(j),i,k},$$

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## Diffusion Limit

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

$$\psi_l^{(0),i,k} = \frac{1}{2} \langle \psi_l^{(0),i,k} \rangle \equiv \frac{\phi^{(0),i,k}}{2}$$

$$\begin{split} \frac{-2}{3\Delta x_i} \left[ \frac{1}{\sigma_{\mathrm{t},i}\Delta x_i} \left( \phi^{(0),i,2} - \phi^{(0),i,1} \right) - \frac{1}{\sigma_{\mathrm{t},i-1}\Delta x_{i-1}} \left( \phi^{(0),i-1,2} - \phi^{(0),i-1,1} \right) \right] \\ + \sigma_{\mathrm{a},i} \phi^{(0),i,1} + \sigma_{\mathrm{a},i} \phi^{(0),i-1,2} = Q^{i,1} + Q^{i-1,2}. \end{split}$$

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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:

$$\begin{aligned} \frac{-2}{3\Delta x_i} \left[ \frac{1}{\sigma_{\mathrm{t},i}\Delta x_i} \left( \phi^{(0),i,2} - \phi^{(0),i,1} \right) - \frac{1}{\sigma_{\mathrm{t},i-1}\Delta x_{i-1}} \left( \phi^{(0),i-1,2} - \phi^{(0),i-1,1} \right) \right] \\ + \sigma_{\mathrm{a},i} \phi^{(0),i,1} + \sigma_{\mathrm{a},i} \phi^{(0),i-1,2} = Q^{i,1} + Q^{i-1,2}. \end{aligned}$$

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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.

**Reed's Problem** Diffusive Problem

# Outline

### **1** Summary and Motivation

#### 2 Derivation

- Choice of Sub-Cell Partioning
- Properties Of The Spectral Volume Method

#### **3** Numerical Results

- Reed's Problem
- Diffusive Problem

#### 4 Conclusions and Future Work

Image: A matrix and a matrix

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**Reed's Problem** Diffusive Problem

### Reed's Problem

• Reed's problem has several different material regions

Vacuum Bound.	Scattering Region	Vacuum	Absorber	Strong Source	Reflect. Bound
	$\Sigma_{a} = 0.1$		$\Sigma_a = 5$	$\Sigma_a = 50$	
	$\Sigma_{s} = 0.9$		$\Sigma_s = 0$	$\Sigma_s = 0$	
			Q = 0	Q = 50	
	$\begin{array}{c c c} Q = 0 & Q = 1 \\ x < 1 & 1 < x < 3 \end{array}$	3 < x < 5	5 < x < 6	6 < x < 8	

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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.

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**Reed's Problem** Diffusive Problem

### Results with K = 2, 3

McClarren Spectral Volume Method

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Reed's Problem Diffusive Problem

### Results with K = 2, 3



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McClarren Spectral Volume Method

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**Reed's Problem** Diffusive Problem

### Results with K = 4, 6

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Reed's Problem Diffusive Problem

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Reed's Problem Diffusive Problem

### Results with K = 4, 6



McClarren Spectral Volume Method

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**Reed's Problem** Diffusive Problem

### Reed's Problem Results

• For  $N_x = 64$  and above, all methods are converged in the view graph norm.

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**Reed's Problem** Diffusive Problem

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- For  $N_x = 64$  and above, all methods are converged in the view graph norm.
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  - The K = 6 solution matches the fine solution.
- This problem is almost ideal for this method as the scalar flux is only non-smooth at the material interfaces.

Reed's Problem Diffusive Problem

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## Diffusive Problem (with boundary layer)

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

Isotropic Boundary	Absorbing Region	Strong Scattering Region	Vacuum Boundary
	$\Sigma_a = 2$	$\Sigma_a = 0$	
	$\Sigma_s = 0$	$\Sigma_{s} = 1000$	
	0 < x < 1	1 < x < 2	

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- This problem has a strong absorber next to a diffusive region
- Particles enter the domain isotropically, travel two mean free paths through an absorber then enter a 1000 mean-free path thick slab.

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

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- For comparison we use a K = 6 and  $N_x = 512$  solution as a reference (max  $\Delta x_{i,k} = .00097656$ ).

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Reed's Problem Diffusive Problem

## Results for K = 2

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#### Results for K = 2



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## Diffusive Problem Results

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Reed's Problem Diffusive Problem

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- 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.

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Reed's Problem Diffusive Problem

## Results for K = 4

McClarren Spectral Volume Method

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#### Results for K = 4



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#### Results for K = 4



McClarren Spectral Volume Method

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Reed's Problem Diffusive Problem

## Diffusive Problem Results

• For K = 4 does a much better job resolving the solution near the interface, including the maximum scalar flux for  $N_x \ge 32$ .

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Reed's Problem Diffusive Problem

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Reed's Problem Diffusive Problem

## Diffusive Problem Results

- For K = 4 does a much better job resolving the solution near the interface, including the maximum scalar flux for  $N_x \ge 32$ .
- There are small oscillations near the boundary layer
  - These are due to interpolating across this sharp change.

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Reed's Problem Diffusive Problem

## Results for K = 6

McClarren Spectral Volume Method

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Reed's Problem Diffusive Problem

#### Results for K = 6



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#### Results for K = 6



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Reed's Problem Diffusive Problem

## Diffusive Problem Results

• For K = 6 the solutions are improved over K = 4

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Reed's Problem Diffusive Problem

## 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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Reed's Problem Diffusive Problem

# 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
  - Small oscillations remain

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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.

Image: A matrix and a matrix

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  - Still work to be done.
- Might be a good candidate for local parallelism.

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#### Well we already know how to solve 1-D problems

• Good point!

McClarren Spectral Volume Method

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- Good point!
- In CFD the method has been extended to 2-D using triangles as the main cells and quads as the sub-cells.

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- Good point!
- In CFD the method has been extended to 2-D using triangles as the main cells and quads as the sub-cells.
- One wrinkle in 2-D is the fact that solutions in a constant material region are not necessarily smooth.

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- Good point!
- In CFD the method has been extended to 2-D using triangles as the main cells and quads as the sub-cells.
- One wrinkle in 2-D is the fact that solutions in a constant material region are not necessarily smooth.
  - Think ray effects, shadows, etc.

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  - Think ray effects, shadows, etc.
- This might necessitate fancier reconstruction schemes.

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# 2-D Spectral Volume on Triangles

• Here's how Wang (2004) divided a triangle into subcells.



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# Acknowledgments

• Thanks to Cory Hauck at Oak Ridge National Lab for showing me this method and getting me interested in it.

References:

Image: A matrix and a matrix

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# Marshak Wave

• This method also works for time-dependent thermal radiative transfer problems.


Summary and Motivation Derivation Numerical Results Conclusions and Future Work

## Marshak Wave

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

