A PieceWise Linear Finite Element Discretization of the Diffusion Equation

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The diffusion equation describes many physical processes.

- Diffusion is used in heat transfer, atomic migration in materials, and photon and sub-atomic particle interaction with background materials.
- One physical system we want to model is inertial confinement fusion, which requires a solution of the linear Boltzmann transport equation coupled to an energy balance equation (as well as other physics).
- The diffusion equation that we are most interested in solving is an asymptotic limit of the radiation transport equation.

The PWL FEM is a robust and accurate diffusion solution on arbitrary grids.

- PWL has been added to the LLNL KULL multi-physics simulation project as a diffusion discretization.
- Previously, Palmer's finite volume method had been used as the KULL diffusion discretization.
- Palmer's method can be shown to be a Petrov-Galerkin "mass-lumped" PWL FEM.
- Palmer's method has an asymmetric matrix.
- PWL has many of the same attributes as Palmer's method, but has a symmetric matrix.

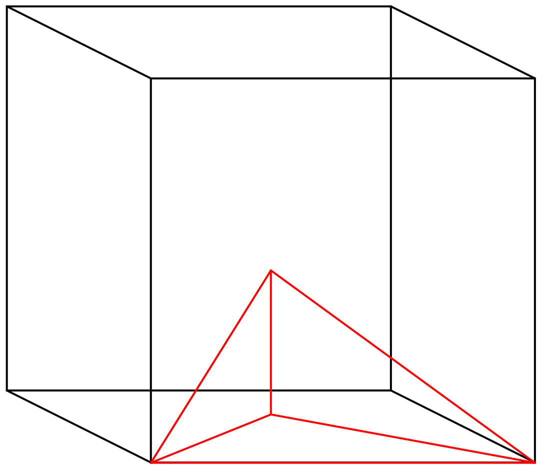
Other methods for these types of problems have disadvantages.

- Wachspress basis functions in the FEM discretization
  - ⇒ *Wachspress FEM has the same potential for working on arbitrary polyhedral meshes*
  - ⇒ *The integrals in the FEM must be done numerically if Wachspress basis functions are used – potentially cumbersome and costly!*
- Solving the problem on a tetrahedral mesh
  - ⇒ *Polyhedral cells can be divided into tetrahedra*
  - ⇒ *This either adds more unknowns or destroys the symmetry of the grid*
- Developing cell centered methods
  - ⇒ *The Support-Operator formalism may produce a cell centered method that works well on an arbitrary polyhedral mesh (but it could be expensive)*
  - ⇒ *Morel developed a finite-volume method; little testing to date*
  - ⇒ *For some classes of problems, cell-centered methods have some intrinsic advantages over vertex-centered.*

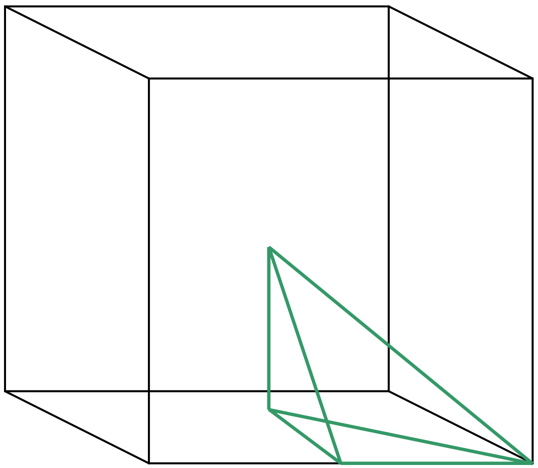
KULL is a software project for simulating inertial confinement fusion.

- KULL is a three-dimensional, time dependent, massively parallel multi-physics code being developed at Lawrence Livermore National Laboratory
- KULL solves coupled systems of hydrodynamics, radiation transport, and diffusion equations
- KULL can be used as a method test bed
- KULL is written mainly in C++

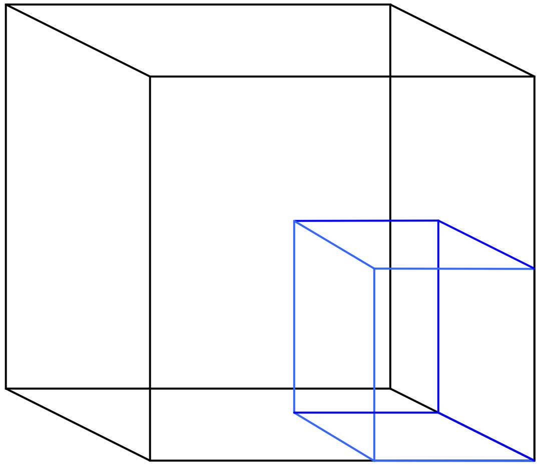
These figures show the basic building blocks of a polyhedral mesh in 3D.



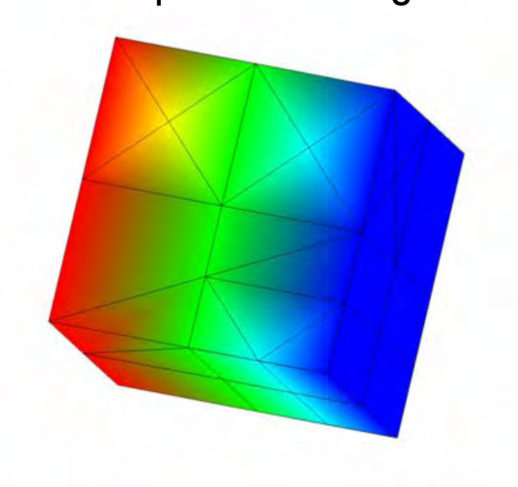
Example of a side



Example of a wedge



Example of a corner



Example of a polyhedral mesh

We have implemented a Galerkin FEM in KULL to solve the diffusion equation.

- The Diffusion Equation is

$$-\vec{\nabla}\cdot D(\vec{r})\vec{\nabla}E(\vec{r})+\sigma(\vec{r})E(\vec{r})=S(\vec{r})$$

- Ignoring boundary conditions, the Galerkin method results in the final form of

$$\sum_{j}E_j\left\{\int_{z\,at\,i} d^3r\left[D\vec{\nabla}b_j(\vec{r})\cdot\vec{\nabla}b_i(\vec{r})+\sigma b_j(\vec{r})b_i(\vec{r})\right]\right\}=\int_{z\,at\,i} d^3r\,b_i(\vec{r})S(\vec{r})$$

- The integration over the cells can be divided into an integration over “side” subcells.

- Galerkin methods produce SPD coefficient matrices.

Galerkin FEMs have significant advantages as diffusion discretizations.

- FEMs have nice properties:
  - ⇒ *allow the physical data to vary in a cell.*
  - ⇒ *are successful for diffusion problems with other kinds of spatial grids.*

- We "lump" the collision term for simplicity, robustness, convenience, and ease of comparison with Palmer's method.
  - ⇒ *Enhances diagonal dominance*

- It is difficult to define basis functions for arbitrary polyhedral cells.
  - ⇒ *Wachspress developed (in the 1970's) rational-polynomial functions that can be applied.*
  - ⇒ *Stone & Adams recently developed "PieceWise Linear" (PWL) functions that can be applied.*

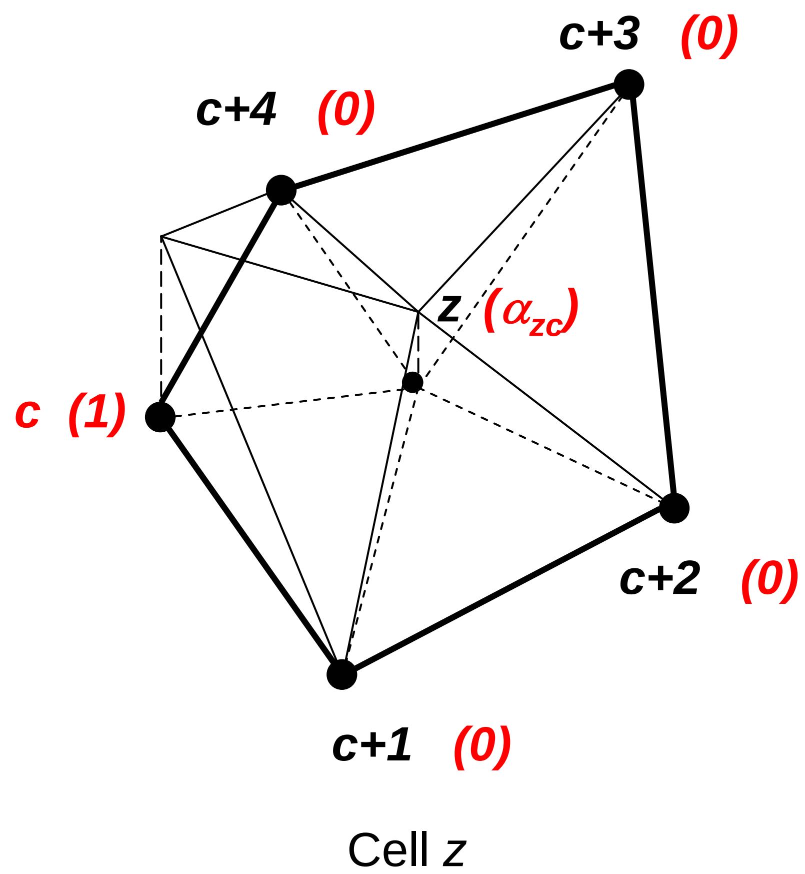
PWL basis functions are linear on each "side" subcell.

- The basis functions are constructed of standard linear functions [t(r)] on tetrahedra (sides).

$$b_j(r) = t_{j,p}(r) + \sum_{faces\ at\ p} \beta_f t_f(r) + \alpha_{j,z} t_z(r)$$

- α and β are coefficients that force the basis-function expansion to exactly reproduce any linear function. These coefficients represent interpolants.

- These basis functions and their products are easily integrable. (Wachspress rational functions are not analytically integrable.)



A PWL basis function in 2D. Figure Courtesy of Hiromi Stone

We can mathematically prove many properties of PWL.

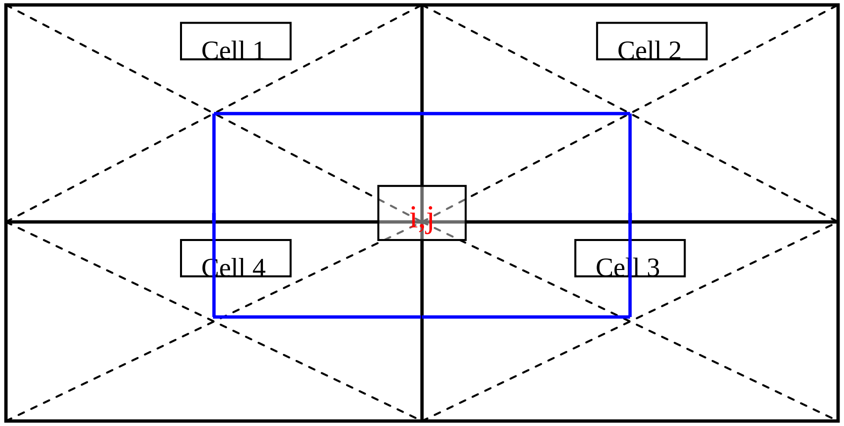
- Using the Lax-Milgram Lemma, we can prove that the PWL method produces a well-posed discrete problem.

- Using the results from the proof of well-posedness and the Bramble-Hilbert Lemma, we can show that Standard linear FEM is second order in the L_2 norm.

- We can show that PWL interpolant is within second order of standard linear (2D and 3D), which means that the PWL method is also second order in the L_2 norm.

Palmer's method is a finite volume method.

- Palmer's method was first derived by integrating the diffusion equation over a dual cell.



- The flux gradient in each half-side is determined by the flux at (i,j), the edge midpoint, and the cell center point.
- Coupling to the other vertex on the edge is created by conservation of particle flow.
- Cell center values are approximated as an interpolant of all vertex values.

Palmer's method is also a Petrov-Galerkin lumped PWL FEM!

- The weight functions that define this method are constant in the dual cell and zero elsewhere.
- As previously noted, the approximation for the flux gradients in each side are constant (if D is constant on each side), which is partially what defines the PWL basis functions.
- The interpolation chosen by Palmer (to preserve linear solutions) is exactly the same as if he had used PWL basis functions. Because Palmer's method is a non-Galerkin FEM, it is easy to see that it is not forced to produce a symmetric matrix.

$$\sum_j E_j \left\{ -\int_{\partial z\, at\, i} d^2 r\, w_i(\vec{r})\vec{n}\cdot D(\vec{r})\vec{\nabla} b_j(\vec{r}) + \int_{z\, at\, i} d^3 r \left[\sigma b_j(\vec{r}) w_i(\vec{r})\right] \right\} = \int_{z\, at\, i} d^3 r\, w_i(\vec{r}) S(\vec{r})$$

We have performed a simple mode analysis on these methods.

- The diffusion equation can be written as

$$-D\left[\frac{\partial^2\phi(\vec{r})}{\partial x^2}+\frac{\partial^2\phi(\vec{r})}{\partial y^2}+\frac{\partial^2\phi(\vec{r})}{\partial z^2}\right]+\sigma_a\phi(\vec{r})=S(\vec{r})$$

- The source can be expanded as

$$S(\vec{r})=\int_{-\infty}^{\infty}dw_z\int_{-\infty}^{\infty}dw_y\int_{-\infty}^{\infty}dw_x S(w)\exp(i\vec{w}\cdot\vec{r})$$

- The solution can also be expanded:

$$\phi(\vec{r})=\int_{-\infty}^{\infty}dw_z\int_{-\infty}^{\infty}dw_y\int_{-\infty}^{\infty}dw_x\phi(w)\exp(i\vec{w}\cdot\vec{r})$$

- Each mode can be separated out of the solution resulting in a single mode analytic solution of

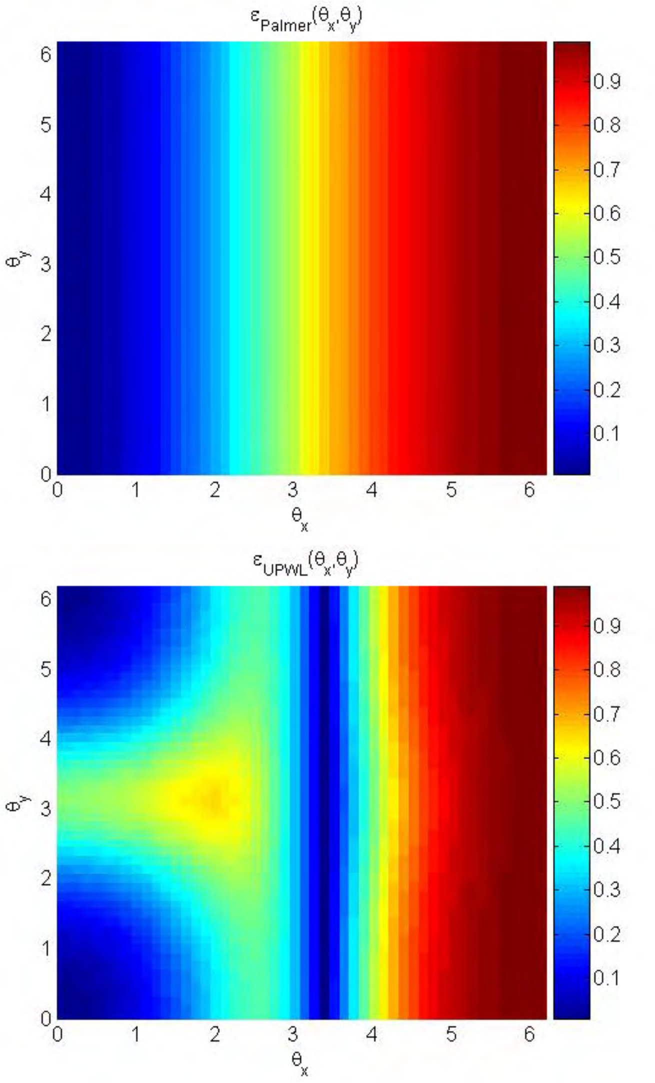
$$\phi_w=\frac{S_w}{D\left\{w_x^2+w_y^2+w_z^2\right\}+\sigma_a}$$

This same analysis can be performed on a discretization of the diffusion equation.

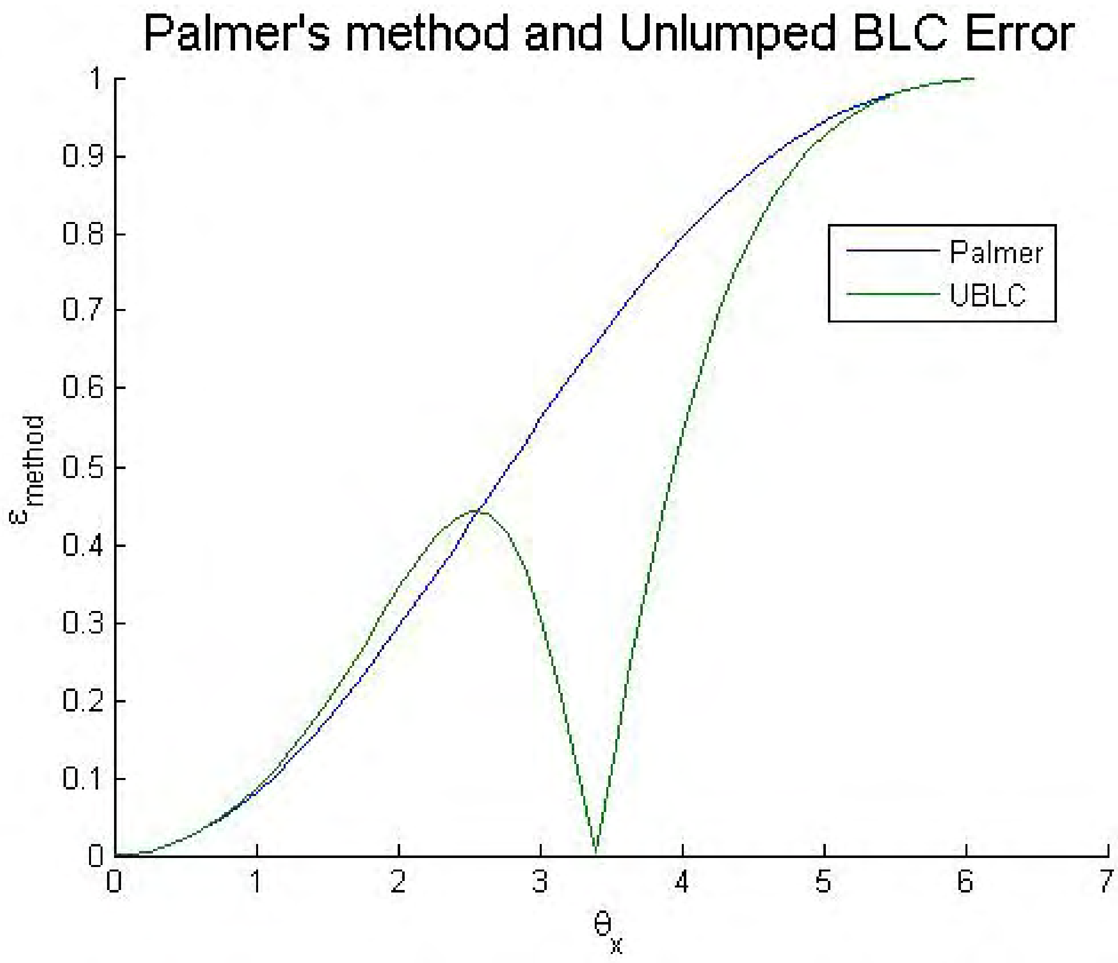
- We analyzed five methods in x-y geometry on an orthogonal grid.
  - ⇒ *Palmer's method*
  - ⇒ *Lumped PWL*
  - ⇒ *Unlumped PWL*
  - ⇒ *Lumped Bilinear Continuous FEM (BLC)*
  - ⇒ *Unlumped Bilinear Continuous FEM*
- The solution for all methods had the form

$$\phi_w = \frac{S_w}{D\left\{w_x^2 f_x\left(\theta_x,\theta_y\right)+w_y^2 f_y\left(\theta_x,\theta_y\right)\right\}+\sigma_a}$$

- $\theta_x = w_x \Delta x$ and $\theta_y = w_y \Delta y$
- When the $f_x(\theta_x,\theta_y)$ and $f_y(\theta_x,\theta_y)$ terms are 1, the methods produce the analytic solution. As (θ_x,θ_y) approach zero, the methods approach the fine mesh solution and the f-coefficients should approach 1 in this limit. We plotted $\varepsilon=|1-f|$ for each method.



εPalmer(θx,θy)
εLBL(θx,θy)
εUPWL(θx,θy)
εLPWL(θx,θy)
θx
θy



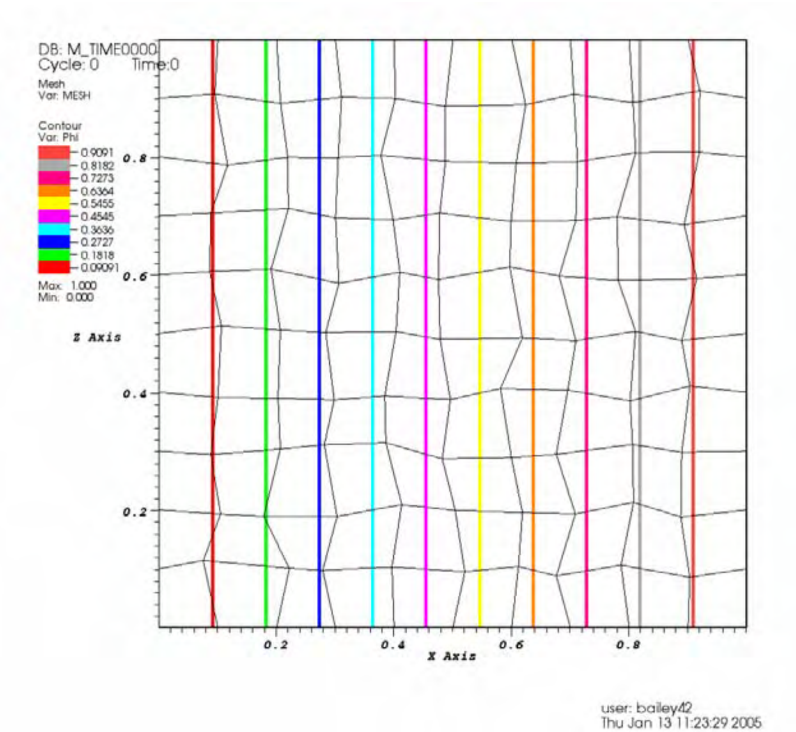
Palmer's method and Unlumped BLC Error
1
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0
ε_{method}
0
1
2
3
4
5
6
7
θ_x
Palmer
UBLC

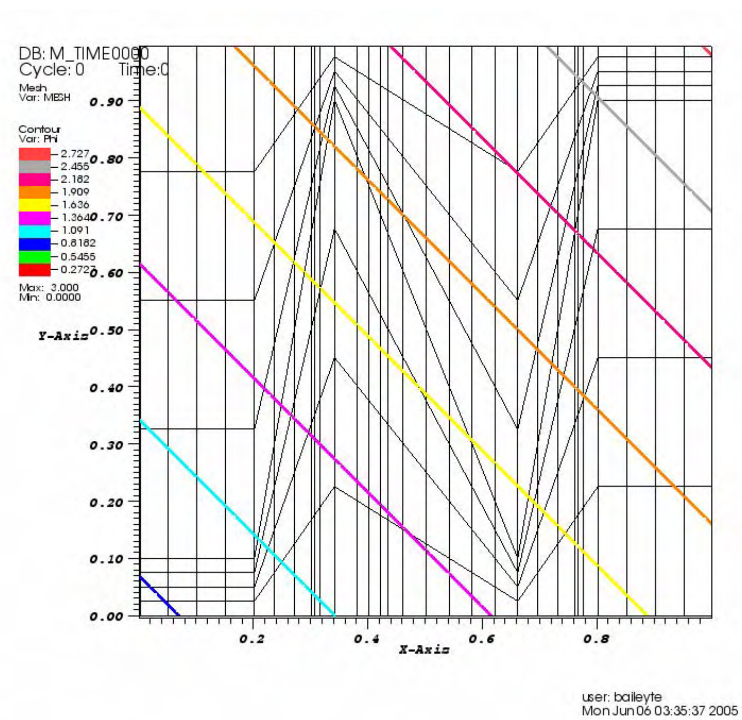
Analysis shows that the PWL method has some advantages to Palmer's method.

- Galerkin weighting makes the PWL system symmetric.
  - ⇒ *Need to build only ~ half the coefficients*
  - ⇒ *Can prove that the method is positive definite, well-posed, and second order convergent*
    - Ensures good behavior for all time steps
  - ⇒ *Can use Conjugate Gradient to solve system*
    - Fast and robust
    - Uses very little storage
- The mode analysis shows that for certain problems Palmer's method is slightly more accurate than various FEMs.
- The properties of the piecewise linear basis functions yield the following advantages:
  - ⇒ *method is exact if exact solution is linear*
  - ⇒ *it can be applied to arbitrary polyhedral meshes*
  - ⇒ *the needed integrals are simple to perform analytically*

Testing confirms that PWL reproduces a linear solution.

- The first test problems are problems with linear solutions in 1D and 3D. The two meshes shown here are a random mesh with a 1D linear solution and a z-mesh with a 3D linear solution.





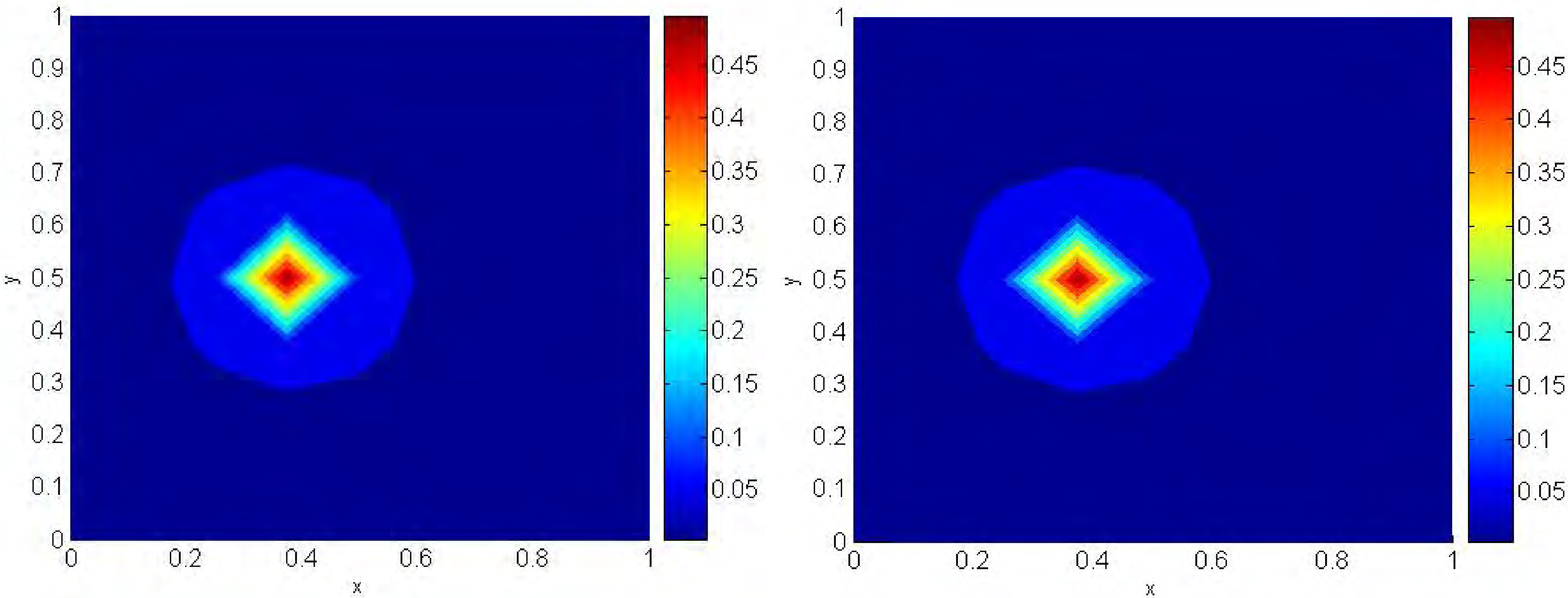
A potential source of problems for PWL is a mesh with high-aspect-ratio cells.

- We analyzed the coupling coefficients for a 2D rectangular grid with non-square cells.
- Some coefficients have the “wrong” sign when:

$$\Delta x / \Delta y \text{ or } \Delta y / \Delta x > \sqrt{3}$$

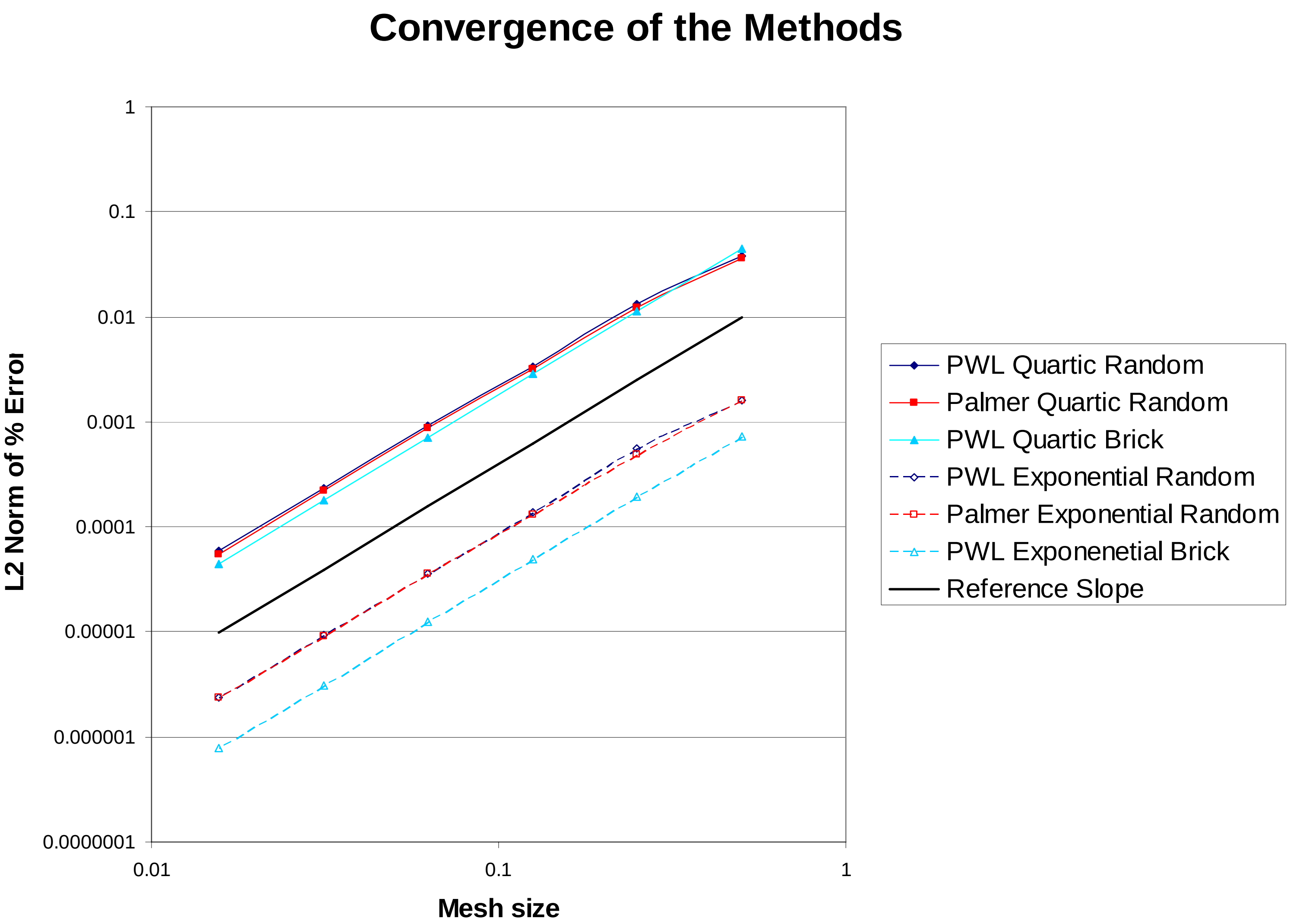
- To test this, we developed a problem with a point source inserted into a homogeneous domain without absorption. This problem has a non-smooth source vector, so it can effectively test the method’s ability to handle cells with high aspect ratios.

The results of the aspect-ratio tests are promising for the PWL method.



- The figure on the left has square cells. The figure on the right has 1000:1 aspect ratio cells located at about x = 0.375.
- There is little effect on the solution. In particular, there are no negative solution values, which means the inverse of the coefficient matrix has no negative entries.

The convergence rates of both methods are about the same.

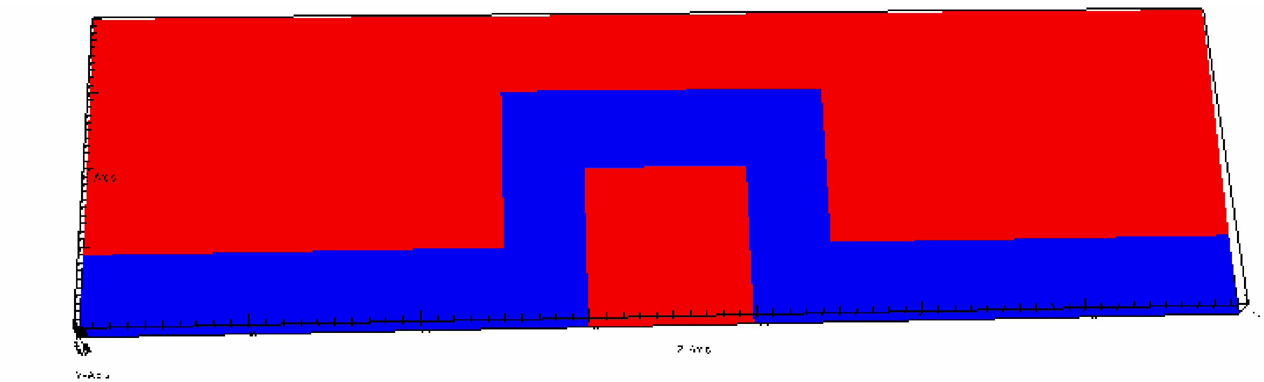


A more complex problem was needed to test the efficiency of PWL.

- PWL's main advantage is that is produces a symmetric positive-definite coefficient matrix, which can be solved by Conjugate Gradient instead of GMRES.
- To assess the difference in efficiency, we compare the iteration count for each matrix solution from the "top-hat" radiation-flow problem.
- Successfully running the tophat problem also demonstrates that both methods can be integrated into KULL completely and solve real applications with coupled physics.

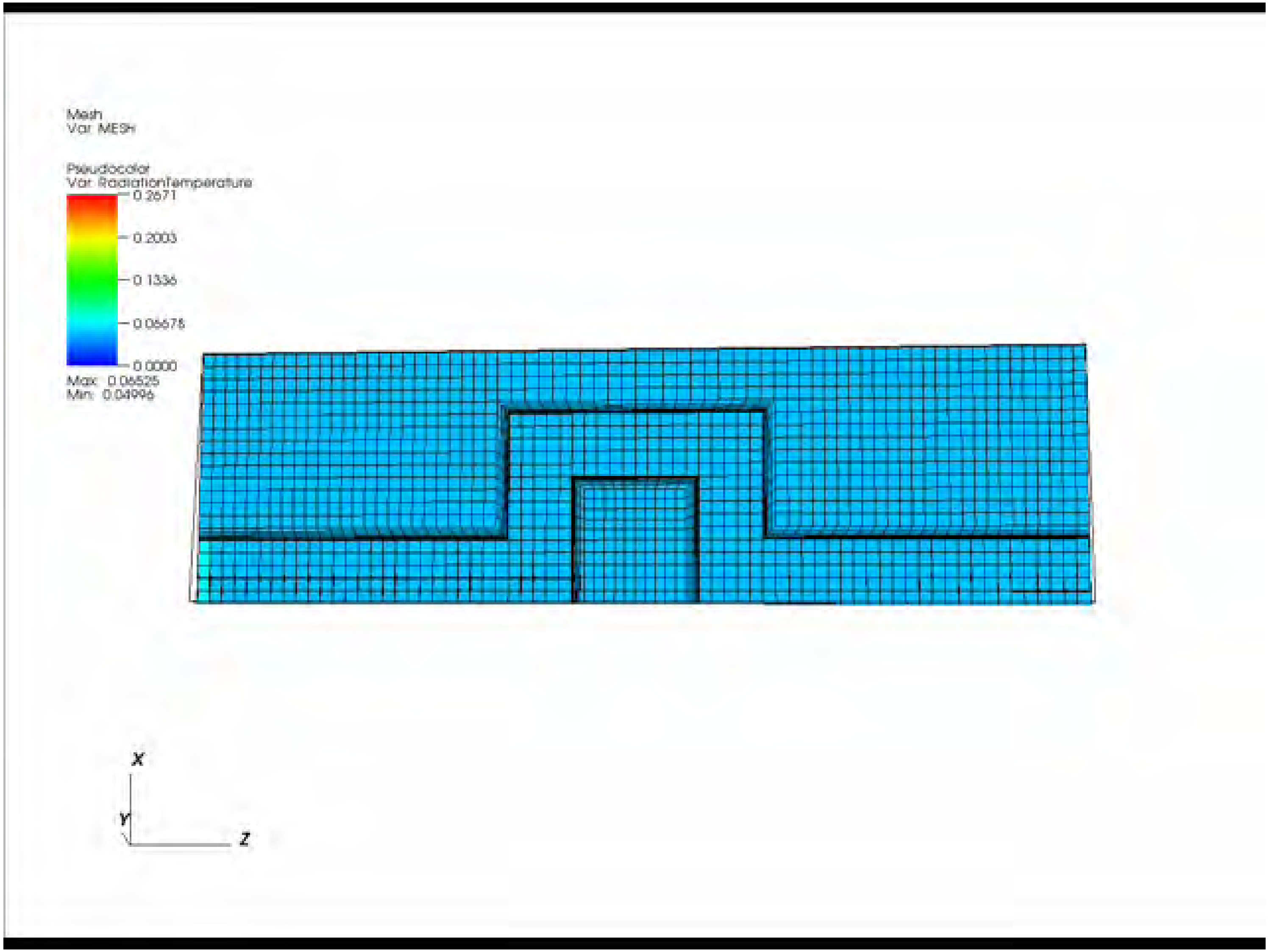
The Top Hat Problem

- The top hat simulation is a radiation diffusion problem with two material regions. One region has high density, which makes it optically thick. The other region has low density, which makes it optically thin. Red is high density, blue is low density.



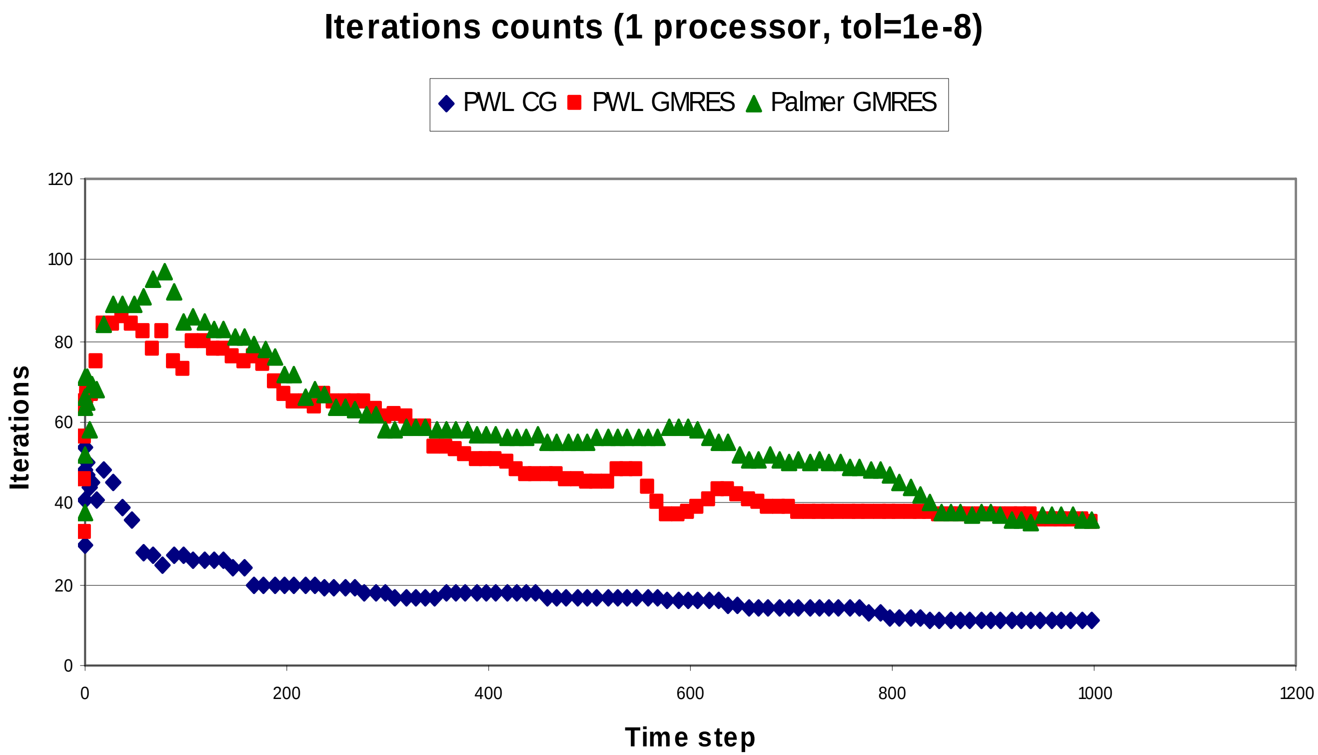
- Particles are inserted into the problem at the left boundary. The initial temperature is 0.05, and the opacity is the same for both materials.
- The simulation was run for 1000 time units.

Top Hat Simulation



Comparison of Linear Solver performance

- When Conjugate Gradient is used for PWL, it decrease the number of iterations for matrix inversion by a factor of 3 relative to Palmer’s method with GMRES. For multiple processors the relative performance of CG improves.



The PWL method retains the benefits of Palmer's method, while being symmetric.

- PWL is vertex-centered and exact for linear solutions – it is very similar to Palmer's method.

- Unlike Palmer's method, PWL is symmetric, which allows us to give it a firmer theoretical foundation. We have more confidence that PWL won't "break" on unusual problems.
  - ⇒ *We can show it is SPD*
  - ⇒ *We can prove the problem is well-posed using the Lax-Milgram Lemma*
  - ⇒ *We can derive the convergence rate of PWL*

- PWL has the potential to solve large-scale problems more efficiently than Palmer's method.

We have a few suggestions for future work.

- An extensive comparison needs to be made between cell-centered methods and vertex-centered methods. The goal of this comparison would be to determine which class of problems are suited to each type of discretization.
- Higher order piecewise basis functions need to be developed, implemented, and analyzed.
- PWL basis functions appear to be uniquely suited to adaptive mesh refinement problems, and need to be tested on these problems.

Acknowledgements

- Krell Institute and the CSGF program

The coefficients

- Palmer's method

$$f_{Palmer}\left(\theta_u,\theta_v\right)=2\left[\frac{1-\cos\left(\theta_u\right)}{\theta_u^2}\right]$$

- PWL

⇒ ***Lumped***

$$f_{LPWL}\left(\theta_u,\theta_v\right)=\left[2\left(\frac{1-\cos\left(\theta_u\right)}{\theta_u^2}\right)\right]\left[\frac{3+\cos\left(\theta_v\right)}{4}\right]$$

Unlumped

$$f_{UPWL}\left(\theta_u,\theta_v\right)=\left[2\frac{1-\cos\left(\theta_u\right)}{\theta_u^2}\right]\left[\frac{3}{1+\left[1+\cos\left(\theta_u\right)\right]\dfrac{5+3\cos(\theta_v)}{6+2\cos(\theta_v)}}\right]$$

- BLC

⇒ ***Lumped***

$$f_{LBL}\left(\theta_u,\theta_v\right)=\left[2\left(\frac{1-\cos\left(\theta_u\right)}{\theta_u^2}\right)\right]\left[\left(\frac{2+\cos\left(\theta_v\right)}{3}\right)\right]$$

Unlumped

$$f_{UBL}\left(\theta_u,\theta_v\right)=\left[2\left(\frac{1-\cos\left(\theta_u\right)}{\theta_u^2}\right)\right]\left[\left(\frac{3}{2+\cos\left(\theta_u\right)}\right)\right]$$