PhD Dissertation Proposal

Stability and Effectiveness of Multi-Frequency Grey Acceleration for DFEM S_N Radiative Transfer Calculations with Spatially Varying Opacities

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Abstract

Linear discontinuous finite element methods (LDFEM) have been widely used to solve the discrete ordinates (S_N) thermal radiative transfer (TRT) equations. While higher order discontinuous finite element methods (DFEM) have been applied to the S_N neutron transport equation, they have not been applied to the S_N TRT equations. The ultimate goal of this dissertation is to effectively solve the multi-frequency S_N TRT equations using an arbitrary order DFEM spatial discretization that explicitly accounts for the spatial variation of cross section within individual mesh cells.

Progress towards this goal has been made in several phases. First, novel self-lumping techniques were developed and applied to the S_N neutron transport equation to improve the robustness of arbitrary order DFEM radiation transport schemes. Next, the accuracy of different cross section spatial treatments for problems with spatially varying cross sections were studied for the S_N neutron transport equation. This investigation revealed previously undocumented, non-physical behavior of the most common spatial treatment used for problems with spatially varying cross sections.

To complete this project, we will extend the mono-energetic radiative transfer code we developed in MATLAB to a multi-frequency radiative transfer code in C++. Most importantly, we will use this code to examine the stability and effectiveness of the linear multi-frequency grey acceleration (LMFGA) technique in accelerating the absorption/re-emission convergence. In particular, we are interested in the possibility of using low-order LMFGA diffusion operators to accelerate higher order DFEM discretizations of the S_N TRT equations.

1. Previous Work

The linear discontinuous finite element method (LDFEM) has long been used to solve the discrete ordinates (S_N) neutron transport equation [1]. LDFEM has achieved wide spread acceptance in the neutronics community because it is accurate [2] and highly damped. Because it possesses the thick diffusion limit [3], LDFEM has also been applied to the S_N thermal radiative transfer (TRT) equations. Morel, Wareing, and Smith first considered the application of LDFEM to the S_N TRT equations in [4]. Mass matrix lumped LDFEM was shown to preserve the thick equilibrium diffusion limit [4]. This suggests that discontinuous finite element (DFEM) schemes could be used to accurately solve the TRT equations in both diffusive and transport effects dominated regions.

The DFEM weak formulation does not limit DFEM solutions of the neutron transport or TRT problems to a linear trial space [1]. However, the robust and well characterized behavior of mass matrix lumped and unlumped LDFEM has resulted in only limited interest in higher degree DFEM trial space solutions. Notable early investigations of using higher degree DFEM trial spaces for the neutron transport equation include the works of Walters [5] and Hennart and Del Valle [6, 7]. More recent investigations of higher order DFEM include those by Wang and Ragusa [8] and Warsa and Prinja [9]. To our knowledge higher degree DFEM trial spaces have not been considered for DFEM S_N TRT applications.

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For a large number of applications, particularly TRT, computations are limited to using optically thick cells in both highly diffusive and strongly absorbing regions. Optically thick cells in highly diffusive regions implies that spatial discretizations must posses the thick equilibrium diffusion limit to be viable computational tools. Optically thick, strong absorbing regions can cause LDFEM to produce negative angular flux solutions which has been well documented in [10, 11, 12]. These negativities do not affect LDFEM's order of convergence, and can be tolerated for certain applications [13], but TRT is particularly sensitive to negative angular intensities. If the angular intensity negativities are large enough, the overall solution procedure can diverge. Several methods to eliminate or inhibit negative solutions have been developed and can be categorized into one of three categories: ad-hoc fix-ups [11], strictly non-negative solution representations [12], and matrix lumping [10]. The first two methods result in nonlinear systems of equations, while matrix lumping yields linear systems of equations. By their definition, ad-hoc fix-ups and strictly non-negative solution representations generate strictly non-negative outflows in 1-D, 2-D, and 3-D geometries, regardless of cell optical thickness. Mass matrix lumping, applied to LDFEM, yields strictly positive outflows only for 1-D source-free, purely absorbing media. When combined with gradient operator lumping in multiple spatial dimensions mass matrix lumping does not eliminate, but does otherwise inhibit negative angular flux solutions [10]. To enable the solution process to progress with negative TRT solutions, modifications must be made to the Planckian, $B(T)$, derivative of the Planckian with respect to temperature, $\frac{\partial B(T)}{\partial T}$, and opacity/cross section. When $T < 0$, we define the Planckian and its derivative as follows:

$$B(T) = B(-T) \tag{1}$$

$$\frac{\partial B(T)}{\partial T} = -\frac{\partial B(-T)}{\partial T}\,. \tag{2}$$

Additionally we require that opacity remain finite and positive fort all material temperatures. For example, we modify the canonical $\sigma_a = T^{-3}$ as:

$$\sigma_a(T) = \min\left(\sigma_{max}\,,\ |T|^{-3}\right)\,. \tag{3}$$

The radiation transport community has often considered matrix lumping to be the process of making a given matrix diagonal by collapsing all off diagonal entries to the main diagonal [10]. Alternatively, a diagonal mass matrix can be obtained through quadrature-based methods. So called self-lumping (SL) methods, first introduced in [14] and [15] for parabolic problems, obtain a diagonal mass matrix by numerically integrating only at the finite element interpolation points. Restricting ourselves to equally-spaced interpolation points, self-lumping numerical integration with the greatest degree of accuracy is achieved through the use of closed Newton-Cotes formulae [16]. However, Newton-Cotes formulas with a large number of integration points are known to be oscillatory and are of relatively low-order accuracy. We need not limit ourselves to equally-spaced Lagrange points to define our DFEM basis functions; the choice of Lagrange interpolatory point does not change the DFEM weight space. By considering different DFEM interpolatory points, for example Gauss-Legendre quadrature [16] or Lobatto-Gauss-Legendre quadrature [16], it is possible to generate new classes of DFEM S_N transport schemes that are arbitrarily accurate and robust.

Many problems of interest to the nuclear science and engineering community have cross sections that are not accurately described as piecewise constants in space. Cross sections can vary in space because they are functions of spatially varying quantities such as temperature, density, fuel burn-up history, etc. [17]. Examples of simulations with space-dependent cross sections include nuclear reactor depletion calculations and TRT calculations for high energy density physics experiments. The majority of neutron transport literature has only considered the case of cell-wise constant cross sections, see [10], [18], and [19]. Work by Kavenoky and Lautard [20] and more recently Santandrea and Bellier [21] are notable exceptions. In [20], continuous cubic finite element diffusion calculations that assume a linearly varying spatial cross section within each mesh cell were compared to results obtained using the same spatial discretization, but with cell-wise constant cross sections in each cell. Similarly, Santandrea and Bellier compared the results of a linear characteristic scheme that assumes a linearly varying cross section in each spatial cell to a linear characteristic scheme that assumes cell-wise constant cross sections [21]. The thermal radiative transfer community has explicitly accounted for the spatial variation of cross sections more frequently than the neutronics community. First proposed by Adams in [22] and demonstrated with computational results in [23], "simple" corner balance (SCB) spatial discretization methods were the first to explicitly account for the spatial variation of cross section within individual cells. The practice of accounting for the spatial variation of cross section is now common place in TRT simulations. Cross-section spatial variation within each cell has typically been accounted for in DFEM TRT and

radiation diffusion simulations via vertex-based quadrature evaluation, as in [24] and [25]. Since higher order DFEM has not been widely applied to S_N radiative transfer, higher order spatial treatments of spatially varying cross sections have not been investigated.

The multigroup thermal radiation diffusion and radiative transfer equations are generally solved iteratively. The simplest iteration scheme is a fixed point scheme, where the thermal absorption/re-emission source is lagged, and the radiation intensity is updated assuming the lagged re-emission source [26]. As shown by Morel, et. al, in [26], this iteration process can converge arbitrarily slowly as the time step size grows infinitely large or the material heat capacity goes to zero. However, the Fourier analysis of Morel also showed that the thermal re-emission iteration error was largest for the slowly varying Fourier modes, similar to the behavior of source iteration in neutron transport. This suggested that a diffusion like synthetic acceleration step would be effective in improving thermal re-emission convergence. Indeed, it was shown in [26] that this linear multi-frequency grey acceleration (LMFGA) greatly improved the convergence of the thermal re-emission source for radiation diffusion. LMFGA has since become an integral part of all radiative transfer solution techniques, and was applied to LDFEM S_N TRT in [4], and was used as a Krylov preconditioner for solving the radiative diffusion equations in [25].

Gelbard and Hageman first showed in [27] that diffusion synthetic acceleration (DSA) could be used to accelerate the convergence of source iteration in neutron transport since the diffusion operator effectively attenuates the slowly varying error modes that hinder the convergence of source iteration. To be unconditionally effective, Larsen showed that DSA needed to be derived in a method consistent with the spatial and angular discretization of the transport equation [28]. Adams and Martin first showed that partially consistent diffusion discretizations could be used to effectively accelerate DFEM spatial discretizations of the neutron transport equation [29]. Though shown to be unconditionally stable for certain geometries the M4S DSA proposed in [29] has been shown to be unstable for unstructured multi-dimensional geometries [30]. To allow more general applicability, we wish to consider a more advanced DSA discretization. Alternative DSA discretizations that have been applied successfully to unstructured multi-dimensional geometries include: the partially consistent WLA DSA proposed in [31], the fully consistent DSA (FCDSA) proposed in [30], and the partially consistent MIP DSA proposed in [32]. WLA DSA produces a symmetric positive definite (SPD) diffusion matrix and is unconditionally stable, but the spectral radius of the WLA DSA scheme increases on distorted mesh cells and for optically thick cells with scattering ratios very close to unity [31, 30]. While the FCDSA scheme remains effective in optically thick cells, it creates a diffusion operator that is very difficult and costly to invert. The MIP DSA discretization [32] of Wang and Ragusa generates a SPD diffusion operator, remains effective for all cell optical thicknesses, has been successfully applied to high order DFEM S_N transport, and can be used with adaptive mesh refinement. Further, it was shown in [33] that the MIP DSA diffusion operator can be inverted very quickly using advanced preconditioners such as algebraic multi-grid.

To increase the computational efficiency of DSA and LMFGA, one would invert as small of a diffusion operator as possible. One possible method to reduce the size of diffusion operator is to use a low order DFEM discretization to accelerate a higher order DFEM discretization of the transport operator. The low order DSA error estimate would then be projected onto the higher order transport iterate. Though using a low order diffusion operator to accelerate a higher order DFEM transport discretization is not guaranteed to be stable when used as a fixed point acceleration technique, the use of Krylov methods could result in a stable, efficient preconditioning method. Using DSA re-cast as a preconditioner for Krylov methods has allowed for the solution of problems where DSA used in a fixed point iteration scheme fails. For instance, in [19], DSA used as a fixed point iteration scheme method failed for problems with large material discontinuities, but when recast as a Krylov preconditioner, problems with large material discontinuities could be efficiently solved. Thus, it may be possible to use low order DFEM diffusion discretization preconditioners in conjunction with Krylov methods to efficiently solve high order DFEM transport discretizations.

2. Current Work

We now briefly go over work that has already been completed for the dissertation project. Two major elements of this dissertation have already been developed and are in various stages of publication.

The first, quadrature-based lumping techniques for arbitrary order DFEM radiation transport, was first presented in [34], and expanded upon in [35]. Interested readers are directed to [34] and [35] for detailed derivations and results. In [34] and [35] we demonstrated the following for problems with cell-wise constant cross section:

1. traditional mass matrix lumping [10] DFEM S_N radiation transport schemes are at most second or third order accurate, for odd and even degree trial spaces, respectively,
2. self-lumping schemes that use equally-spaced DFEM interpolation points are at most second or third order accurate, for odd and even degree trials spaces, respectively,
3. self-lumping schemes that used Lobatto or Gauss quadrature as the DFEM interpolation points can be made arbitrarily accurate
4. self-lumping schemes using Gauss quadrature are more accurate than self-lumping schemes using Lobatto quadrature as the DFEM interpolation points, for equivalent degree polynomial trial spaces,
5. self-lumping schemes using Gauss quadrature yield strictly positive outflow for even degree polynomial spaces, and
6. self-lumping schemes using Lobatto quadrature yield strictly positive outflow for odd degree polynomial trial spaces.

The positivity results in [34] and [35] assume cell-wise constant cross sections.

Treatments for spatially varying cross section have been considered in [36]. Key results from [36] include:

1. linear self-lumping schemes using Lobatto interpolation points are the only schemes that can produce strictly positive angular flux outflow in source-free pure absorber while explicitly accounting for the spatial variation of cross sections within a cell,
2. higher order DFEM schemes that explicitly account for the spatial variation of cross section cannot be guaranteed to yield strictly positive angular flux outflows,
3. exact integration of the true spatial variation of cross section within each cell is unnecessary to create arbitrarily accurate DFEM schemes,
4. self-lumping schemes using equally-spaced DFEM interpolation points are limited to at most second or third order accuracy for odd and even degree polynomial degree trial spaces, respectively,
5. self-lumping schemes that use either Gauss or Lobatto quadrature and explicitly account for the spatial variation of cross section within each cell can be made arbitrarily accurate
6. DFEM schemes which impose cell-wise constant cross sections for problems where cross section is not cell-wise constant are at most second order accurate, regardless of angular flux trial space degree, and
7. imposing cell-wise constant cross sections leads to a highly non-physical, non-monotonic interaction rate solution.

Though not yet published, we have also applied our self-lumping numerical quadrature and explicit treatment of cross-section spatial variation to the grey radiative transfer equations. We omit the actual equations now for brevity, but discuss our process for deriving the equations now:

1. start with the spatially analytic grey radiative transfer equations and linearize the Planck function about some temperature iterate, T^*
2. discretize the radiation and material energy equations assuming arbitrary order DFEM,
3. manipulate the material energy DFEM moments equations to solve for the vector of unknown temperatures, T_k (k-th stage temperature of the SDIRK scheme), and
4. eliminate the explicit temperature dependence in the radiation moment equations using the manipulated material energy moment equations,

yielding a set of equations for the angular intensity that is similar to the DFEM neutron transport equations with fission. We have tested our methods using a Marshak wave test problem adapted from a radiation diffusion problem given by Ober and Shadid [24]. The problem consists of an initially cold material with a beam of radiation impinging on the left hand side of the slab and vacuum boundary conditions on the right side of the slab. Opacity is assumed to vary as $1/T^3$, there no conduction, and no photon scattering.

In the results that follow, we use an S_2 Gauss angular quadrature, and implicit Euler time differencing. Figure 1 gives an example of the radiation and temperature profiles at time $t = 1.0$. To obtain Fig. 1, we used 100 mesh cells,

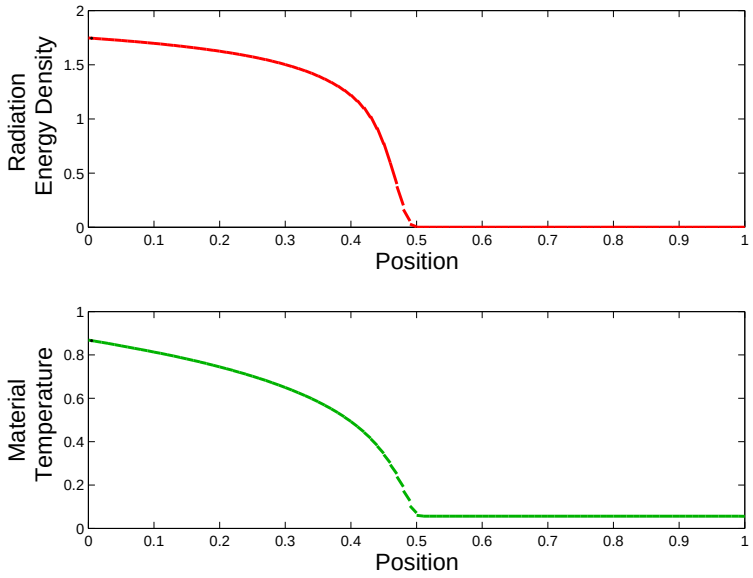


Figure 1: Example solution of the Marshak wave problem.

a linear trial space, and self-lumping Lobatto quadrature that explicitly accounted for the variation of cross section in each cell.

We now demonstrate the effects of assuming a constant opacity in each cell. In Fig. 2, we use the same computational mesh, trial space, and lump the mass matrix, but assume a cell-wise constant opacity, equal to the cell average opacity. Obviously, the large, persistent non-monotonic discontinuities in the temperature profile are non-physical.

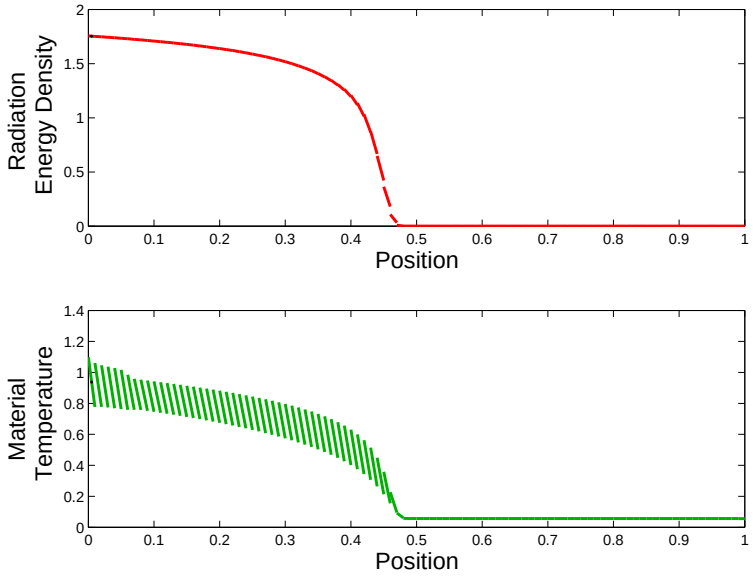


Figure 2: Lumped linear discontinuous solution assuming cell-wise constant opacity.

However, this “blading” phenomena has gone unnoticed due to historical choices in data presentation. If instead of presenting the true, discontinuous approximation of the temperature profile, as in Fig. 2, we plot cell average quantities at cell centers, the blading effect cannot be seen, as shown in Fig. 3.

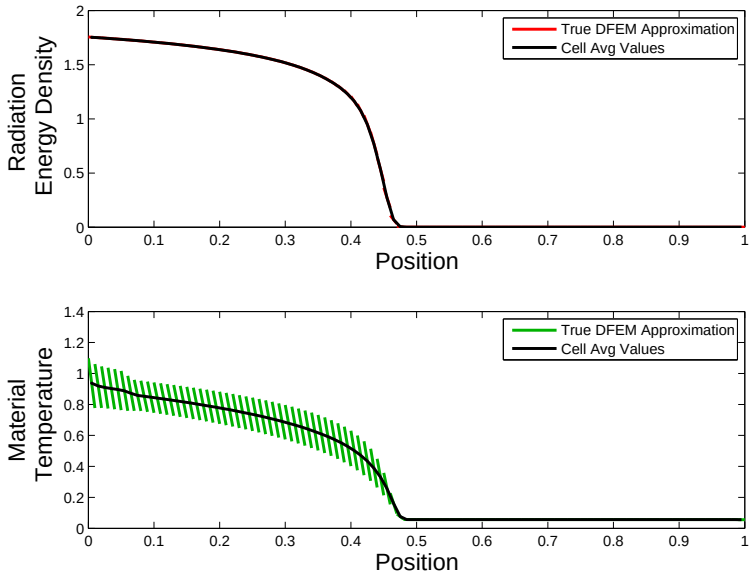


Figure 3: Constant opacity, lumped linear discontinuous DFEM approximation solution. Comparison of cell averages interpolated at cell centers versus true discontinuous solution approximation.

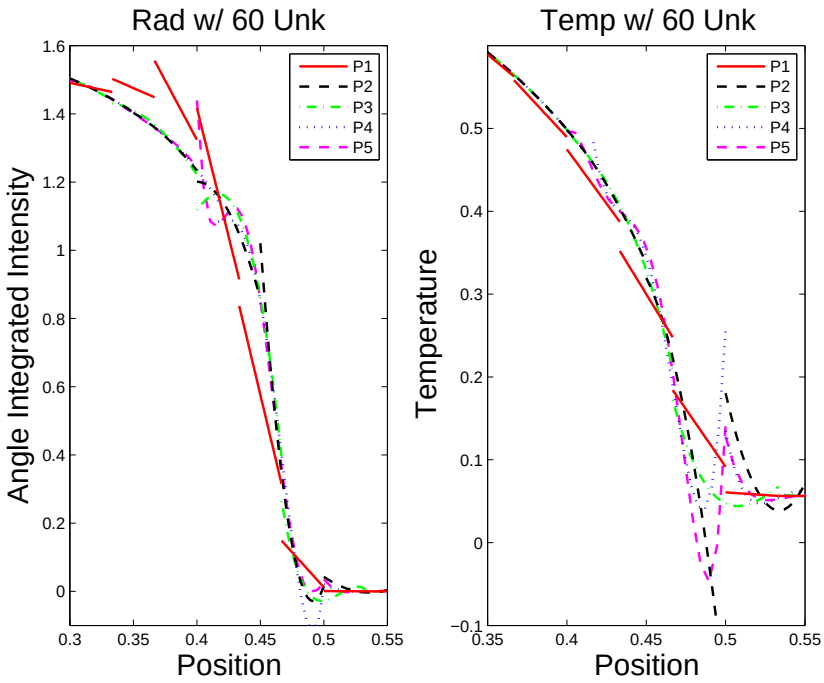
The effects of using higher degree polynomial trial spaces for radiative transfer have also been explored using the grey Marshak wave test problem. As an example, consider Fig. 4 that shows numerical results for DFEM schemes with different trial space degrees, but using the same total number of unknowns in each scheme.

3. Future Work

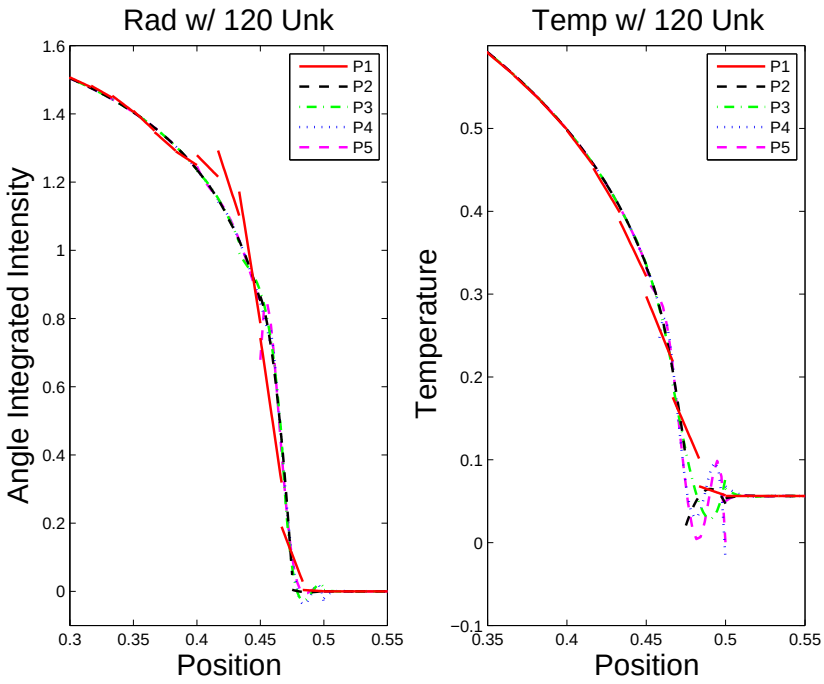
To complete the project, we will use C++ to write a multi-frequency radiative transfer code. The code will incorporate all of the work we have developed and implemented in the grey radiative transfer code: SDIRK time integration, arbitrary order DFEM, and self-lumping quadrature that accounts for the spatial variation of cross section in each cell using equally-spaced, Lobatto, or Gauss quadrature points. We will use preconditioned Krylov methods, using both sweep and DSA [32] preconditioners, to iteratively solve the within group scattering problem. Likewise, we will iterate on the absorption rate density using Krylov methods with LMFGA as in [25]. The effectiveness and efficiency of a low order diffusion operator used to accelerate high order DFEM discretizations will be examined.

The Trilinos code package [37] will be used to invert the diffusion operator. Though the 1-D diffusion operator is block diagonal and can be directly inverted, using Trilinos offers direct solvers, iterative solvers, and the ability to use powerful preconditioners such as algebraic multi-grid. Additionally, Trilinos has a GMRES Krylov solver that can be used to solve the scattering and absorption/re-emission iterations efficiently.

Given the complexity of thermal radiative transfer, benchmark solutions are difficult to find. The most commonly used benchmarks come from the work of Su and Olson [38, 39]. While the Su and Olson benchmarks offer analytic solutions that can be used for code verification, they are not ideal for comparing the relative accuracy or convergence rates of different numerical schemes. To be used as convergence comparison tools requires that the analytic integrals in [38] and [39] be numerically evaluated to a very tight tolerance, a non-trivial task. The Su and Olson benchmark solutions are given in terms of two-dimensional improper integrals with an integrand that is a composite function of a trigonometric function of a slowly decaying function. Even with the use of advanced, recursive numerical techniques [40], the evaluation of the Su and Olson integrals for even a single state point, that is the temperature or radiation energy density at one point in space, at one instance in time is a computationally intense task. Thus, using analytical benchmarks to measure and compare the accuracy of our different numerical schemes is not practical.



(a) 60 Unknowns



(b) 120 Unknowns

Figure 4: Comparison of numerical solutions at the wave front using the same total number of unknowns and different DFEM trial space degrees.

An alternative to using analytical solutions as a benchmarking tool is to use code-to-code comparisons. One can use published results, for instance the results in [4], but these comparisons are again of limited utility in determining order of convergence/relative accuracy of numerical methods. The difficulty in using published results is that the results are not necessarily reproduced with their full accuracy, may have been found using limited tolerances, used non-comparable solution methodologies, or give only a few data points. Like comparing against analytical results, comparison of our schemes to published numerical results of other schemes offers opportunities for validation, but is most likely insufficient for our purposes.

The most appropriate tool for quantifying our new methods' performance will be the Method of Manufactured Solutions (MMS) [41]. By first defining a desired solution, then solving the analytic TRT equations assuming the manufactured solution, we generate an inhomogeneous driving source. Using this manufactured source, we can then study the convergence of our methods to the manufactured solution.

Judging the effectiveness of our low order LMFGA acceleration technique/preconditioner is not as difficult as measuring the convergence and accuracy of our spatial discretization schemes. To measure the effectiveness, we need data that is readily available: CPU timing data and iteration counts. Using expert judgment, we will then choose different problems that have historically challenged iterative schemes. We can then compare timing data and iteration counts to determine the efficiency and effectiveness of equal order DFEM DSA acceleration schemes to the respective values obtained using LDFEM diffusion operators.

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