HIGHER ORDER DISCONTINUOUS FINITE ELEMENT METHODS FOR DISCRETE ORDINATES THERMAL RADIATIVE TRANSFER

A Dissertation

by

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DOCTOR OF PHILOSOPHY

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ABSTRACT

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DEDICATION

To my wife, Kelli, for traveling with me along all the unforeseen curves of life. To my mom and dad, for providing my foundation and inspiration.

ACKNOWLEDGEMENTS

I am thankful for the years of teaching and guidance provided by my co-chairs Dr. Jean Ragusa and Dr. Jim Morel; you convinced me long ago that a career in research was worth the extra challenges, costs, and years of work. I would also like to thank Dr. Marvin Adams for initially guiding me to the Computational Methods Group at Texas A&M and for encouraging me to consider Lawrence Livermore National Laboratory for post-graduation employment. Additionally, I thank I would like to thank Dr. Jean-Luc Guermond for your time and feedback on this dissertation and the master's thesis that preceeded it. Finally, I wish to thank the Department of Energy Computational Science Graduate Fellowship (administered by the Krell institute under grant number DE-FG02-97ER25308) for financial support during this work.

NOMENCLATURE

B/CS	Bryan/College Station
HSUS	Humane Society of the United States
P	Pressure
T	Time
TVA	Tennessee Valley Authority
TxDOT	Texas Department of Transportation

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1. INTRODUCTION

This dissertation is dedicated to the solution of thermal radiative transfer (TRT) equations. The TRT equations:

$$\frac{1}{c}\frac{dI}{dt} + \vec{\Omega}\cdot\vec{\nabla} I + \sigma_t I = \int_0^\infty \int_{4\pi} \sigma_s(\vec{\Omega}' \rightarrow \vec{\Omega}, E' \rightarrow E) I, d\vec{\Omega}' dE' + \sigma_a B \quad (1.1a)$$

$$C_v \frac{dT}{dt} = \int_0^\infty \sigma_a \left(\phi - 4\pi B\right) dE\,, \quad (1.1b)$$

are a nonlinear system of equations that describe the exchange of energy between a photon radiation field and a non-moving material. The radiation intensity, I, is a seven dimensional field dependent upon spatial location, $\vec{x}$; photon energy, E; photon direction of travel, $\vec{\Omega}$; and time t. c is the speed of light. Material opacities for all interactions, σ_t; absorption, σ_a; and scattering, σ_s are functions of photon energy and material temperature, T. Material heat capacity, C_v, is also a function of material temperature. The angle integrated radiation intensity is an integral over all photon directions of the the photon intensity and is a function of space and photon energy. Finally, the Planck function, B, is a function of photon energy and material temperature. While materials at all temperatures emit photon radiation, the radiation emission is proportional to T^4. Thus, solution of the radiative transfer equations is most important in situations where materials are very hot. Solving the thermal radiative transfer equations is an important component of the simulation of different scientific and engineering problems including astrophysics supernova explosions and high energy density laboratory physics experiments like those conducted at the National Ignition Facility.

1.1 Simplifications of the Thermal Radiative Transfer Equations

In this dissertation, we we make a number of simplifying assumptions to make solution of Eqs. (1.1) more tractable. First, we limit our focus to 1-D Cartesian (slab) geometry. The assumption of slab geometry is not required, but slab geometry radiation transport simulations require significantly less computational time. Further, any methods that have a possibility of being viable for radiation transport in multiple spatial dimensions must also work well in slab geometry.

Second, we approximate the continuous angle dependence of the intensity using the discrete ordinates (S_N) method. The S_N method approximates the true definition of the angle integrated intensity,

$$\phi(\vec{x}, E, t) = \int_{4\pi} I(\vec{x}, \vec{\Omega}, E, t) d\vec{\Omega}\,,$$

using quadrature integration,

$$\phi(\vec{x}, E, t) \approx \sum_{d=1}^{N_{dir}} w_d I(\vec{x}, \vec{\Omega}_d, E, t)\,. \tag{1.2}$$

In Eq. (1.2), $\{w_d, \vec{\Omega}_d\}_{d=1,\dots N_{dir}}$ is the set of N_{dir} quadrature weights w_d and discrete directions, $\vec{\Omega}_d$ and corresponding intensities I_d.

Finally, we treat the photon energy dependence using the multi-frequency method. The multi-frequency method approximates photon energy dependence by discretizing the continuous photon energy dependence with G discrete groups such that:

$$\int_0^\infty I(\vec{x}, \vec{\Omega}, t, E) dE = \sum_{g=1}^{G} I_g\,, \tag{1.3}$$

where

$$I(\vec{x},\vec{\Omega},t)_g = \int_{E_{g+1/2}}^{E_{g-1/2}} I(\vec{x},\vec{\Omega},t,E)dE\,, \tag{1.4}$$

$E_{g+1/2}$ is the lower photon energy bound of group g, $E_{g-1/2}$ is the upper photon energy bound of group g, and we have maintained the traditional neutron transport number of higher energy particles belonging to lower number energy groups.

1.2 Spatial and Temporal Discretization

To complete a description of the approach we will take to solve Eqs. (1.1), we now describe how we will discretize the spatial and temporal variables.

1.2.1 Time Integration

The appearance of the speed of light in Eq. (1.1) results in the TRT equations being very stiff. To solve the such a stiff system of equations would require either an impractically small time step, or the use of implicit methods. We elect to use Diagonally Implicit Runge-Kutta (DIRK) methods to advance our TRT solution in time. The simplest of DIRK scheme is the first order implicit Euler scheme, but more advanced DIRK higher order methods in time [4].

1.2.2 Spatial Discretization with Discontinuous Finite Elements

The linear discontinuous finite element method (LDFEM) has long been used to solve the discrete ordinates neutron transport equation [13]. LDFEM has achieved wide spread acceptance in the neutron transport community because it is accurate [8] and highly damped. Because it possesses the thick diffusion limit [7], LDFEM has also been applied to the S_N TRT equations. Morel, Wareing, and Smith first considered the application of LDFEM to the S_N TRT equations in [10]. Mass matrix lumped LDFEM was shown to preserve the thick equilibrium diffusion limit [10]. This suggests that discontinuous finite element (DFEM) schemes can 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 [13]. However, the robust and well characterized behavior of mass matrix lumped and unlumped LDFEM, along with historical limits on computational resources, 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 [14] and Hennart and Del Valle [5, 6]. More recent investigations of higher order DFEM include those by Wang and Ragusa [15] and Warsa and Prinja [16]. To our knowledge higher degree DFEM trial spaces have not been considered for DFEM S_N TRT applications.

Thermal radiative transfer interaction opacities can be rapidly varying functions of temperature. For example, consider Marshak wave problems and the canonical T^{-3} dependence [12] of absorption opacity. Opacity variations of several orders of magnitude near the heated/cold material interface are easily possible. Historically, the neutron transport and thermal radiative transfer communities assumed interaction cross section and opacities, respectively, were cell-wise constant [2, 9, 10]. Adams first described [1] and then presented computational results [3] for a "simple" corner balance (SCB) spatial discretization method that explicitly accounted for the spatial variation of opacity within individual spatial cells. The SCB scheme (which can be shown to be related to a LDFEM for certain geometries) accounts for opacity spatial variation within each cell via vertex-based quadrature evaluation. Similar strategies have been adapted to LDFEM radiative diffusion [12] and LDFEM TRT [11] calculations. For accurate TRT solutions, use of higher order DFEM will requires the development of corresponding higher order strategies for treating the within cell spatial variation of opacities.

1.3 A Natural Progression to Accurate DFEM Radiative Transfer Solutions

In Chapter 2

2. LITERATURE REVIEW: THE IMPORTANCE OF RESEARCH PART TWO- THIS IS DESIGNED TO TEST LONG TITLES IN THE TOC

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2.1 New Section

2.1.1 Subsection

2.1.2 Subsection

2.1.2.1 This is a subsubsection

2.2 Another Section

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Table 2.1: This is a table template - This is an example of a long table title. Table titles need to be single-spaced within and double spaced between in the list of tables.

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Guarantee [years]	1	2	-	3	1
Rating	89%	84%	51%		45%
Recommended	yes	yes	no	no	no

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Recommended	yes	yes	no	no	no

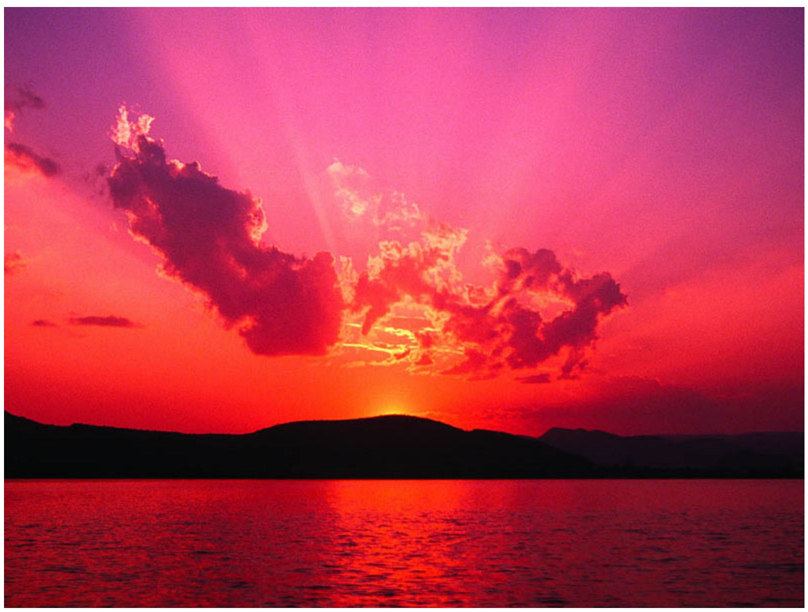

Figure 2.2: Sunset figure

3. LAST CHAPTER: THE IMPORTANCE OF RESEARCH

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3.1 New Section

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Rating	89%	84%	51%		45%
Recommended	yes	yes	no	no	no

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APPENDIX A

FIRST APPENDIX

Text for the Appendix follows.

Figure A.1: TAMU figure

APPENDIX B

SECOND APPENDIX WITH A LONGER TITLE - MUCH LONGER IN FACT

Text for the Appendix follows.

B.1 Appendix Section

Figure B.1: TAMU figure