

A HIGH-ORDER LOW-ORDER ALGORITHM WITH
EXPONENTIALLY-CONVERGENT MONTE CARLO FOR THERMAL
RADIATIVE TRANSFER PROBLEMS

A Dissertation

by

SIMON RAY BOLDING

Submitted to the Office of Graduate and Professional Studies of
Texas A&M University
in partial fulfillment of the requirements for the degree of

DOCTOR OF PHILOSOPHY

Chair of Committee,	Jim Morel
Committee Members,	Ryan McClarren
	Jean Ragusa
	Jean-Luc Guermond
Head of Department,	Yassin Hassan

December 2016

Major Subject: Nuclear Engineering

Copyright 2016 Simon Ray Bolding

ABSTRACT

We have implemented a new high-order low-order (HOLO) algorithm for solving thermal radiative transfer problems. The low-order (LO) system is based on spatial and angular moments of the transport equation and a linear-discontinuous finite-element spatial representation, producing equations similar to the standard S_2 equations. The LO solver is fully implicit in time and efficiently resolves the non-linear temperature dependence at each time step. The HO solver utilizes exponentially-convergent Monte Carlo (ECMC) to give a globally accurate solution for the angular intensity to a fixed-source, pure absorber transport problem. This global solution is used to compute consistency terms, which require the HO and LO solutions to converge towards the same solution. The use of ECMC allows for the efficient reduction of statistical noise in the MC solution, reducing inaccuracies introduced through the LO consistency terms. We compare results with an implicit Monte Carlo (IMC) code for one-dimensional, gray test problems and demonstrate the efficiency of ECMC over standard Monte Carlo in this HOLO algorithm.

DEDICATION

This is an optional page. Lorem ipsum dolor sit amet, consectetur adipiscing elit. Integer lectus quam, condimentum quis bibendum eu, sollicitudin eget lacus. Praesent non sodales odio. Class aptent taciti sociosqu ad litora torquent per conubia nostra, per inceptos himenaeos. Nulla ac luctus sapien. Morbi cursus sapien eget lorem fermentum hendrerit. Nam ac erat dui, in cursus velit. Vivamus hendrerit porttitor nisi, ut porttitor lorem volutpat eget. In ligula ligula, euismod ut condimentum sit amet, pulvinar sit amet diam. Pellentesque interdum, ipsum ullamcorper consequat dignissim, sem arcu egestas mauris, vitae interdum sem tortor ut ante. Nunc blandit laoreet nisi, non rutrum lorem hendrerit quis. Cras nunc diam, convallis et feugiat at, auctor id libero. Nunc facilisis massa eu eros imperdiet vestibulum. Vestibulum ante ipsum primis in faucibus orci luctus et ultrices posuere cubilia Curae; Donec non velit vitae tortor blandit semper.

Etiam vitae dolor nulla. Ut eros odio, rhoncus eget placerat vitae, elementum ac ante. Proin vitae odio eu nisl pharetra mattis. Pellentesque habitant morbi tristique senectus et netus et malesuada fames ac turpis egestas. Phasellus fermentum lacus consectetur neque consequat ullamcorper. Cras blandit urna non dui consequat molestie. Curabitur viverra nibh at nisi semper faucibus. Nam egestas mauris a enim dignissim nec consectetur tortor rutrum. Mauris at nisi in est luctus congue ut mattis est. Ut pretium, mi quis elementum cursus, ante eros suscipit ligula, ut porttitor elit leo sed turpis. Nam sed dui ligula.

ACKNOWLEDGEMENTS

Lorem ipsum dolor sit amet, consectetur adipiscing elit. Integer lectus quam, condimentum quis bibendum eu, sollicitudin eget lacus. Praesent non sodales odio. Class aptent taciti sociosqu ad litora torquent per conubia nostra, per inceptos himenaeos. Nulla ac luctus sapien. Morbi cursus sapien eget lorem fermentum hendrerit. Nam ac erat dui, in cursus velit. Vivamus hendrerit porttitor nisi, ut porttitor lorem volutpat eget. In ligula ligula, euismod ut condimentum sit amet, pulvinar sit amet diam. Pellentesque interdum, ipsum ullamcorper consequat dignissim, sem arcu egestas mauris, vitae interdum sem tortor ut ante. Nunc blandit laoreet nisi, non rutrum lorem hendrerit quis. Cras nunc diam, convallis et feugiat at, auctor id libero. Nunc facilisis massa eu eros imperdiet vestibulum. Vestibulum ante ipsum primis in faucibus orci luctus et ultrices posuere cubilia Curae; Donec non velit vitae tortor blandit semper.

Etiam vitae dolor nulla. Ut eros odio, rhoncus eget placerat vitae, elementum ac ante. Proin vitae odio eu nisl pharetra mattis. Pellentesque habitant morbi tristique senectus et netus et malesuada fames ac turpis egestas. Phasellus fermentum lacus consectetur neque consequat ullamcorper. Cras blandit urna non dui consequat molestie. Curabitur viverra nibh at nisi semper faucibus. Nam egestas mauris a enim dignissim nec consectetur tortor rutrum. Mauris at nisi in est luctus congue ut mattis est. Ut pretium, mi quis elementum cursus, ante eros suscipit ligula, ut porttitor elit leo sed turpis. Nam sed dui ligula.

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

This page is optional.

TABLE OF CONTENTS

	Page
ABSTRACT	ii
DEDICATION	iii
ACKNOWLEDGEMENTS	iv
NOMENCLATURE	v
TABLE OF CONTENTS	vi
LIST OF FIGURES	vii
LIST OF TABLES	viii
0.1 Preservation of the Discrete Maximum Principle	ix
REFERENCES	xiv
APPENDIX A FIRST APPENDIX	xiv
APPENDIX B SECOND APPENDIX WITH A LONGER TITLE - MUCH LONGER IN FACT	xv
B.1 Appendix Section	xv

LIST OF FIGURES

FIGURE		Page
1	Simulation of MP violation problem with IMC method and $\Delta t = 0.001$ sh.	xi
2	Simulation of MP violation problem with IMC method for various time step sizes.	xi
3	Simulation of MP violation problem with HOLO-ECMC method for various time step sizes.	xii
A.1	TAMU figure	xiv
B.1	TAMU figure	xv

LIST OF TABLES

TABLE		Page
1	Problem specifications for maximum principle violation. Absorption cross section has form $\sigma_a = \sigma_{a,0}/T^3$	xii
2	Comparison of LO Newton iterations for different time step sizes and MP problem. For $\Delta t = 0.1$, damping has $\zeta = 1$. For all other cases $\zeta = 0.5$	xiii

0.1 Preservation of the Discrete Maximum Principle

An important property for a discretization of the TRT equations is preservation of the discrete maximum principle (MP). The maximum principle states that the material temperature and mean intensity in the interior of the domain should be bounded by the solution at the boundaries of the domain, in the absence of interior energy sources [?, ?]. The analytic solution to the TRT equations satisfies a maximum principle [?], so we desire numerical approximations that preserve the MP in a discrete sense, for each time step. For IMC simulations, violation of the maximum principle results in the material temperature being artificially higher than the boundary conditions and sources should physically allow. As discussed in Sec. ??, IMC can violate the MP due to the approximate linearization of the emission source in the time discretization; it is not truly implicit in time. We expect our method, with a fully implicit time discretization, to preserve the MP with sufficient convergence of the nonlinear emission source [?].

To numerically demonstrate that our method preserves the MP, we have simulated problems similar to those in [?]. We modify the Marshak wave problem in Sec. ??, by decreasing c_v and increasing σ_a , to produce a problem which results in MP violations for IMC at various fixed time step sizes. The spatial and temporal discretization determine the occurrence of MP violations for IMC. In particular, if time steps are too large or spatial mesh cells are too small, IMC will demonstrate MP violations [?]. Here, we have kept the spatial mesh size fixed and increased time step to make MP violations occur. The material specifications for the problem are given in Table 1. The domain width is 2.0 cm with $N_c = 150$ uniform spatial mesh cells. The radiation and material energies are initially in equilibrium at 0.01 keV, before an isotropic boundary source of 1 keV is applied at the left boundary at $t = 0$. The simulation

is ran until $t = 0.1$ sh.

The material and radiation temperature are plotted for an IMC simulation with $\Delta t = 0.025$ sh in Figure 1. Figure 2 depicts the material temperature for various time step sizes and a fixed mesh size of 150 equally spaced cells. All IMC simulations used 100,000 histories per time step. As demonstrated in Fig. 1, the material temperature exceeds the specified boundary temperature and is artificially hotter than the radiation temperature. This artificial “temperature spike” also leads to a slower propagation of the wave [?]. As shown in Fig. 2, as larger timestep sizes are taken the nonphysical results worsen. It is noted that although the final solution for $\Delta t = 0.0001$ sh obeys the MP, during the first few time steps the temperature spikes are present.

The simulations are repeated with the same specifications for the HOLO method. All HOLO simulations used a fixed mesh of 8μ cells by $150 x$ cells, 3 batches per time step, and 6,000 histories per batch. As seen in Figure 3, the TRT solution does not violate the maximum principle. For these simulations, it was necessary to use a damped Newton’s method to converge the solutions. A damping factor of 0.5 was used for all these simulations, and found to stably converge.

Table 2 demonstrates the LO Newton iteration counts for the HOLO method. For reference, the solution at $\Delta t = 0.00001$ sh requires no damping. Clearly damping increases the number of iteration counts per step as the Newton solve is taking more conservative steps, but the overall increase is not dramatic.

NO FIXUP APPLIED, NEWTON CONVERGENCE OF 10e-06. MODIFIED MARSHAK WAVE PROBLEM.

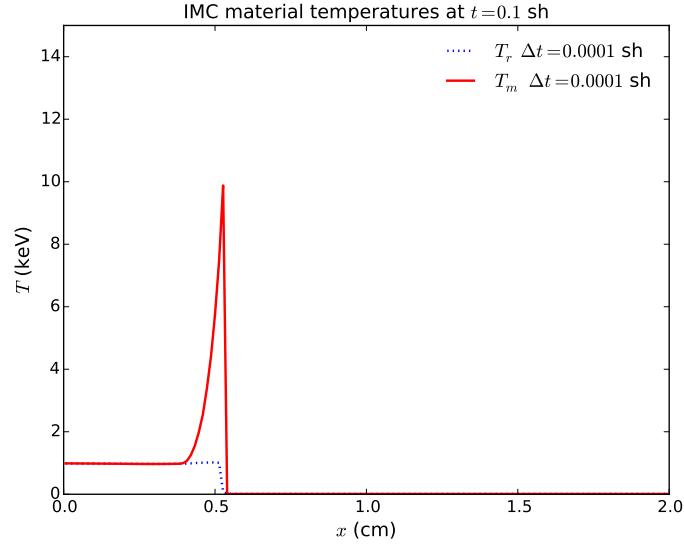


Figure 1: Simulation of MP violation problem with IMC method and $\Delta t = 0.001$ sh.

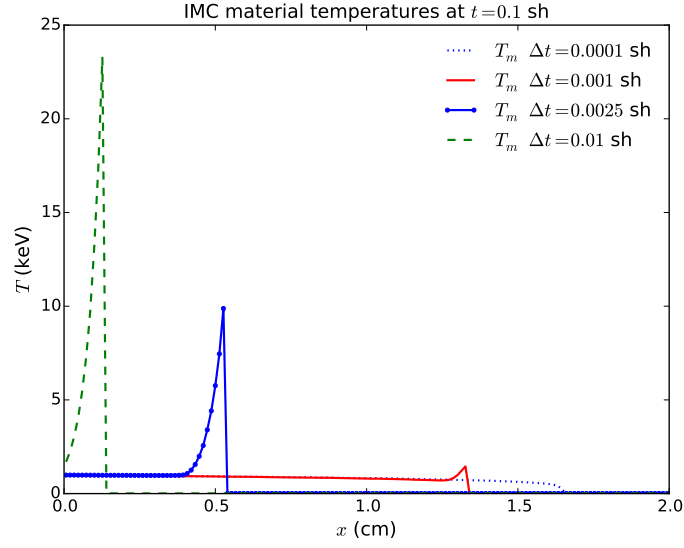


Figure 2: Simulation of MP violation problem with IMC method for various time step sizes.

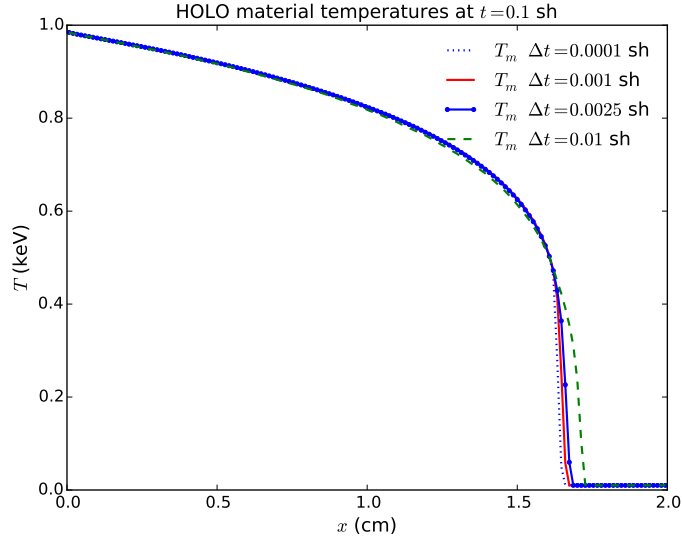


Figure 3: Simulation of MP violation problem with HOLO-ECMC method for various time step sizes.

Table 1: Problem specifications for maximum principle violation. Absorption cross section has form $\sigma_a = \sigma_{a,0}/T^3$.

$\sigma_{a,0}$ ($\text{cm}^{-1} \text{ keV}^3$)	4.0
σ_s (cm^{-1})	0.0
ρ (g cm^{-3})	1.0
c_v (jks/keV-g)	0.0081181

Table 2: Comparison of LO Newton iterations for different time step sizes and MP problem. For $\Delta t = 0.1$, damping has $\zeta = 1$. For all other cases $\zeta = 0.5$.

Δt	Avg. Iters / Time Step
σ_s (cm ⁻¹)	0.0
ρ (g cm ⁻³)	1.0
c_v (jks/keV-g)	0.0081181

An isotropic incident intensity of 0.150 keV is applied at $x = 0$; the incident intensity on the right boundary is 2.5×10^{-5} keV. The material properties are $\rho = 1$ g cm⁻³ and $c_v = 0.013784$ jks/keV-g. The absorption cross section varies as $\sigma(T) = 0.001 \rho T^{-3}$ (cm⁻¹). The simulation was advanced until $t = 5$ sh (1 sh $\equiv 10^{-8}$ s) with a fixed time step size of 0.001 sh. For comparison purposes, we have not used adaptive mesh refinement, only performed one HOLO iteration per time step, and use a fixed 3 HO batches with equal number of histories per batch. A relative tolerance of 10^{-6} for the change in $\phi(x)$ and $T(x)$ was used for the LO newton solver for all results. Radiation energy distributions are plotted as an equivalent temperature given by $T_r = (\phi/(ac))^{0.25}$. Cell-averaged quantities are plotted. Although isotropic scattering can be included in the LO solver with this method [?], we have only considered problems with $\sigma_s = 0$ here.

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.



Figure B.1: TAMU figure

B.1 Appendix Section