A High-Order Low-Order Algorithm with Exponentially-Convergent Monte Carlo for Thermal Radiative Transfer

Simon Bolding and Jim Morel

22 November 2016

NEUP Nuclear Energy University Programs
U.S. Department of Energy

CERT
Center for Exascale Radiation Transport

We are interested in modeling thermal radiation transport in the high energy density physics regime

Modeling materials under extreme conditions

Temperatures $\mathcal{O}(10^6)$ K or more

Photon radiation transports through a material

Significant energy may be exchanged

We want to improve efficiency of Monte Carlo calculations

e.g., inertial confinement fusion, supernovae, et. al.

Our method has been applied to a simplified model: the 1D frequency-integrated radiative transfer equations

Energy balance equations for radiation and material.
Radiation intensity $I(x, \mu, t)$, material temperature $T(x, t)$

$$\frac{1}{c}\frac{\partial I}{\partial t} + \mu\frac{\partial I}{\partial x} + \sigma_t I(x, \mu, t) = \frac{1}{4\pi}\sigma_a ac T^4,$$
$$C_v \frac{\partial T(x,t)}{\partial t} = \boxed{\sigma_a \phi(x,t)} - \boxed{\sigma_a ac T^4}$$

TRT equations are nonlinear and may be tightly coupled
Absorption opacity (σ_a) can be a strong function of T

Typically solved with implicit Monte Carlo (IMC)
which partially linearizes the system over a time step

Basic idea is a nonlinear low-order system with high-order angular correction from Monte Carlo transport solves

The **LO system** is space-angle moment equations,
on a fixed finite-element (FE) spatial mesh

- Reduced dimensionality in angle
  allows for solution with Newton's method
- **Output:** linear-discontinuous $\phi(x)$ and $T(x)$,
  Construct LDFE scattering and emission source

The **HO system** is a pure-absorber transport problem

- Solved with exponentially-convergent MC (ECMC)
  for *efficient* reduction of statistical noise
- **Output:** consistency terms

Our high-order low-order (HOLO) method improves on several drawbacks of standard IMC

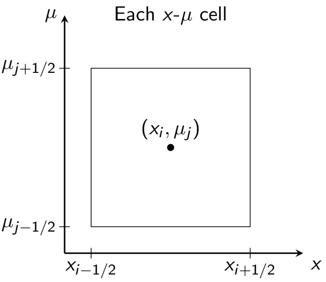
Standard IMC	**HOLO Method**
Large statistical noise possible	ECMC is efficient for TRT
Effective scattering can make MC tracking very expensive	MC solution has no scattering
Linearization can cause non-physical results (maximum principle violations)	Fully implicit time-discretization and LO solution resolves nonlinearities
Reconstruction of linear emission shape limits artificial energy propagation	Linear-discontinuous FE for $T(x)$ preserving equilibrium diffusion limit

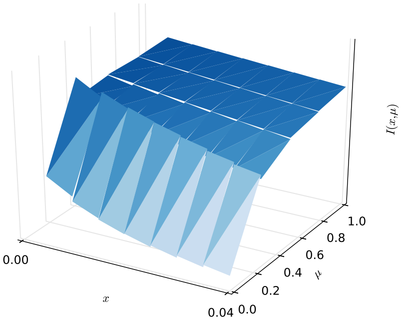
A HOLO Algorithm for Thermal Radiative Transfer

ECMC uses a projection $\tilde{I}(x,\mu)$ onto a space-angle LDFE mesh to represent the solution

local volumetric tallies

$$\tilde{I}_{ij}(x,\mu) = I_a + \frac{2}{h_x} I_x (x - x_i) + \frac{2}{h_\mu} I_\mu (\mu - \mu_i)$$





We apply the ECMC algorithm to the pure-absorber time-discrete transport equation

$$\left[\mu\frac{\partial}{\partial x} + \left(\sigma_t + \frac{1}{c\Delta t}\right)\right] I^{n+1} = \frac{1}{4\pi}\left[\sigma_a ac\left(T_{LO}^{n+1}\right)^4 + \sigma_s\phi_{LO}^{n+1}\right] + \frac{\tilde{I}^n}{c\Delta t}$$

$$\mathbf{L} I^{n+1} = q$$

For each **batch** m:

- Evaluate residual source: $r^{(m)} = q - \mathbf{L}\tilde{I}^{n+1,(m)}$
- Estimate $\epsilon^{(m)} = \mathbf{L}^{-1} r^{(m)}$ via MC simulation
- Update solution: $\tilde{I}^{n+1,(m+1)} = \tilde{I}^{n+1,(m)} + \tilde{\epsilon}^{(m)}$

Our HO system allows for straight-forward variance reduction and source biasing

$I^n(x, \mu)$ is often an **excellent** estimate of $I^{n+1}(x, \mu)$

No MC sampling from thermal equilibrium regions

Histories stream without collision

along path s, weight reduces as $w(s) = w_0 e^{-\sigma_t s}$

Use cell-wise systematic sampling for $|r^{(m)}|$ source

Particularly effective in thick cells

- Particles in each x-μ cell $\propto |r^{(m)}|$ in cell
- No sampling from cells in thermal equilibrium

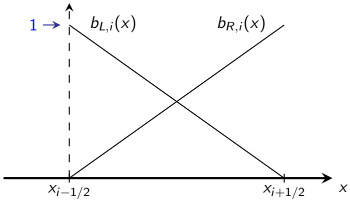
A HOLO Algorithm for Thermal Radiative Transfer

The LO equations are formed as *consistently* as possible with spatial and angular moments of TRT equations

The time discretization is backward Euler

for both the HO and LO equations

Spatial moments are weighted with FE basis functions:



$$\boxed{\langle\cdot\rangle_{L,i} = \frac{2}{h_i}\int_{x_{i-1/2}}^{x_{i+1/2}} b_{L,i}(x)(\cdot)\mathrm{d}x}$$

Half-range integrals reduce angular dimensionality

$$\boxed{I^+(x) = 2\pi\int_0^1 I(x,\mu)\mathrm{d}\mu}$$

Apply moments to the TRT equations and manipulate to form angular consistency terms

Ultimately, we get six **exact** moment equations
for each spatial element i

For example, apply $\langle\cdot\rangle_{L,i}$ and $(\cdot)^{+}$ to streaming term
and perform algebra to form angular averages

$$\begin{aligned}
\frac{h_i}{2}\left\langle\mu\frac{\partial I}{\partial x}\right\rangle_L^{+} &= \frac{1}{2}\left[\langle\mu I\rangle_{L,i}^{+} + \langle\mu I\rangle_{R,i}^{+}\right] - (\mu I)_{i-1/2}^{+} \\
&= \frac{1}{2}\left[\boxed{\frac{\langle\mu I\rangle_{L,i}^{+}}{\langle I\rangle_{L,i}^{+}}}\langle I\rangle_{L,i}^{+} + \boxed{\frac{\langle\mu I\rangle_{R,i}^{+}}{\langle I\rangle_{R,i}^{+}}}\langle I\rangle_{R,i}^{+}\right] - \boxed{\frac{(\mu I)_{i-1/2}^{+}}{I_{i-1/2}^{+}}} I_{i-1/2}^{+}
\end{aligned}$$

Apply moments to the TRT equations and manipulate to form angular consistency terms

Ultimately, we get six **exact** moment equations

for each spatial element i

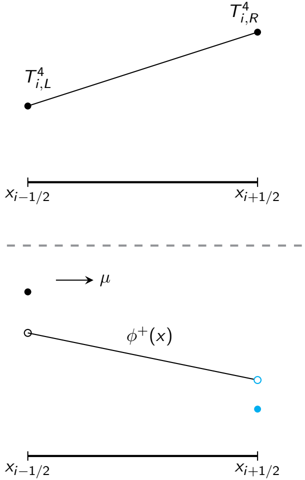
For example, apply $\langle \cdot \rangle_{L,i}$ and $(\cdot)^{+}$ to streaming term

and perform algebra to form angular averages

$$
\begin{aligned}
\frac{h_i}{2}\left\langle \mu \frac{\partial I}{\partial x} \right\rangle_L^{+} &= \frac{1}{2}\left[\langle \mu I \rangle_{L,i}^{+} + \langle \mu I \rangle_{R,i}^{+}\right] - (\mu I)_{i-1/2}^{+} \\
&= \frac{1}{2}\left[\boxed{\frac{\langle \mu I \rangle_{L,i}^{+}}{\langle I \rangle_{L,i}^{+}}} \langle I \rangle_{L,i}^{+} + \boxed{\frac{\langle \mu I \rangle_{R,i}^{+}}{\langle I \rangle_{R,i}^{+}}} \langle I \rangle_{R,i}^{+} \right] - \boxed{\frac{(\mu I)_{i-1/2}^{+}}{I_{i-1/2}^{+}}} I_{i-1/2}^{+}
\end{aligned}
$$

Now, approximate angular consistency terms with $\tilde{I}_{HO}^{n+1}(x, \mu)$ from previous HO solve

We eliminate auxillary spatial unknowns with a linear-discontinuous (LD) representation



1. Assume $T(x)$ and $T^4(x)$ are LD
   preserving equi. diff. limit
2. Assume $\phi^{\pm}$ linear on interior
3. Eliminate outflows with parametric closure from HO solution, e.g.,

   $$\boxed{\phi^+_{i+1/2} = \gamma^+_{i,HO}\langle\phi\rangle^+_{a,i} + \langle\phi\rangle^+_{x,i}}$$

   where $\gamma^+_{i,HO} = 1$ gives LD
4. Global system solved with Newton's method and lagged **implicit opacities**.
   Energy is always conserved

Apply source-iteration with linear diffusion-synthetic acceleration (DSA) to solve LO system

Source iteration with WLA-DSA
for (effective) scattering source of each Newton step

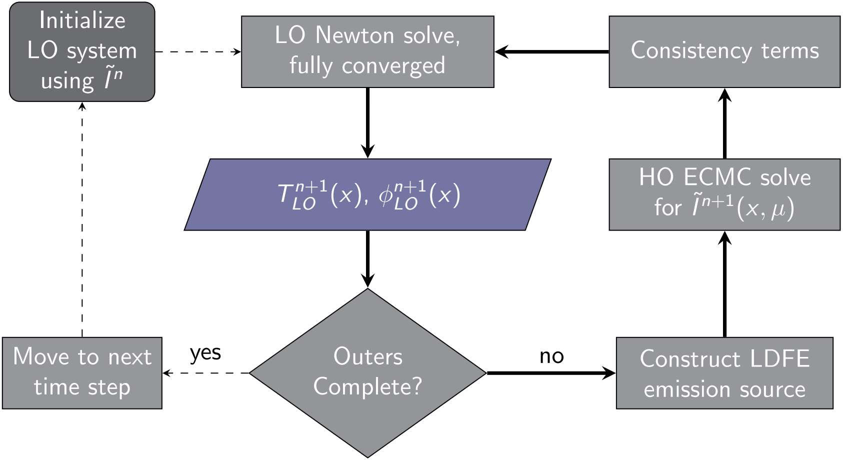
1. Sweep for a new $\phi^{\pm}$
   with a lagged scattering source

2. Solve approximate spatially continuous diffusion equation for error in scattering iterations

3. Update with local balance equations over elements

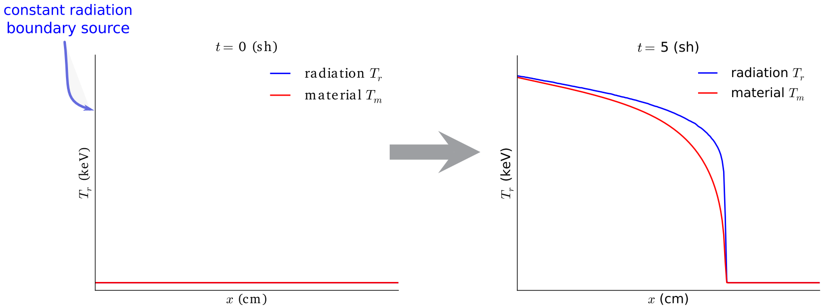
Recast as a GMRES solution with DSA-preconditioning

Iterations between the HO and LO systems can be performed each time step



A HOLO Algorithm for Thermal Radiative Transfer

We will test our method with several standard **Marshak Wave** problems



Figures depict radiation temperature $T_r = \sqrt[4]{\phi/ac}$

Implementation specifics for most results are given below:

- HOLO method is stand-alone C++ code (??? lines)
  IMC results from Jayenne (LANL code)

- One HO solve per time step, with two LO solves
  - *each HO* solve has 3 ECMC batches
    no adaptive mesh refinement

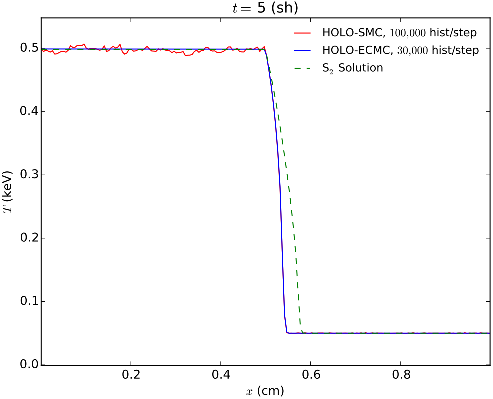
- Lumped LD discretization for $T(x)$ and $\phi(x)$

- Figure of Merit: $\boxed{\mathrm{FOM} = \dfrac{1}{\left(\dfrac{\|\sigma(\phi_i)\|}{\|\phi_i\|}\right)^2 N_{\mathrm{total}}}}$

  normalized so IMC FOM=1

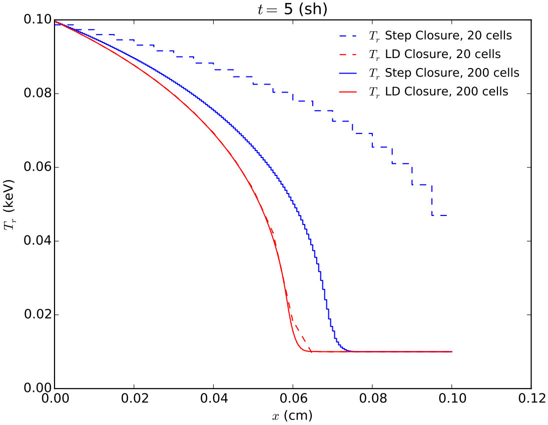
ECMC is more efficient than standard MC as a HO solver

- Left half is optically thin ($\sigma = 0.2$ cm^{-1}), right half is thick ($\sigma_a = 2000$ cm^{-1}). 8 μ cells
- Results for HOLO with different HO solvers: ECMC (FOM=10,000), standard MC (FOM=0.46), and S_2



The LDFE discretization for the LO equations preserves the equilibrium diffusion limit

- Large, constant σ_a and small c_v

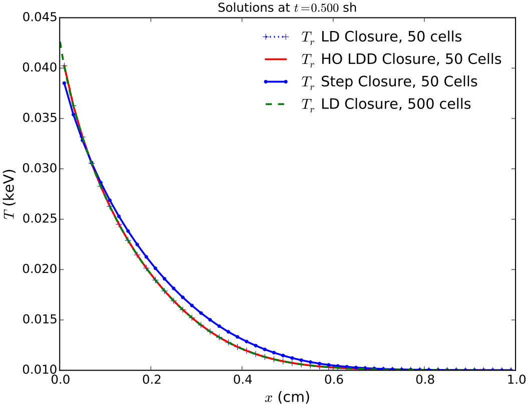


Tested the HO spatial closure for a simpler TRT problem

Fairly diffusive domain so that
linear discontinuous $T(x)$ is positive

- Problem is approaching state, $\Delta t_{\text{max}} = 0.01$ sh

Use ECMC with adaptive refinement
and 585,000 histories per time step



The HO spatial closure improves L_2 error and consistency, but does not decrease error in cell averages

- Compute error for 50 cells, compared to 500 cell reference
  Average results from 20 independent simulations

Spatial Closure	$\|e(x)\|_{rel}$	$\|e_i\|_{rel}$	$\|\phi_{HO}(x) - \phi_{LO}(x)\|_{rel}$
LDFE Closure	1.60%	0.59%	0.76%
HO Closure	1.40%	0.67%	0.013%

*$1\sigma \leq 0.01\%$ for all results

- For ECMC, $\tilde{\phi}_{HO}(x)$ does *not satisfy* moment equations
- Issues with using HO spatial closure and lumping
  but standard lumped LDFE is accurate

Negative intensities can occur in optically thick cells and mesh refinement is of minimal use

- Desire a positive $\tilde{I}_{HO}(x,\mu)$ for consistency terms
  to produce a physical, stable LO solution

- Rotate negative $\tilde{I}(x,\mu)$ to positive at end of batch:

$$\tilde{I}_{\text{pos}} = I_a + C\left[\frac{2}{h_x} I_x (x - x_i) + \frac{2}{h_\mu} I_\mu (\mu - \mu_j)\right], \quad (x,\mu) \in \mathcal{D}_{ij},$$

Negative intensities can occur in optically thick cells and mesh refinement is of minimal use

- Desire a positive $\tilde{I}_{HO}(x,\mu)$ for consistency terms
  to produce a physical, stable LO solution

- Rotate negative $\tilde{I}(x,\mu)$ to positive at end of batch:

$$\tilde{I}_{\text{pos}} = I_a + C\left[\frac{2}{h_x} I_x(x - x_i) + \frac{2}{h_\mu} I_\mu(\mu - \mu_j)\right], \quad (x,\mu) \in \mathcal{D}_{ij},$$

- Optionally add artificial source to next batch to attempt to mitigate stagnation

$$\mathbf{L} I^{(m+1)} = q_{LO} + \mathbf{L}\left(\tilde{I}^{n+1,(m)} - \tilde{I}_{\text{pos}}^{n+1,(m)}\right),$$

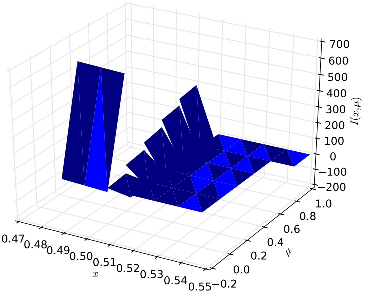
- If we apply $\mathbf{L}^{-1}$ to both sides

$$I^{n+1} = \mathbf{L}^{-1} q + (\tilde{I}^{n+1,(m)} - \tilde{I}_{\text{pos}}^{n+1,(m)}). \tag{1}$$

Apply rotation and artificial source to an analytic fixed-source problem

- Thin ($\sigma_a = 0.2$ cm^{-1}) and thick ($\sigma_a = 1000$ cm^{-1}) regions, $q(x) = I_{\text{floor}}\sigma_a(x)$

NEED A PICTURE OF FIXED SOURCE PROBLEM???



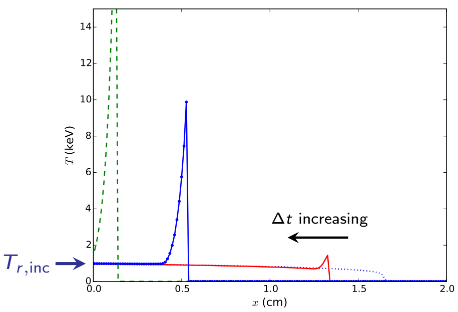
Artificial source does not improve solution for analytic neutronics problem

- Thin ($\sigma_a = 0.2$ cm^{-1}) and thick ($\sigma_a = 1000$ cm^{-1}) regions, $q(x) = I_{\text{floor}}\sigma_a(x)$

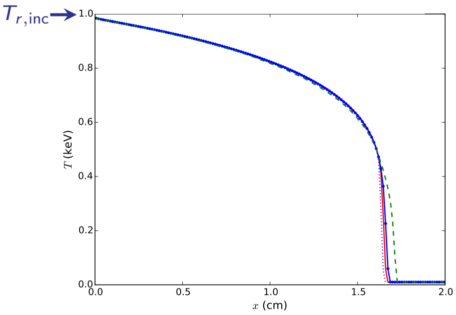
Our HOLO method preserves the maximum principle with sufficient nonlinear convergence

- **Material temperatures** plotted; all simulations end at $t = 0.1$ sh
  $\sigma_a \propto T^{-3}$, c_v small, $\Delta t \in [10^{-4}, 10^{-2}]$ sh
- LO Newton iterations required damping

IMC T_m



HOLO T_m



DSA allows for efficient iterative solution of the low-order equations

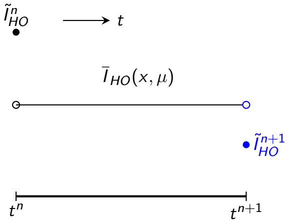
Apply iterative solution methods to two material problem with diffusivity of the thick region increased

Method	Avg. Sweeps/Time step
SI	25,900
SI-DSA	273
GMRES	292
GMRES-DSA	151

*25.1 **damped** Newton iterations per time step
Scattering iteration relative tolerance 10^{-10}

A HOLO Algorithm for Thermal Radiative Transfer

The time variable can be included in the ECMC trial space with a consistent LO time closure



Include continuous $\frac{1}{c}\frac{\partial}{\partial t}(\cdot)$ in **L** for residual source
leaving $T(x)$ still implicit

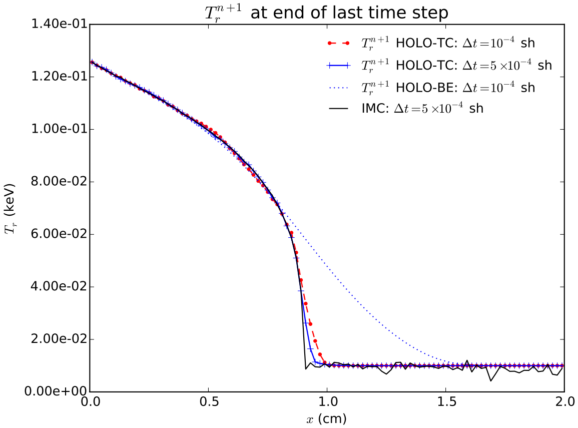
Sample and track particle histories in time.
Tally the time-averaged and t^{n+1} error

In LO equations, parameterize ϕ^{n+1}_{LO}
in terms of **time-averaged** unknowns, e.g.,

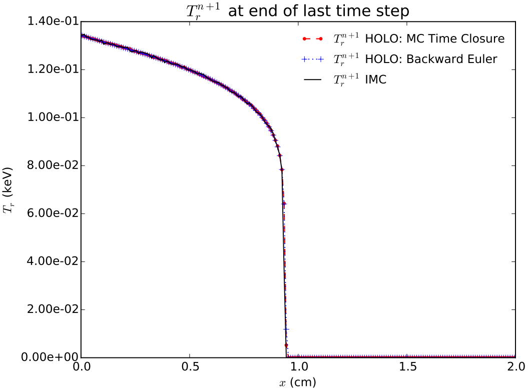
$$\langle\phi\rangle^{n+1}_{L,i} = 2\,\gamma^{HO}_{L,i}\,\overline{\langle\phi\rangle}_{L,i} - \langle\phi\rangle^{n}_{L,i}$$

The time-closure parameters preserve accuracy of MC time integration in the LO solution

- Material has $\sigma_a = 10^{-6}$ cm^{-1}, so temperature uncouples
  take 3 large time steps and compare $E_R^{n+1} = \phi^{n+1}/c$
- 300,000 histories/step, 100 spatial cells, **FOM=0.53**



With sufficient histories in a mix of optical thicknesses HOLO-TC is stable



- Figure: Comparison of HOLO-TC, HOLO-BE, and IMC methods for the Marshak Wave problem, with 10^6 histories per time step.

A HOLO Algorithm for Thermal Radiative Transfer

ECMC is very efficient for TRT simulations
and fits well in global HOLO method

The LO system can resolve nonlinearities
with bounded angular consistency terms

Next step is to extend to higher dimensions
main hurdle to overcome is infrastructure

A HOLO Algorithm for Thermal Radiative Transfer

ECMC is very efficient for TRT simulations
and fits well in global HOLO method

The LO system can resolve nonlinearities
with bounded angular consistency terms

Next step is to extend to higher dimensions
main hurdle to overcome is infrastructure

Future Work

Extend time treatment to a linear variable

Backup Slides

Simon Bolding and Jim Morel

NEUP Nuclear Energy University Programs
U.S. Department of Energy

CERT
Center for Exascale Radiation Transport

Implicit Monte Carlo (IMC) is the standard Monte Carlo transport method for TRT problems

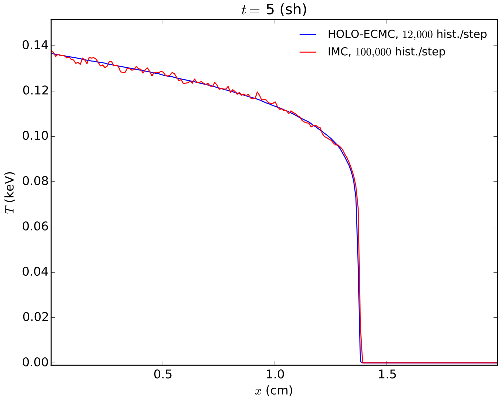
The system is *linearized* over a time step $t \in [t^n, t^{n+1}]$
Opacities are evaluated with $T(t^n)$

- Produces a linear transport equation
  with effective emission and scattering terms
- MC particle histories are simulated
  tallying radiation energy deposition
- Emission source is **not** fully time-implicit.
  Uses MC integration over Δt for intensity

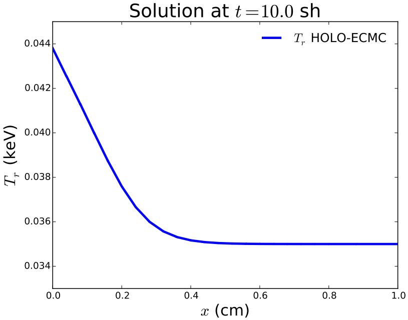
The HOLO method produces significantly less noise than IMC for a typical Marshak Wave: **FOM=145**

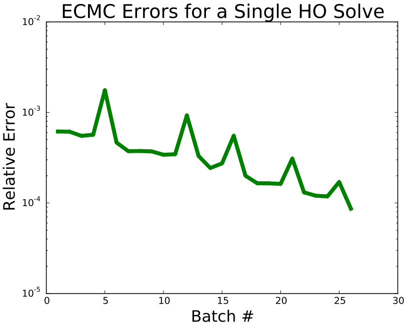
- $\sigma_a \propto T^{-3}$

- Transient solution after 5 shakes ($\sim$ 520 steps)
  200 x cells (and 4 μ cells for ECMC)



Exponential convergence can be maintained if the LDFE mesh resolves the solution reasonably





We need a way to resolve issues when the LDFE representation of the intensity is negative

Negative intensities can occur in optically thick cells
Mesh refinement is of minimal use

$\tilde{I}_{HO}(x,\mu)$ must be positive for consistency terms
to produce a physical, stable LO solution

Independent fix up for LO solution
E.g., lumping or preserving balance with floored $\phi(x)$

Can add source δ to produce a positive projection $\tilde{I}_{pos}$ such that $\tilde{I}_{pos}$ satisfies the latest residual equation

Produce $\tilde{I}_{\text{pos}}$ by scaling $x - \mu$ moments equally,
to estimate source for the next iteration

$$\mathbf{L}\tilde{I}^{(m)} = q - r^{(m)}$$
$$\mathbf{L}\tilde{I}^{(m)}_{\text{pos}} = q - r^{(m)} + \delta^{(m+1)}$$

$$\Rightarrow$$

$$\delta^{(m+1)} = \mathbf{L}\left(\tilde{I}^{(m)} - \tilde{I}^{(m)}_{\text{pos}}\right)$$
$$q \to q + \delta^{(m+1)}$$

We can delay error stagnation
Investigating alternative positive projection of I

Tried importance sampling on the interior of the time step

Ensure that p_{surv} of particles sampled from interior are 2 mfp from census

p_{surv}	FOM
No Bias	1
0.05	0.001
0.1	0.005
0.25	0.179
0.5	0.003

Solving LO System with Newton's Method

- Linearization:
  $\underline{B}(T^{n+1}) = \underline{B}(T^*) + \left(T^{n+1} - T^*\right) \frac{\partial \underline{B}}{\partial t}\Big|_{t^*}$
- Modified system

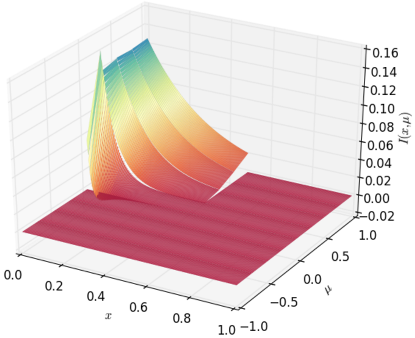
$$\left[\mathbf{D}(\mu^{\pm}) - \sigma_a^*(1-f^*)\right] \underline{\Phi}^{n+1} = f^* \underline{B}(T^*) + \frac{\underline{\Phi}^n}{c\Delta t}$$

$$\boxed{\hat{\mathbf{D}}\Phi^{n+1} = \underline{Q}}$$

$$f = \left(1 + \sigma_a^* c\Delta t \frac{4aT^{*3}}{\rho c_v}\right)^{-1} \qquad T_i^* = \frac{T_{L,i}^* + T_{R,i}^*}{2}$$

- Equation for T^{n+1} based on linearization that is conservative
- Converge T^{n+1} and $\langle\phi\rangle$ with Newton Iterations

The angular flux for the two material problem is difficult to resolve near $\mu = 0$



Timing Results For Two Material Problem

hists./step	$\Delta t (sh)$	IMC (μs/hist.)	HOLO-ECMC (μs/hist)	Newt
100,000	0.001	17	3.5	
30,000	0.001	18	6.9	
30,000	0.005	59	7.4	

Forming the LO System

- Taking moments of TE yields 4 equations, per cell i, e.g.

$$-2\mu_{i-1/2}^{n+1,+}\phi_{i-1/2}^{n+1,+}+\{\mu\}_{L,i}^{n+1,+}\langle\phi\rangle_{L,i}^{n+1,+}+\{\mu\}_{R,i}^{n+1,+}\langle\phi\rangle_{R,i}^{n+1,+}+$$

$$\left(\sigma_t^{n+1}+\frac{1}{c\Delta t}\right)h_i\langle\phi\rangle_{L,i}^{n+1,+}-\frac{\sigma_s h_i}{2}\left(\langle\phi\rangle_{L,i}^{n+1,+}+\langle\phi\rangle_{L,i}^{n+1,-}\right)$$

$$=\frac{h_i}{2}\langle\sigma_a^{n+1}acT^{n+1,4}\rangle_{L,i}+\frac{h_i}{c\Delta t}\langle\phi\rangle_{L,i}^{n,+}, \quad (2)$$

- Cell unknowns: $\langle\phi\rangle_{L,i}^{+}$, $\langle\phi\rangle_{R,i}^{+}$, $\langle\phi\rangle_{L,i}^{-}$, $\langle\phi\rangle_{R,i}^{-}$, T_L, T_R

- Need angular consistency terms and spatial closure (LD)