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

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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 $T(x, t)$

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

$$C_v \frac{\partial T(x, t)}{\partial t} = \boxed{\sigma_a \phi(x, t)} - \boxed{\sigma_a a c T^4}$$

TRT equations are nonlinear and may be tightly coupled
Absorption cross section (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

A HOLO Algorithm for Thermal Radiative Transfer

Exponentially Convergent Monte Carlo (ECMC) can efficiently reduce noise globally

ECMC is an iterative form of residual Monte Carlo
applied to particle transport problems

Each MC batch tallies the **error** in solution estimate

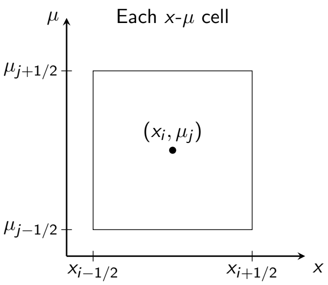
- standard MC particle transport, but a complex source
- ECMC requires a functional representation for all phase space variables being sampled

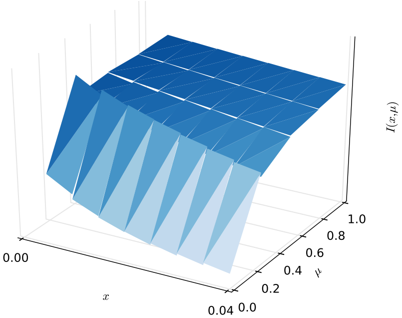
Can reduce solution error globally $\propto e^{-\alpha N}$
Adaptive *h*-refinement can help represent error

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
- Set minimum N for each cell
  except for zero from cells in thermal equilibrium

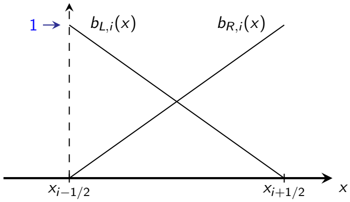
A HOLO Algorithm for Thermal Radiative Transfer

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

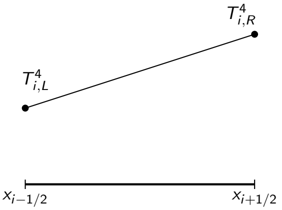
Ultimately, we get six **exact** moment equations
for each spatial element i

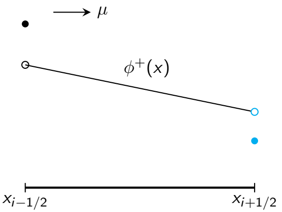
For example, apply $\langle\cdot\rangle_{L,i}$ and $(\cdot)^+$ to streaming term
and perform algebra to form angular averages

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

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

We eliminate auxillary spatial unknowns to close global system of equations





1. Assume $T(x)$ and $T^4(x)$ are LD
   preserving equi. diff. limit

2. Assume $\phi^{\pm}(x)$ linear
   over each cell

3. Can 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

HO closure improves consistency
Requires face tallies in ECMC

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

Used source iteration (SI) 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 moments w/ local balance equations
   over each spatial element

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Recast as a GMRES solution with DSA-preconditioning

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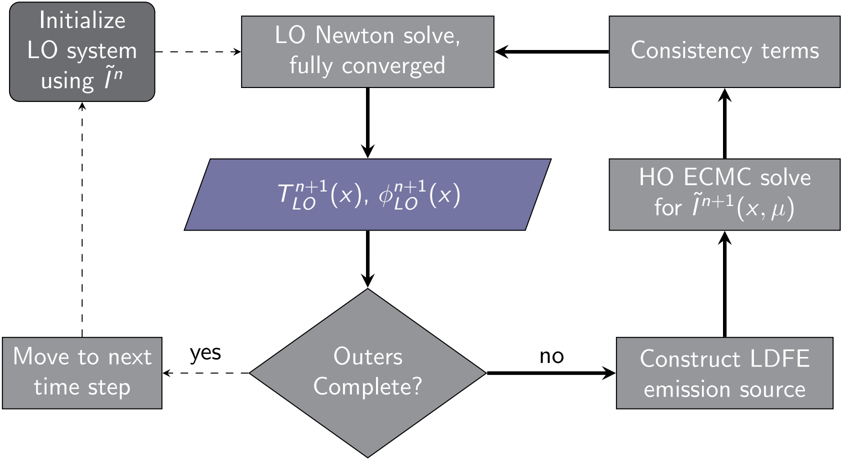
Iterations between the HO and LO systems can be performed each time step



A HOLO Algorithm for Thermal Radiative Transfer

Implementation specifics for results are:

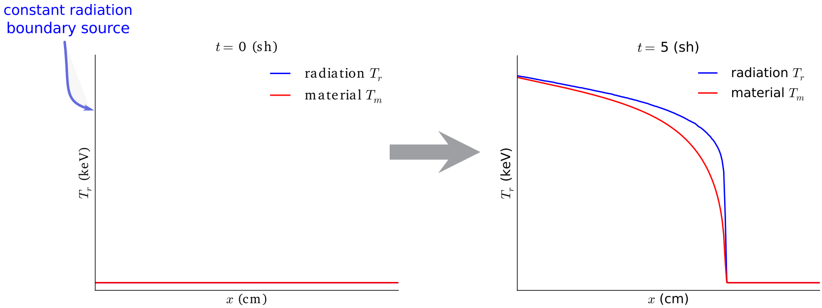
- HOLO method is written in stand-alone C++ (15k lines)
  IMC results from Jayenne (LANL code)

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

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

  normalized so IMC FOM=1

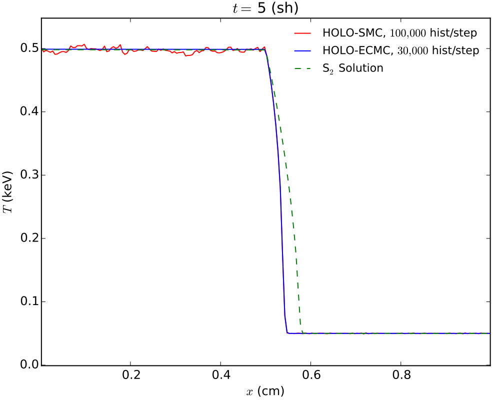
We will test our method with several standard **Marshak Wave** problems



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

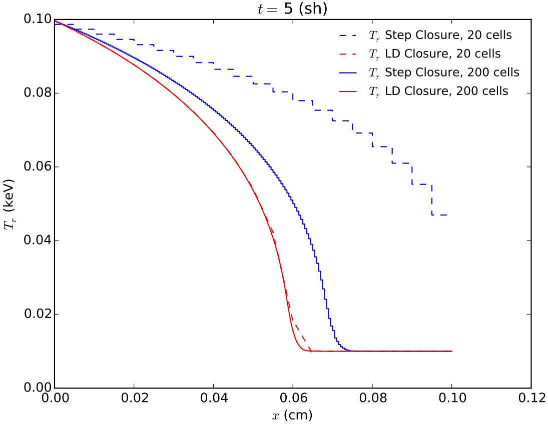
ECMC is more efficient than standard MC as a HO solver

- Left half is optically thin ($\sigma = 0.2$ cm^{-1}), right half is thick ($\sigma_a = 2000$ cm^{-1}). 8 μ cells, $\Delta t = 0.001$ sh
- Results for HOLO with different HO solvers: ECMC (FOM=10,000), standard MC (FOM=0.46), and S_2



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

- **EDL Problem:** Large, constant σ_a and small c_v
- Apply HOLO algorithm, 12k histories per step



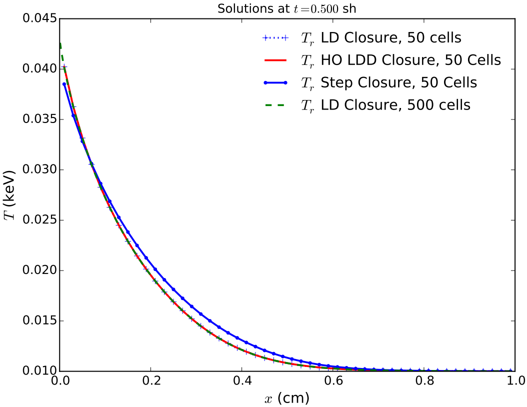
Tested the HO spatial closure for a easier TRT problem

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

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

- Use ECMC with adaptive refinement, 2 HOLO iters

  and 585k histories per HO solve



The HO spatial closure improves L_2 error and consistency but does not decrease error in cell-averaged quantities

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

	$\|e(x)\|_{2,rel}$	$\|e_i\|_{2,rel}$	$\|\phi_{HO}(x) - \phi_{LO}(x)\|_{2,rel}$
LDFE Closure	1.60%	0.59%	0.76%
HO Closure	1.40%	0.67%	0.013%

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

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- For ECMC, $\tilde{\phi}_{HO}(x)$ does *not satisfy* moment equations

$$\mathbf{L}\tilde{I}(x,\mu) = q - r(x,\mu)$$

- 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 $\tilde{I}(x,\mu)$ above I_{floor} at end of batch:

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

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

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

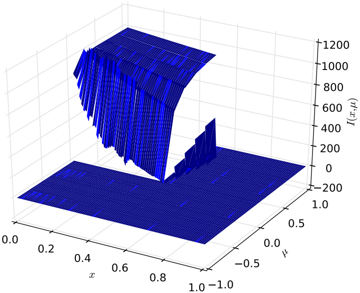
  If we apply $\mathbf{L}^{-1}$ to both sides

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

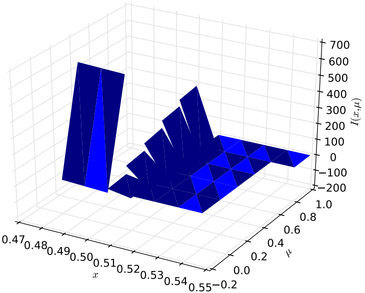
Apply rotation and artificial source methods to steady state, pure-absorber neutronics problem

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

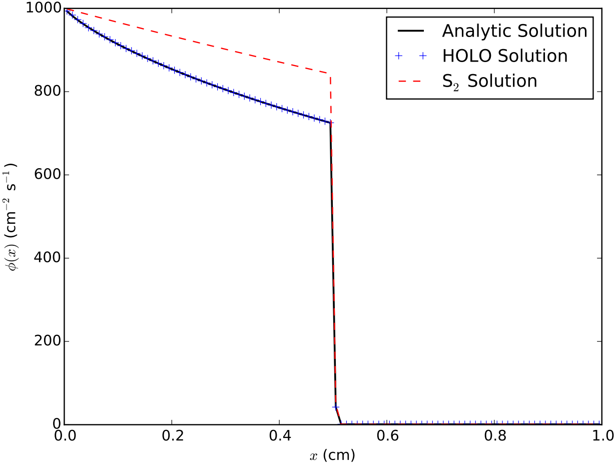
$\underline{\tilde{I}(x, \mu)}$



$\underline{\tilde{I}(x, \mu) < I_{\text{floor}}}$ (zoom)



Plot of cell-averaged mean intensities $\phi(x)$ for analytic problem and 100 spatial cells



Artificial source does not improve solution for analytic neutronics problem

- Compute cell-averaged error norms for HO and LO solutions, with 4 batchs, 10^5 histories per batch

Fixup Method	$\|e_i^{LO}\|_{2,rel}$	$\|e_i^{HO}\|_{a,rel}$	FOM
Rotate every Batch	0.232%	0.265%	1.76
Rotate Last Batch	0.267%	0.302%	1.30
Artificial Source	0.261%	0.304%	1.34

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

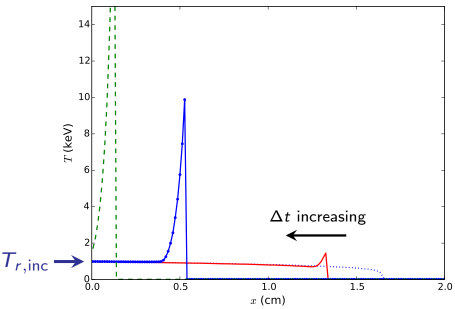
- The artificial source reduces magnitude of local residual, but can produce inaccurate solutions down stream

- Mixed results for TRT problems
  but all results have similar and high efficiency

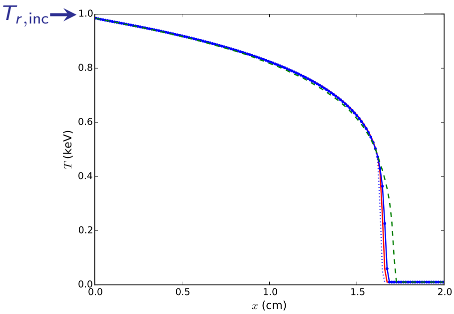
Our HOLO method preserves the maximum principle with sufficient nonlinear convergence

- **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



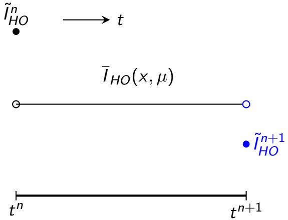
DSA allows for efficient iterative solution of the low-order equations

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

Method	Avg. Sweeps/Newton Iter.
SI	1037
SI-DSA	10.9
GMRES	11.6
GMRES-DSA	6

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

The time variable can be included in the ECMC trial space allowing for accurate time integration of intensity



Introduce trial space representation for $I(x, \mu, t)$
step doubly discontinuous in t, LDFE in x & μ

Include continuous $\frac{1}{c}\frac{\partial}{\partial t}(\cdot)$ in $\mathbf{L}$ for residual source
leaving $T(x)$ and $T^4(x)$ implicit:

$$r(x, \mu, t) = \frac{1}{2}\sigma_a^{n+1} ac \left(T^{n+1}\right)^4 - \frac{1}{c}\frac{\partial \tilde{I}}{\partial t} - \mu\frac{\partial \tilde{I}}{\partial x} - \sigma_t \frac{\partial \tilde{I}}{\partial x}$$

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

The LO equations must be closed consistently by eliminating t^{n+1} unknowns with HO information

1. Form LO Equations with space-angle moments as before, but integrated over a time step
   Treat $T(x)$ terms implicitly

2. Angular consistency terms are now time-averaged
   evaluated with time-averaged projection $\bar{I}_{HO}(x,\mu)$

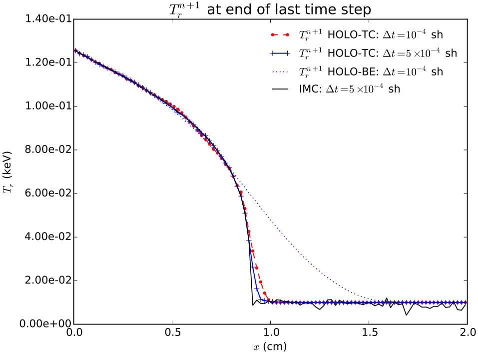
3. Eliminate moments of ϕ_{LO}^{n+1} in terms of **time-averaged** moments, e.g.,

$$\langle\phi\rangle_{L,i}^{n+1,+} = \boxed{\gamma_{L,i}^{HO,+}}\,\langle\overline{\phi}\rangle_{L,i}^{+}$$

4. Use closure to advance to next time step
   after solving for time-averaged unknowns

The time closure preserves the accuracy of MC time integration in LO solution

- Material has $\sigma_a = 0.2\ \text{cm}^{-1}$, temperature mostly uncouples
  Plots depict T_r^{n+1} at $t = 0.1$
- For HOLO w/ time closure (HOLO-TC)
  smaller time steps decrease noise but increase projection error
- HOLO Backward Euler (HOLO-BE) is inaccurate



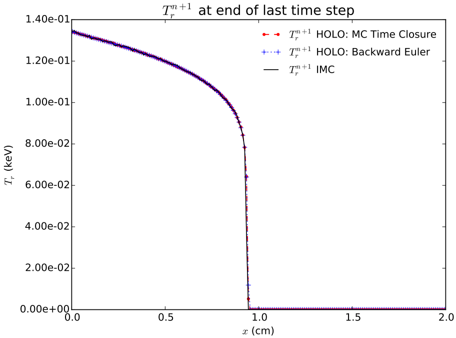
The HOLO-TC method is more efficient than IMC with sufficiently fine mesh

- Results for 200 x cells, HOLO-TC has 60 μ cells
  $\Delta t = 0.001$ sh
- Error computed against IMC reference answer with 4×10^8 histories/step, 100 x cells

	$\|\mathbf{e_i}\|_{\mathbf{2,rel}}$		**FOM**	
hists./step	IMC	HOLO-TC (1)	IMC	HOLO-TC(1)
30,000	2.93%	14.00%	1	0.10
300,000	0.99%	0.37%	0.92	14.2
1,000,000	0.49%	0.18%	1.02	81.7

The HO temporal closure is stable in a mix of optical thicknesses with sufficient histories

- Marshak wave problem, 10^6 hists/step over 2 batches



- Multiple batches are more efficent at estimating census
- HOLO-BE (FOM=1800) more efficient than HOLO-TC (FOM=15)
  step doubly-discontinuous trial space inaccurate

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... very distant future

Need consistent way to resolve negativities
strictly positive trial space for moments

Extend time treatment to a linear trial space
sampling is significantly complicated

Improve efficiency of ECMC
with asymmetric mesh refinement

Consider Kernel Density Estimators for ECMC
to improve efficiency within a batch

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FOM and error norm definitions

Cell-averaged error norms

$$\|e_i\|_{rel}^{(l)} = \left(\frac{\sum_{i=1}^{N_c^{(l)}} \left(\phi_i^{n+1,(l)} - \phi_i^{n+1,ref} \right)^2}{\sum_{i=1}^{N_c^{(l)}} \left(\phi_i^{n+1,ref} \right)^2} \right)^{1/2}, \quad (1)$$

FOM is based on the following variance

$$\sigma(\phi_i)^2 = \frac{1}{N_{sim} - 1} \sum_{l=1}^{N_{sim}} \left(\overline{\phi_i} - \phi_i^{(l)} \right)^2, \quad (2)$$

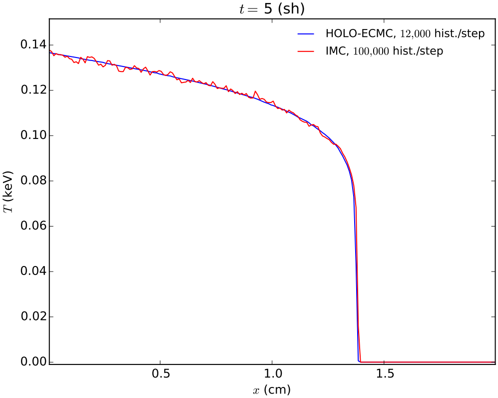
Implicit Monte Carlo (IMC) is the standard Monte Carlo transport method for TRT problems

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)



Time-integrated moment equation for L, $+$

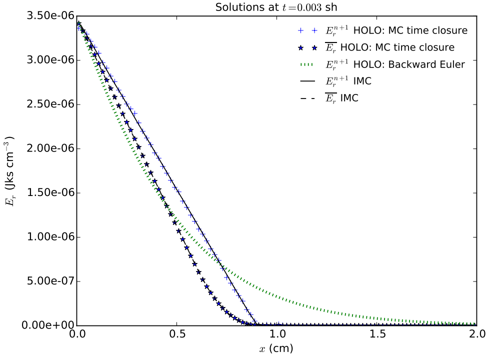
$$\frac{\langle\phi\rangle_{L,i}^{+,n+1} - \langle\phi\rangle_{L,i}^{+,n}}{c\Delta t} - 2\overline{\mu}_{i-1/2}^{+}\overline{\phi}_{i-1/2}^{+} + \overline{\{\mu\}}_{L,i}^{+}\langle\overline{\phi}\rangle_{L,i}^{+} + \overline{\{\mu\}}_{R,i}^{+}\langle\overline{\phi}\rangle_{R,i}^{+}$$
$$+ \sigma_{t,i}^{n+1} h_i \langle\overline{\phi}\rangle_{L,i}^{n+1,+} - \frac{\sigma_{s,i} h_i}{2}\left(\langle\overline{\phi}\rangle_{L,i}^{+} + \langle\overline{\phi}\rangle_{L,i}^{-}\right)$$
$$= \frac{h_i}{2}\langle\sigma_a^{n+1} acT^{n+1,4}\rangle_{L,i}, \quad (3)$$

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

Near-void problem, $\sigma_a = 10^{-6}$ cm^{-1}

take 3 **large** time steps

- Comparison radiation energy densities $E_r = \phi(x)/c$ for time-averaged and census values
- 3 batches of 100,000 hists./step, 100 x cells, **FOM=0.53**



Projection error for near-void problem

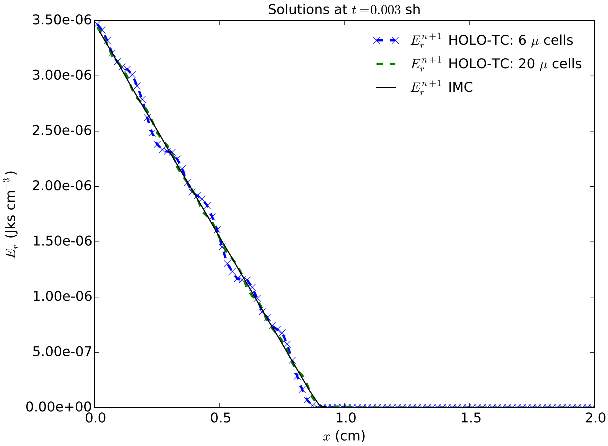
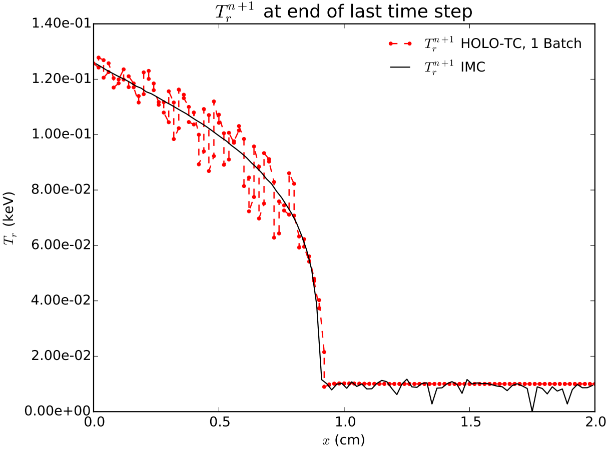
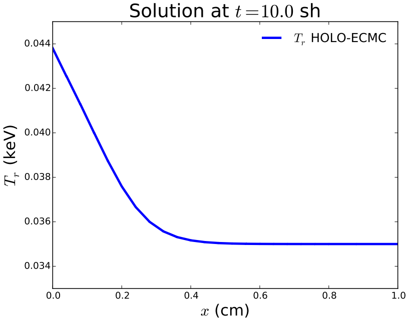


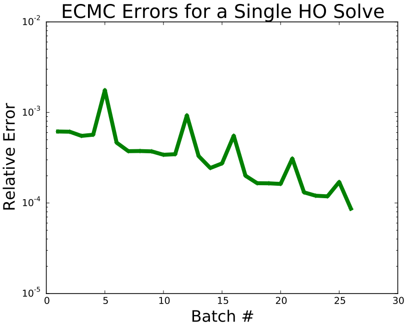
Figure: Comparison of radiation energy densities for the HOLO method with different numbers of μ cells. $\Delta t = 0.001$ sh, for near-void problem.

Without sufficient histories, time closure can introduce instabilities



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





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

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

$$\Rightarrow$$

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

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

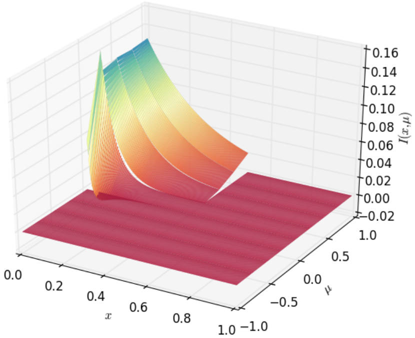
$$\left[\mathbf{D}(\mu^{\pm}) - \sigma_a^*(1 - f^*)\right] \underline{\Phi}^{n+1} = f^* \underline{B}(T^*) + \frac{\underline{\Phi}^n}{c\Delta t}$$

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

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

- 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.

$$-2\mu_{i-1/2}^{n+1,+}\phi_{i-1/2}^{n+1,+}+\{\mu\}_{L,i}^{n+1,+}\langle\phi\rangle_{L,i}^{n+1,+}+\{\mu\}_{R,i}^{n+1,+}\langle\phi\rangle_{R,i}^{n+1,+}+ \left(\sigma_t^{n+1}+\frac{1}{c\Delta t}\right)h_i\langle\phi\rangle_{L,i}^{n+1,+}-\frac{\sigma_s h_i}{2}\left(\langle\phi\rangle_{L,i}^{n+1,+}+\langle\phi\rangle_{L,i}^{n+1,-}\right) = \frac{h_i}{2}\langle\sigma_a^{n+1}acT^{n+1,4}\rangle_{L,i}+\frac{h_i}{c\Delta t}\langle\phi\rangle_{L,i}^{n,+}, \quad (4)$$

- 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)