Residual Monte Carlo Transport in Time with Consistent Low-Order Acceleration for 1D Thermal Radiative Transfer

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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, e.g., supernovae

Photon radiation transports through a material

Significant energy may be exchanged

This work increases time-integration accuracy

of the radiation variable in optically thin regions

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 $T(x,t)$

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

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

As $\sigma_a \to 0$, the equations become linear
and the radiation uncouples from the material

We will compare our time-integration accuracy to the **Implicit Monte Carlo** (IMC) method

TRT equations are often solved with IMC
which partially linearizes the system over a time step

Linearized *radiation* equation is integrated continuously
via MC sampling and tracking in time

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We have extended a high-order low-order (HOLO) method:

- Previously shown to be statistically efficient in optically thick problems
- Use MC time-integration for radiation terms
  instead of pure backward Euler in time

A HOLO Algorithm for Thermal Radiative Transfer

Exponentially Convergent MC High-Order Solver

Derivation of the LO equations

Summary of algorithm

Computational Results

Produce a nonlinear low-order system with high-order angular and temporal correction from MC transport solve

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

- Reduced dimensionality in angle
  allows for solution with Newton's method
- **Output:** linear-discontinuous $\phi^{n+1}(x)$ and $T^{n+1}(x)$,
  Construct LDFE 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 to close LO equations

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

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

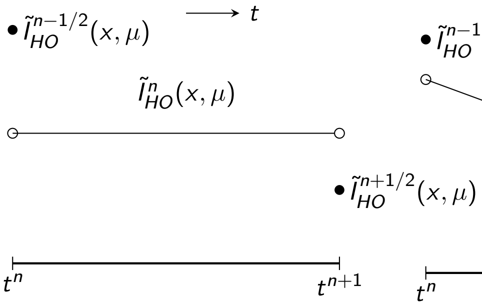
- A complex residual source
  with standard MC particle transport
- Residual requires a functional representation
  for all phase space variables being sampled

We can not maintain exponential convergence
without adaptive *h*-refinement of trial space

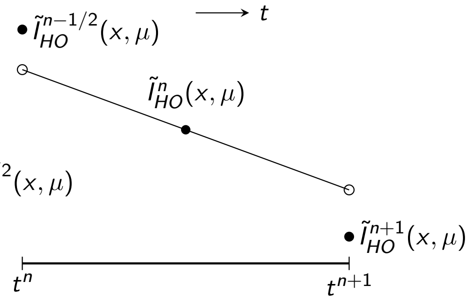
We still gain efficiency from residual formulation
with previous intensity as initial guess each time step

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

- linear-discontinuous FE projection in x and μ
- Tried three different t spaces: SDD, LDD, LD



(a) SDD trial space



(b) LDD trial space

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

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

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

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: $\tilde{I}^{n+1,(m+1)} = \tilde{I}^{n+1,(m)} + \tilde{\epsilon}^{(m)}$

We sample from a simplified FE residual source and importance sampling estimates residual magnitude

Cannot analytically evaluate L_1 norm of x-μ-t residual
because of bi-linear functions with zero-crossings

Sample from piece-wise constant, discontinuous approximation $p^*(x, \mu, t)$:

- Magnitude is quadrature approx. of L_1 norm
  for each volumetric- or δ-function

- Modified weights $w(x, \mu, t) = \frac{r(x,\mu,t)}{p^*(x,\mu,t)}$

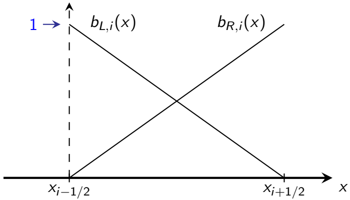
Frequency of element samples $\propto \|r\|_1$ over element,
and this approach is extendable to higher dimensions

A HOLO Algorithm for Thermal Radiative Transfer

The LO equations are formed as *consistently* as possible with space-angle-time moments of TRT equations

Integration over time step $t \in [t^{n-1/2}, t^{n+1/2}]$
with an implicit time discretization for the emission source

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

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

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 $\tilde{I}_{HO}^n(x,\mu)$ from previous HO solve

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

1. Assume LD spatial closure for $T(x)$, $T^4(x)$, and $\phi(x)$

2. Eliminate space-angle moments of $I_{LO}^{n+1/2}$ in terms of **time-averaged** moments $\overline{I}_{LO}$, e.g.,

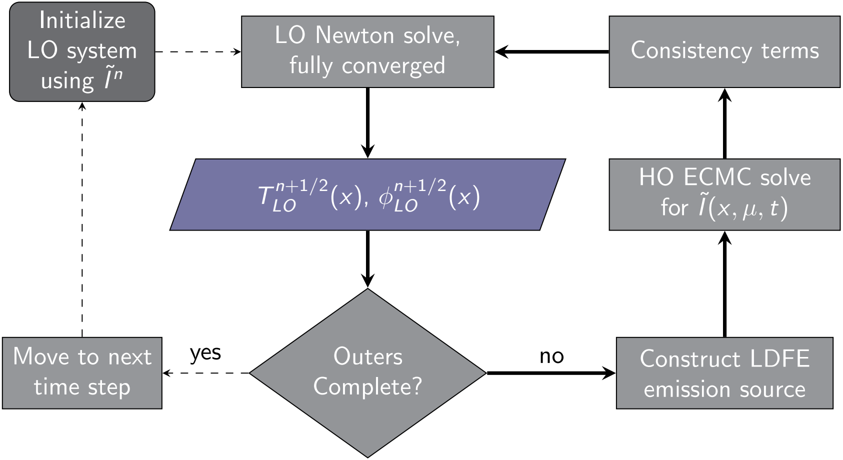
$$\langle \phi \rangle_{L,i}^{n+1/2,+} = \boxed{\gamma_{L,i}^{HO,+}} \langle \overline{\phi} \rangle_{L,i}^{+}$$

3. Coupled equations are solved with Newton's method for time-averaged moment unknowns

4. Use time closure to advance to the next time step

A HOLO Algorithm for Thermal Radiative Transfer

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

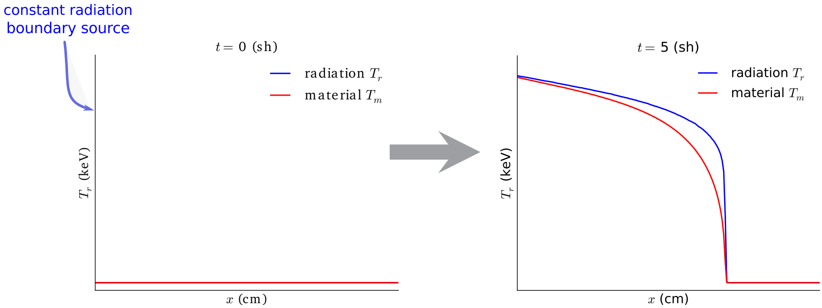


A HOLO Algorithm for Thermal Radiative Transfer

Implementation specifics for results are:

- HOLO method is written in stand-alone C++
  IMC results from Jayenne (LANL code)
- One HO solve per time step,
  with two LO solves
- Figure of Merit: $\boxed{\mathrm{FOM} = \frac{1}{\left(\frac{\|\sigma(\phi_i)\|_2}{\|\phi_i\|_2}\right)^2 N_{\text{total}}}}$
  normalized so IMC FOM=1

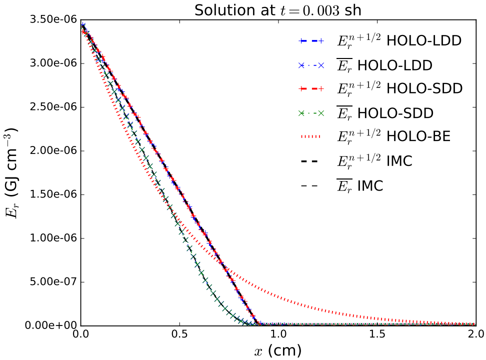
We will test our method with several standard **Marshak Wave** problems



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

HOLO can preserve accuracy of IMC for near-void problem $\sigma_a = 10^{-9}$

- *Three* large time steps, 10^6 histories per time step
- Plots depict Radiation energy densities $\phi(x)/c$
  IMC is more efficient for this problem



The LDFE projection error between time steps does not affect wave front location

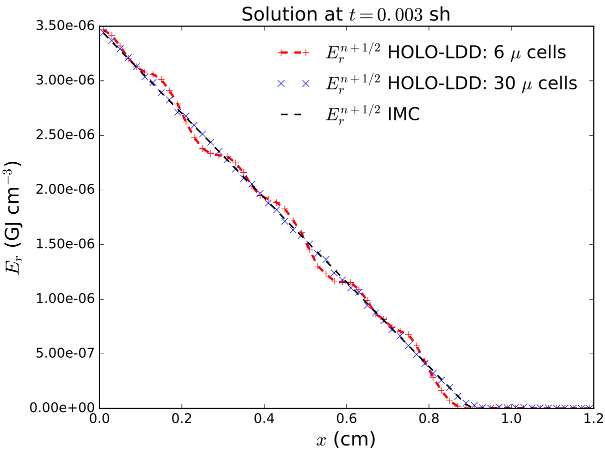
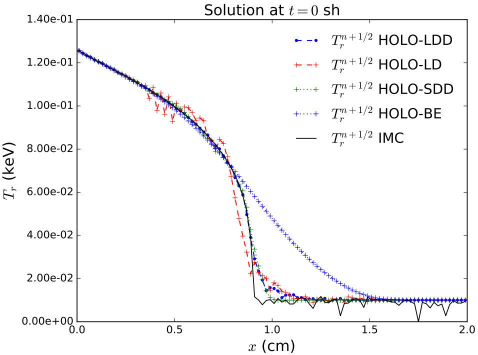


Figure: Comparison of radiation energy densities for the HOLO method with different numbers of μ cells. $\Delta t = 0.001$ sh, for near-void problem.

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

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



Optically thin problem $\sigma_a = 0.2$ cm^{-1}

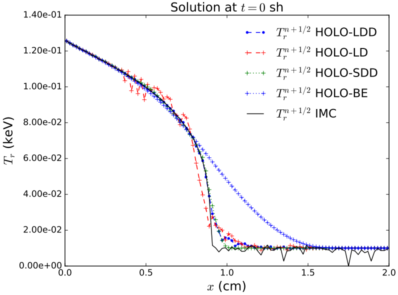
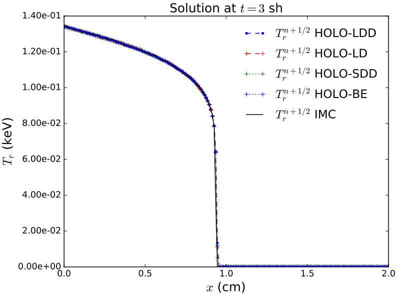


Figure: Comparison of radiation temperatures of IMC and the HOLO method for different time step sizes and numbers of batches, for optically thin problem.

Table: Comparison of $\|e\|_{a,rel}$ and FOM values for the end of time step radiation energy densities, of the last time step, for the optically thin problem, 200 x cells, and $\Delta t = 1 \times 10^{-4}$ sh. The reference IMC result has 100 x cells. Simulation end time is $t = 0.003$ sh. Fractional error in all results below 0.01

$\|\mathbf{e}\|_{\mathbf{a,rel}}$			
hists./step	IMC	HOLO-SDD	HOLO-LDD
30,000	2.93%	14.00%	14.50%
300,000	0.99%	0.37%	0.46%
1,000,000	0.49%	0.18%	0.19%
FOM			
hists./step	IMC	HOLO-SDD	HOLO-LDD
30,000	1	0.11	0.10
300,000	0.90	14.24	8.61
1,000,000	1.01	81.71	71.36



	FOM			
hists./step	IMC	HOLO-SDD	HOLO-LD	HOLO-BE
300,000	1.00	0.43	200	2050
1,000,000	0.94	15.95	201	1806

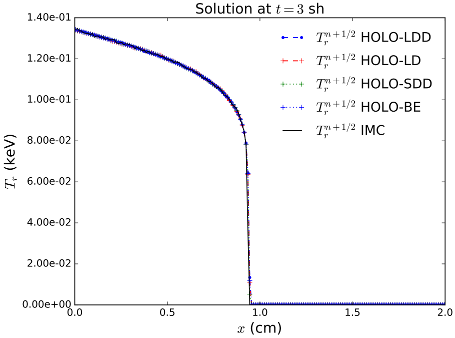
The HOLO-TC method is more efficient than IMC with sufficiently fine mesh

- 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-SDD (FOM=15) but HOLO-LD (FOM=200) is comparable

A HOLO Algorithm for Thermal Radiative Transfer

ECMC was extended to include the time variable
and fits well in global HOLO context

HOLO method can be more efficient than IMC
but would greatly benefit from x-μ adaptivity

The LO system is stable with sufficient statistics
but the time-closure terms are not bounded

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

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EST. 1943

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Backup Slides

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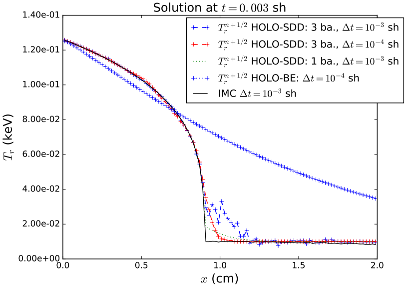
Near-void problem plotted as radiation temperatures



FOM and error norm definitions

Cell-averaged error norms

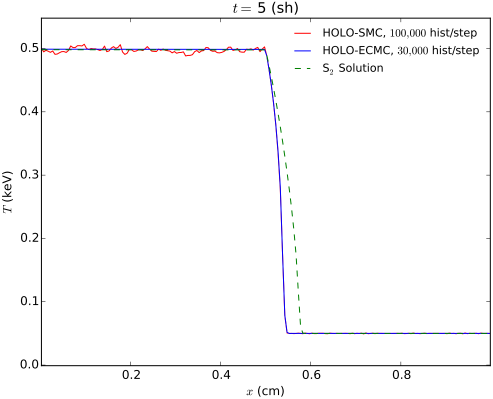
$$\|e_i\|_{rel}^{(l)} = \left(\frac{\sum_{i=1}^{N_c^{(l)}} \left(\phi_i^{n+1,(l)} - \phi_i^{n+1,ref} \right)^2}{\sum_{i=1}^{N_c^{(l)}} \left(\phi_i^{n+1,ref} \right)^2} \right)^{1/2}, \tag{1}$$

FOM is based on the following variance

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

ECMC is more efficient than standard MC as a HO solver

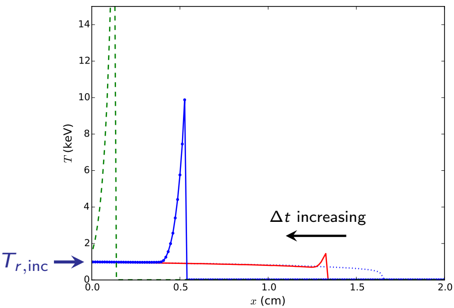
- Left half is optically thin ($\sigma = 0.2$ cm^{-1}), right half is thick ($\sigma_a = 2000$ cm^{-1}). 8 μ cells, $\Delta t = 0.001$ sh
- Results for HOLO with different HO solvers: ECMC (FOM=10,000), standard MC (FOM=0.46), and S_2



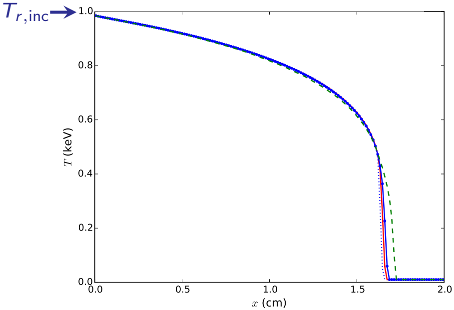
Our HOLO method preserves the maximum principle with sufficient nonlinear convergence

- **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

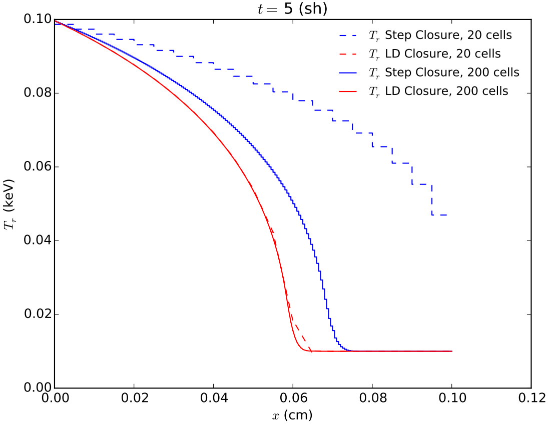
Apply iterative solution methods to TRT two material problem with diffusivity of the thick region increased

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 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



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

Time-integrated moment equation for L, $+$

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

Without sufficient histories, time closure can introduce instabilities