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

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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, 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 $T(x, t)$

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

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

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

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

Overview of HOLO approach

Residual Monte Carlo High-Order Solver

Derivation of the LO equations

Summary of algorithm

Computational Results

We produce a nonlinear low-order system with high-order angular and temporal correction from MC transport solves

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

- Reduced dimensionality and HO closures
  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 residual Monte Carlo (RMC)
  for *efficient* reduction of statistical noise

- **Output:** consistency terms to close LO equations

A HOLO Algorithm for Thermal Radiative Transfer

We apply the RMC algorithm to the HO transport eq., without discretization of the transport operator

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

$$\mathbf{L}\, I(x,\mu,t) = q$$

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

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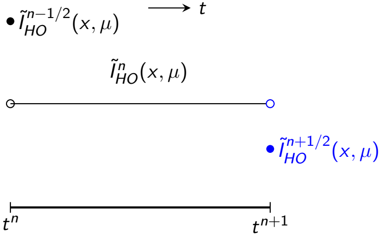
Initialize $\tilde{I}^{(}(0))$ with previous intensity $\tilde{I}^{n-1/2}$
which is very efficient as optical thickness increases

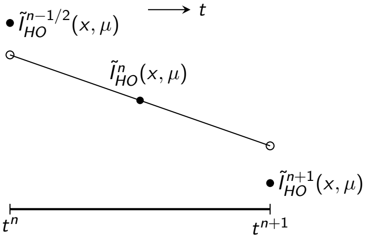
RMC uses a projection $\tilde{I}(x, \mu, t)$ onto a space-angle-time FE mesh to represent the solution

Linear-discontinuous (LD) FE projection in x and μ

Tried three different t spaces: step-doubly discontinuous (SDD), linear doubly-discontinuous (LDD), LD



(a) SDD trial space



(b) LDD trial space

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

Cannot analytically evaluate L_1 norm of x-μ-t residual
because of 3D- and 2D-bi-linear functions

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

- Values are quadrature approx. of L_1 norm
  for each local volumetric- or δ-function
- Modified weights $w^*(x, \mu, t) = \dfrac{r(x, \mu, t)}{p^*(x, \mu, t)}$

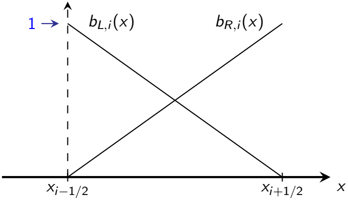
Frequency of element samples $\propto \|r\|_1$ over element,
and this approach is extendable to higher dimensions

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 implicit time discretization for temperature terms

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

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

$$= \frac{1}{2} \left[\frac{\langle \mu I \rangle_{L,i}^{+}}{\langle I \rangle_{L,i}^{+}} \langle I \rangle_{L,i}^{+} + \frac{\langle \mu I \rangle_{R,i}^{+}}{\langle I \rangle_{R,i}^{+}} \langle I \rangle_{R,i}^{+} \right] - \frac{(\mu I)_{i-1/2}^{+}}{I_{i-1/2}^{+}} I_{i-1/2}^{+}$$

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

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

1. Assume lumped-LDFE spatial closure
   for $I^{\pm}(x)$, $T(x)$, & $T^4(x)$
2. Eliminate space-angle moments of $I_{LO}^{n+1/2}$ in terms of **time-averaged** moments $\bar{I}_{LO}^{n}$, e.g.,

$$\langle I \rangle_{L,i}^{n+1/2,+} = \gamma_{L,i}^{HO,+} \langle \bar{I} \rangle_{L,i}^{+,n}$$

   Coupled equations have same numerical complexity as a Backward Euler time-discretization

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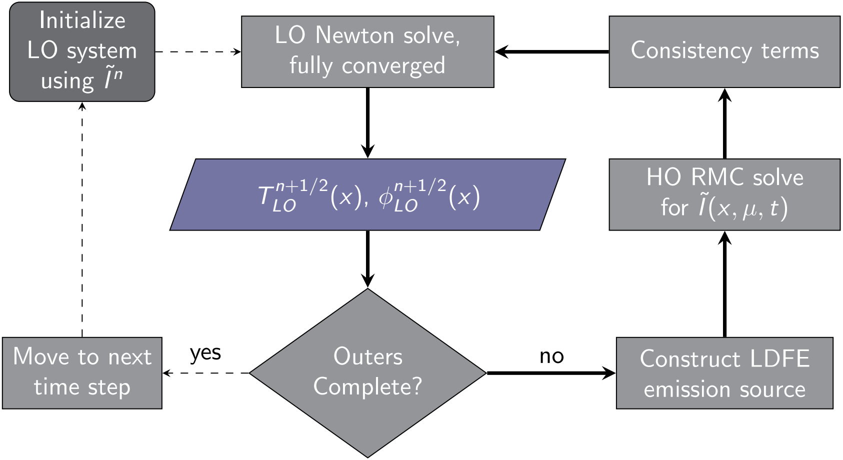
3. After Newton solve for time-averaged moments, use time closures to advance to the next time step

For thin problems, which are nearly linear one outer iteration is often sufficient



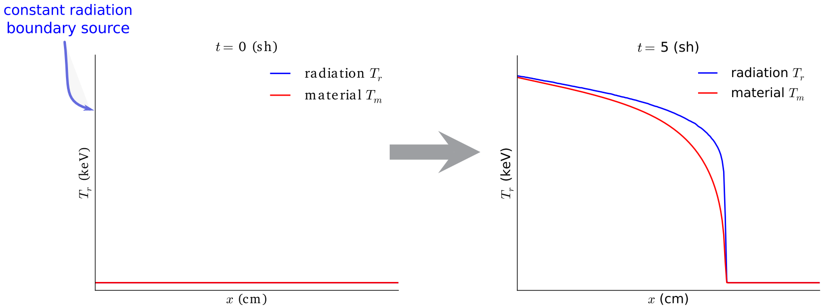
A HOLO Algorithm for Thermal Radiative Transfer

Implementation specifics for results are:

- IMC results from Jayenne (LANL code)
- One HO solve per time step,
  with two LO solves
- Figure of Merit: $\boxed{\mathrm{FOM} = \dfrac{1}{\left(\dfrac{\|\sigma(\phi_i)\|_2}{\|\phi_i\|_2}\right)^2 N_{\mathrm{total}}}}$

  normalized so IMC FOM=1

We will simulate several **Marshak Wave** problems with different values for the absorption cross section



Figures depict radiation temperature $T_r = \sqrt[4]{\phi/ac}$
or radiation energy-density $E_r = \phi/c$

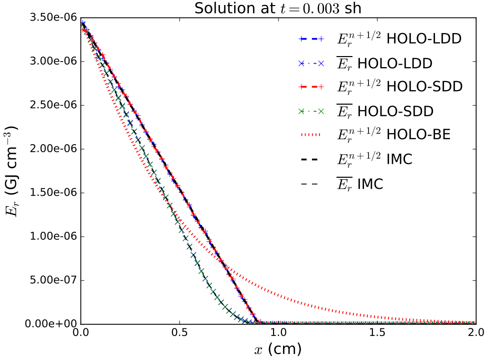
HOLO can preserve accuracy of IMC for near-void problem $\sigma_a = 10^{-9}$ cm^{-1}

Three large time steps, 10^6 histories per time step

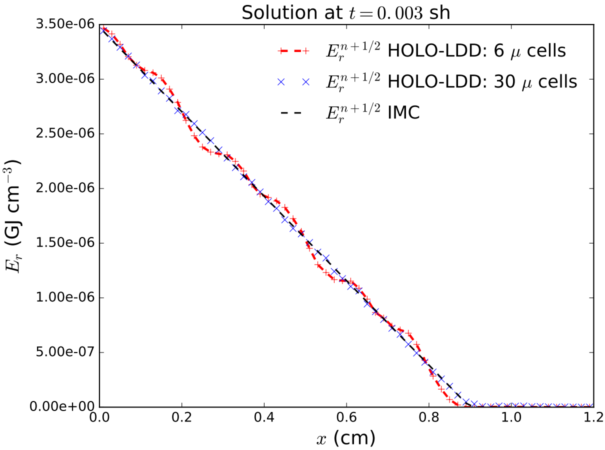
Plots depict radiation energy densities $E_r = \phi(x)/c$

IMC is more efficient for this limiting case

because HOLO resamples intensity between time steps



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

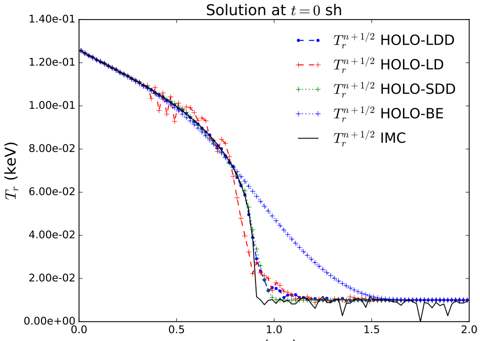


The time closure preserves the accuracy of MC time integration in LO solution

- 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/ doubly-discontinuous spaces, smaller Δt decrease noise but increase projection error

- HOLO Backward Euler (HOLO-BE) is inaccurate
  and HOLO-LD is unstable



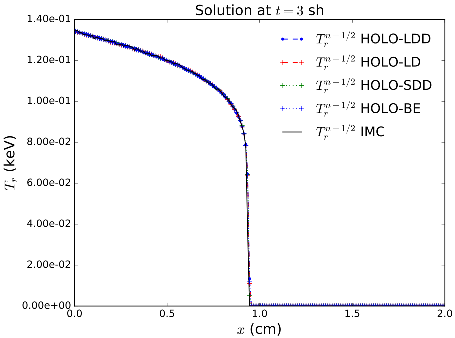
The HOLO method is more efficient than IMC with a sufficiently fine space-angle mesh

- 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-SDD (1)	IMC	HOLO-SDD(1)
30,000	2.93%	14.00%	1	unstable
1,000,000	0.49%	0.18%	1.02	81.7

The HO temporal closures are stable in a mix of thicknesses with sufficient histories

- Marshak wave problem, $\sigma \propto T^{-3}$, 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

RMC 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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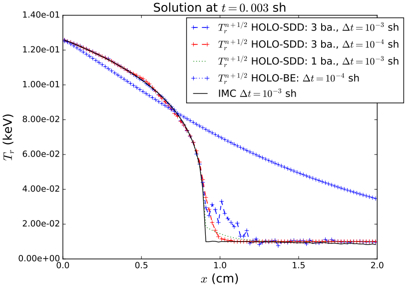
Near-void problem plotted as radiation temperatures



FOM and error norm definitions

Cell-averaged error norms

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

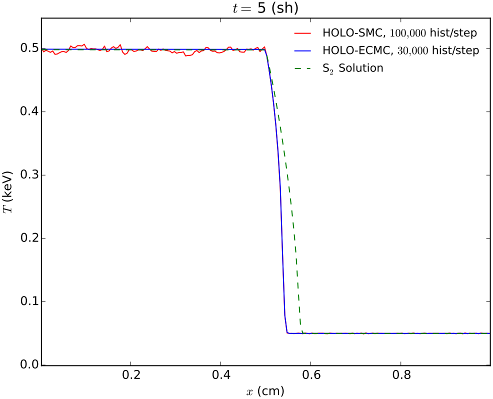
FOM is based on the following variance

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

RMC 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

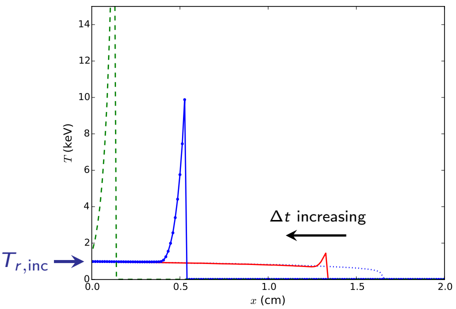
- Results for HOLO with different HO solvers:
  ECMC (FOM=10,000), standard MC (FOM=0.46), and S_2



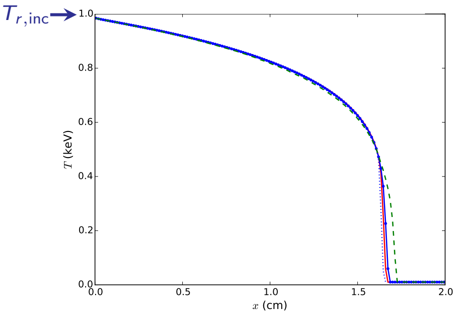
Our HOLO method preserves the maximum principle with sufficient nonlinear convergence

- **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

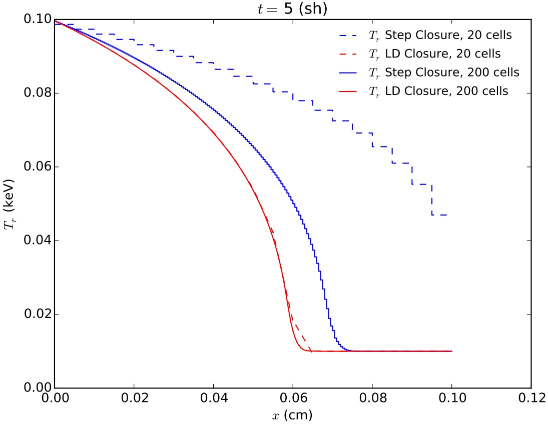
Apply iterative solution methods to TRT two material problem with diffusivity of the thick region increased

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, $+$

$$\frac{\langle\phi\rangle_{L,i}^{+,n+1} - \langle\phi\rangle_{L,i}^{+,n}}{c\Delta t} - 2\overline{\mu}_{i-1/2}^{+}\overline{\phi}_{i-1/2}^{+} + \overline{\{\mu\}}_{L,i}^{+}\langle\overline{\phi}\rangle_{L,i}^{+} + \overline{\{\mu\}}_{R,i}^{+}\langle\overline{\phi}\rangle_{R,i}^{+}$$

$$+ \sigma_{t,i}^{n+1} h_i \langle\overline{\phi}\rangle_{L,i}^{n+1,+} - \frac{\sigma_{s,i} h_i}{2}\left(\langle\overline{\phi}\rangle_{L,i}^{+} + \langle\overline{\phi}\rangle_{L,i}^{-}\right)$$

$$= \frac{h_i}{2}\langle\sigma_a^{n+1} acT^{n+1,4}\rangle_{L,i}, \quad (3)$$

Without sufficient histories, time closure can introduce instabilities