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

Simon Bolding

Advisor: Jim Morel

22 November 2016







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

Modeling materials under extreme conditions Temperatures  $\mathcal{O}(10^6)~\mathrm{K}$  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)

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

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

TRT equations are nonlinear and may be tightly coupled Absorption cross section ( $\sigma_a$ ) 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



Exponentially Convergent MC High-Order Solver

Derivation of the LO equations

Summary of algorithm

Computational Results

Monte Carlo time integration

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

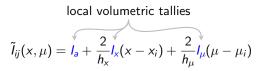
ECMC is an iterative form of residual Monte Carlo applied to particle transport problems

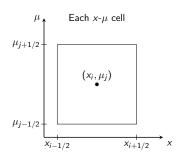
#### Each MC batch tallies the error in solution estimate

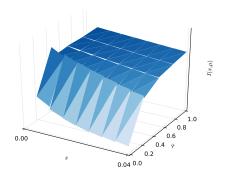
- standard MC particle transport, but a complex source
- ► ECMC requires a functional representation for all phase space variables being sampled

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







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

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

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

#### 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- $\mu$  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



Exponentially Convergent MC High-Order Solver

#### Derivation of the LO equations

Summary of algorithm

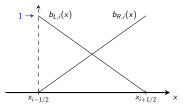
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### The LO equations are formed as *consistently* as possible with spatial and angular moments of TRT equations

The time discretization is backward Euler for both the HO and LO equations

Spatial moments are weighted with FE basis functions:



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

Half-range integrals reduce angular dimensionality

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

### 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

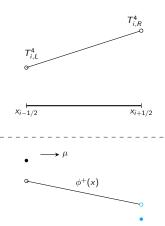
For example, apply  $\langle \cdot \rangle_{L,i}$  and  $(\cdot)^+$  to streaming term and perform algebra to form angular averages

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

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

### We eliminate auxillary spatial unknowns to close global system of equations

 $x_{i+1/2}$ 



 $x_{i-1/2}$ 

- 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.,

$$\phi^+_{i+1/2}=\gamma^+_{i,HO}\langle\phi\rangle^+_{a,i}+\langle\phi\rangle^+_{x,i}$$
 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/ approx. local balance equations over each spatial element

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Recast as a GMRES solution with DSA-preconditioning

### A HOLO Algorithm for Thermal Radiative Transfer



Exponentially Convergent MC High-Order Solver

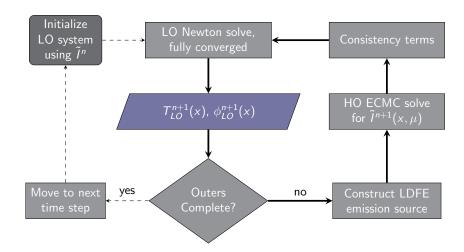
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### Iterations between the HO and LO systems can be performed each time step



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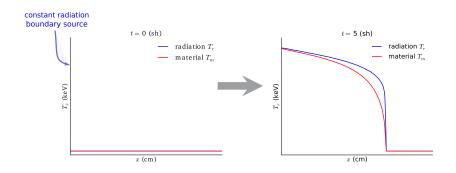
#### Implementation specifics for results are:

- ► 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: 
$$FOM = \frac{1}{\left(\frac{\|\sigma(\phi_i)\|}{\|\phi_i\|}\right)^2 N_{\mathsf{total}} }$$

normalized so IMC FOM=1

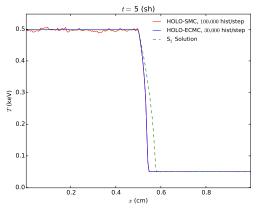
### We will test our method with several standard **Marshak Wave** problems



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

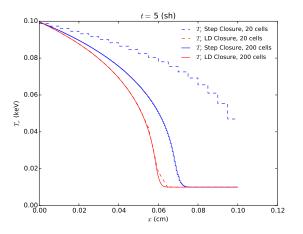
### ECMC is more efficient than standard MC as a HO solver

- ▶ Left half is optically thin ( $\sigma$ =0.2 cm<sup>-1</sup>), right half is thick ( $\sigma_a$ =2000 cm<sup>-1</sup>). 8  $\mu$  cells,  $\Delta t$  = 0.001 sh
- ▶ Results for HOLO with different HO solvers: ECMC (FOM=10,000), standard MC (FOM=0.46), and S<sub>2</sub>



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

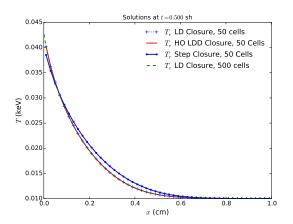
- ▶ EDL Problem: Large, constant  $\sigma_a$  and small  $c_v$
- ► Apply HOLO algorithm, 12k histories per step



#### Tested the HO spatial closure for a easier TRT problem

Fairly diffusive domain so that linear discontinuous T(x) is positive  $\Delta t$  increased from 0.001 sh to  $\Delta t_{\rm max} = 0.01$  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 HO Closure	1.60% 1.40%	0.59% 0.67%	0.76% 0.013%
*1 < 0.010/ C II II			

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

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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,  $\tilde{I}_{HO}(x,\mu)$  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:

$$\tilde{I}_{\mathsf{pos}} = I_{\mathsf{a}} + C \left[ \frac{2}{h_{\mathsf{x}}} I_{\mathsf{x}}(\mathsf{x} - \mathsf{x}_i) + \frac{2}{h_{\mu}} I_{\mu}(\mu - \mu_j) \right], \quad (\mathsf{x}, \mu) \in \mathcal{D}_{ij},$$

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

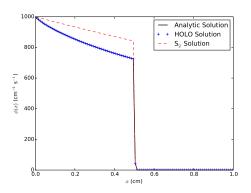
$$\mathsf{L}I^{(m+1)} = q + \mathsf{L}\left(\tilde{I}^{n+1,(m)} - \tilde{I}^{n+1,(m)}_{\mathsf{pos}}\right)$$

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

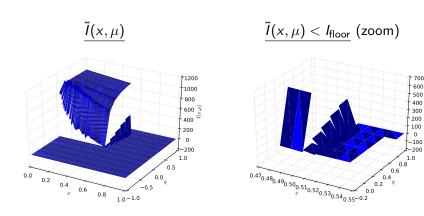
$$\tilde{I}^{(m+1)} = \mathbf{L}^{-1}q + (\tilde{I}^{(m)} - \tilde{I}^{(m)}_{\mathsf{pos}})$$

### 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
- $q(x) = I_{\mathsf{floor}} \sigma_{\mathsf{a}}(x)$



# The angular intensity is difficult to resolve at the material interface and near $\mu=0$



### Artificial source does not improve solution for analytic neutronics problem

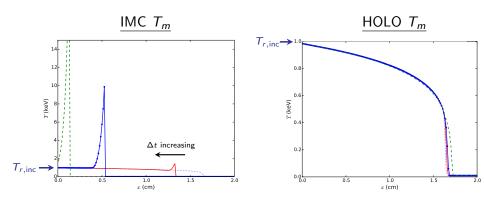
► Compute cell-averaged error norms for HO and LO solutions, with 4 batchs, 10<sup>5</sup> histories per batch

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



### 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

<sup>\*25.1</sup> damped Newton iterations per time step Scattering iteration relative tolerance  $10^{-10}$ 

### A HOLO Algorithm for Thermal Radiative Transfer



Exponentially Convergent MC High-Order Solver

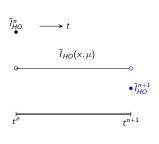
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# The time variable is included in the ECMC trial space allowing for accurate time integration of HO intensity



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

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

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

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

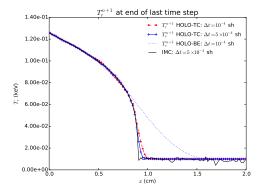
- 1. Form LO Equations with space-angle moments as before, but integrated over a time step Treat T(x) terms implicitly
- 2. Angular consistency terms are now time-averaged evaluated with time-averaged projection  $\bar{I}_{HO}(x,\mu)$
- 3. Eliminate space-angle moments of  $I_{LO}^{n+1}$  in terms of time-averaged moments  $\bar{I}_{LO}$ , e.g.,

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

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 sh
- ► For HOLO w/ time closure (HOLO-TC) smaller time steps decrease noise but increase projection error
- ► HOLO Backward Euler (HOLO-BE) is inaccurate



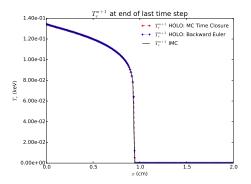
# The HOLO-TC method is more efficient than IMC with sufficiently fine mesh

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

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

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

► Marshak wave problem, 10<sup>6</sup> 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

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

Simon Bolding

Advisor: Jim Morel

22 November 2016





### Backup Slides

Simon Bolding

Advisor: Jim Morel





#### 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

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

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

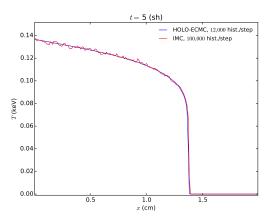
The system is *linearized* over a time step  $t \in [t^n, t^{n+1}]$  Opacities are evaluated with  $T(t^n)$ 

- 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** 

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

► Transient solution after 5 shakes ( $\sim$  520 steps) 200  $\times$  cells (and 4  $\mu$  cells for ECMC)



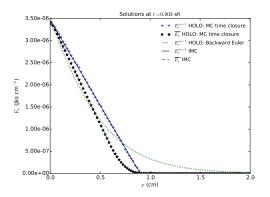
Time-integrated moment equation for L, +

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

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

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

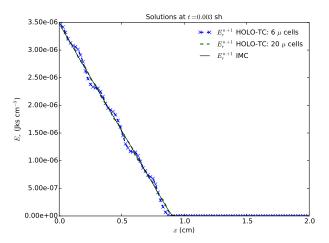
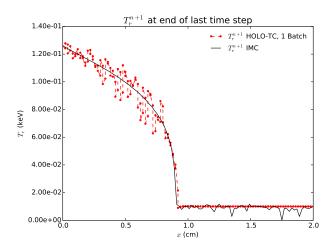
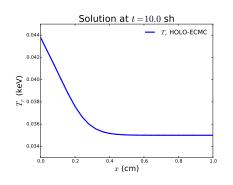


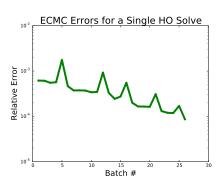
Figure : Comparison of radiation energy densities for the HOLO method with different numbers of  $\mu$  cells.  $\Delta t = 0.001$  sh, for near-void problem.

### Without sufficient histories, time closure can introduce instabilities



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





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

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

$$\mathbf{L}\tilde{I}^{(m)} = q - r^{(m)}$$

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

$$q \to q + \delta^{(m+1)}$$

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 <sub>surv</sub>	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:

$$\underline{B}(T^{n+1}) = \underline{B}(T^*) + (T^{n+1} - T^*) \frac{\partial \underline{B}}{\partial t} \Big|_{t=0}$$

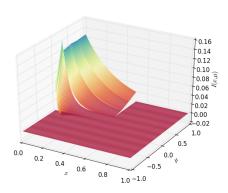
► Modified system

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

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

- ▶ 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  $\mu=\mathbf{0}$ 



### Timing Results For Two Material Problem

	hists./step	$\Delta t(sh)$	IMC ( $\mu$ s/hist.)	HOLO-ECMC ( $\mu$ s/hist)	Newt
	100,000	0.001	17	3.5	
	30,000	0.001	18	6.9	
	30,000	0.005	59	7.4	
- 1					

### Forming the LO System

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

- ► Cell unknowns:  $\langle \phi \rangle_{L,i}^+$ ,  $\langle \phi \rangle_{R,i}^+$ ,  $\langle \phi \rangle_{L,i}^-$ ,  $\langle \phi \rangle_{R,i}^-$ ,  $\langle \phi \rangle_{R,i}^-$ ,  $\langle \phi \rangle_{R,i}^-$
- Need angular consistency terms and spatial closure (LD)