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

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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

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 calculations

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

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

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

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

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

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

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 MC transport problem
  with effective emission and scattering terms

- Emission source is **not** fully implicit.
  Monte Carlo integration over Δt for intensity

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

Standard IMC	HOLO Method
Large statistical noise possible	ECMC is very efficient for TRT problems
Effective scattering can make MC 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

Solve a non-linear low-order system with high-order angular correction from efficient MC simulations

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

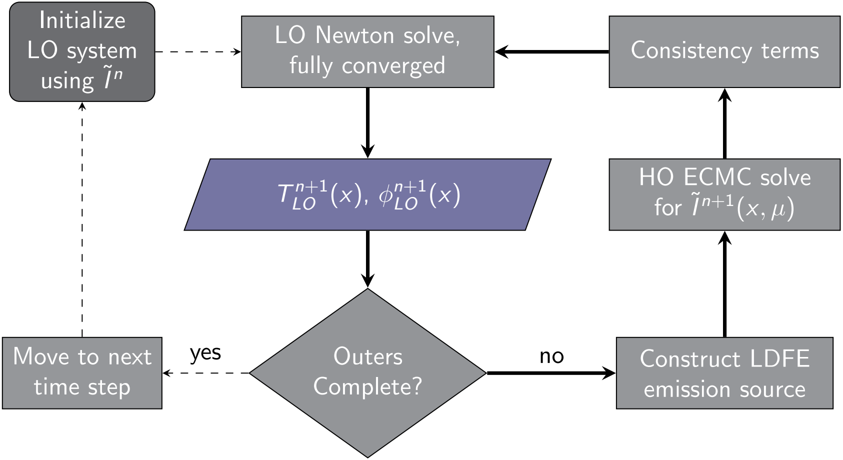
- **Output:** linear-discontinuous $\phi(x)$ and $T(x)$
  Construct LDFE scattering and emission source

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

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

- **Output:** consistency terms

Iterations between the HO and LO systems are performed each time step



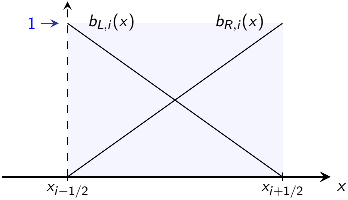
A HOLO Algorithm for Thermal Radiative Transfer

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

FE basis functions weight spatial moments:



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

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

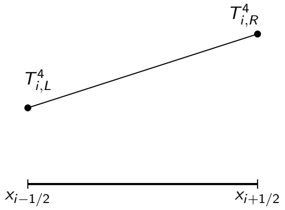
Ultimately, we get 4 radiation and 2 material equations
for each spatial element i

The streaming terms are algebraically manipulated
to form consistency terms (no approximation here)

For example, apply $\langle\cdot\rangle^{+}_{L,i}$ to a streaming term:

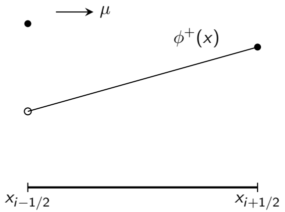
$$\begin{aligned}
\left\langle \mu \frac{\partial I}{\partial x} \right\rangle^{+}_{L} &= -\frac{2}{h_i}\{\mu I\}^{+}_{i-1/2} + \langle \mu I\rangle^{+}_{L,i} + \langle \mu I\rangle^{+}_{R,i} \\
&= -\frac{2}{h_i}\boxed{\frac{\{\mu I\}^{+}_{i-1/2}}{\phi^{+}_{i-1/2}}}\phi^{+}_{i-1/2} + \boxed{\frac{\langle \mu I\rangle^{+}_{L,i}}{\langle\phi\rangle^{+}_{L,i}}}\langle\phi\rangle^{+}_{L,i} + \boxed{\frac{\langle \mu I\rangle^{+}_{R,i}}{\langle\phi\rangle^{+}_{R,i}}}\langle\phi\rangle^{+}_{R,i}
\end{aligned}$$

We can close equations with HO angular information and a linear-discontinuous (LD) spatial discretization



1. Assume $T(x)$ and $T^4(x)$ are LD

2. A lagged $\tilde{I}^{n+1}_{\mathrm{HO}}$ is used
   to evaluate consistency terms



3. Eliminate $\phi^{\pm}_{i+1/2}$ with LD closure
   preserving equi. diff. limit

$$\boxed{\phi^+_{i+1/2} = 2\langle\phi\rangle^+_{R,i} - \langle\phi\rangle^+_{L,i}}$$

4. Global system solved with Newton's method and lagged **implicit opacities**
   Energy is always conserved

A HOLO Algorithm for Thermal Radiative Transfer

Exponentially Convergent Monte Carlo can efficiently reduce noise globally

Each MC batch tallies the error in the solution

- standard MC particle transport, but a complex source
- ECMC requires a functional representation of $I(x, \mu)$

Can reduce solution error globally $\propto e^{-\alpha N}$

Adaptive h-refinement can help represent error

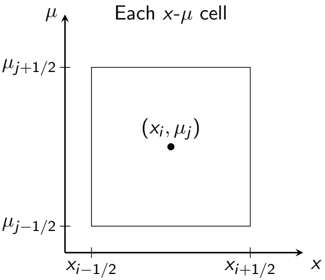
$I^n(x, \mu)$ often provides an **excellent** estimate of $I^{n+1}(x, \mu)$

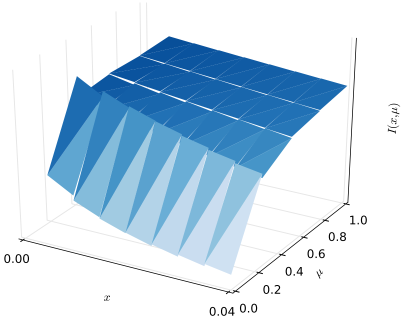
No MC sampling from thermal equilibrium regions

We use a projection $\tilde{I}(x,\mu)$ of the angular intensity onto a LDFE space-angle mesh

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 HO 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 simple variance reduction methods

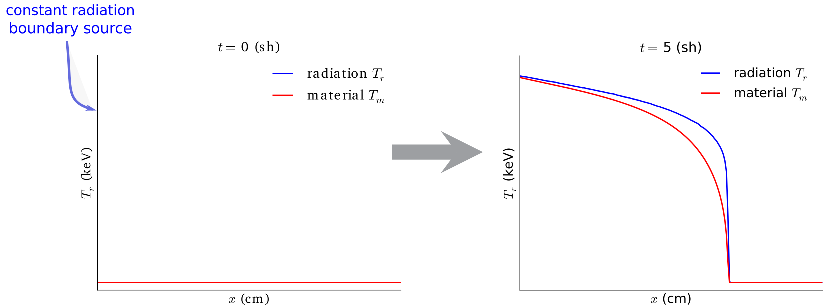
Histories stream without collision
along path s, weight reduces as $w(s) = w_0 e^{-\sigma_t s}$

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 cells
  except for cells in thermal equilibrium

A HOLO Algorithm for Thermal Radiative Transfer

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



Results show radiation temperature $T_r = \sqrt[4]{\phi/ac}$

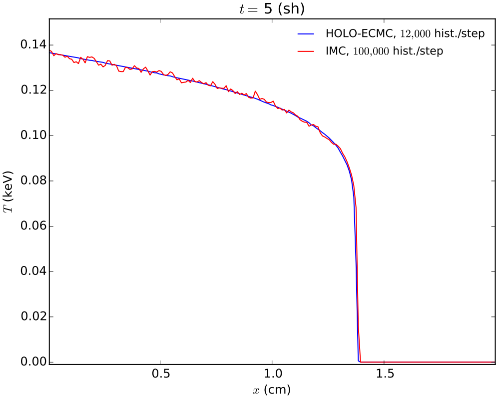
Several specifics for most results shown:

- Initial Δt of 0.001 sh (0.01 ns), linearly increased to 0.01 sh by 15% per step
- One HO solve per time step (predictor-corrector)
  - *each HO* solve has 3 ECMC batches
    no mesh refinement
- FOM$= \dfrac{1}{\|s\|^2 N_{\text{total}}}$, normalized to IMC result

The HOLO method produces significantly less noise than IMC in a Marshak Wave test problem

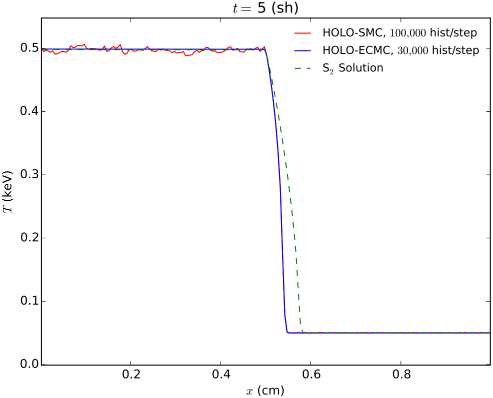
- $\sigma_a \propto T^{-3}$

- Transient solution after 5 shakes
  200 x cells and 4 μ cells (for ECMC)



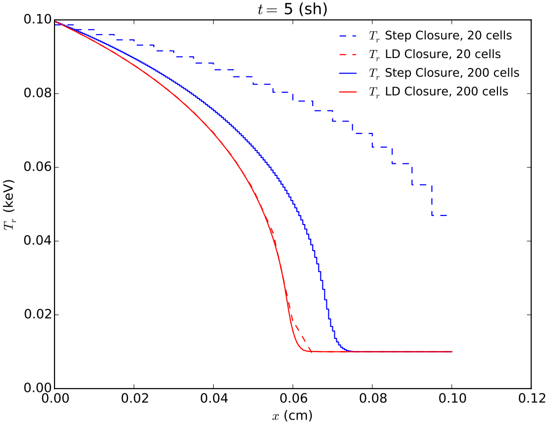
ECMC is more efficient than standard MC (SMC) as a HO solver

- Left half is optically thin ($\sigma = 0.2$ cm^{-1}), right half is thick ($\sigma_a = 2000$ cm^{-1}). 8 μ cells
- Different HO solvers: ECMC with 3 batches, standard MC (SMC), and an S_2 solution



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

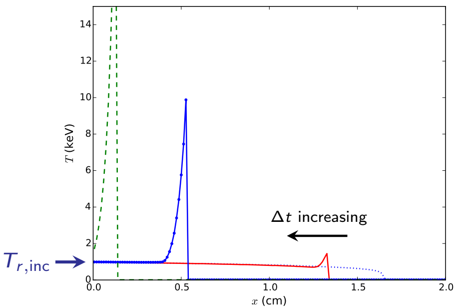
- Large, constant σ_a and small c_v



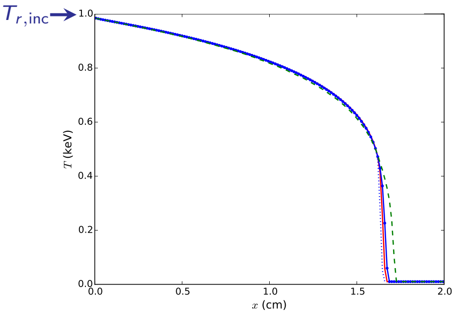
Our HOLO method preserves the maximum principle with sufficient nonlinear convergence

- **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

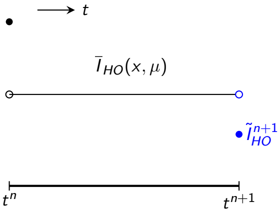


HOLO T_m



A HOLO Algorithm for Thermal Radiative Transfer

A doubly-discontinuous trial space in time allows for a MC temporal closure



Include $\frac{1}{c}\frac{\partial}{\partial t}(\cdot)$ in transport operator $\mathbf{L}$
with $T(x)$ still implicit

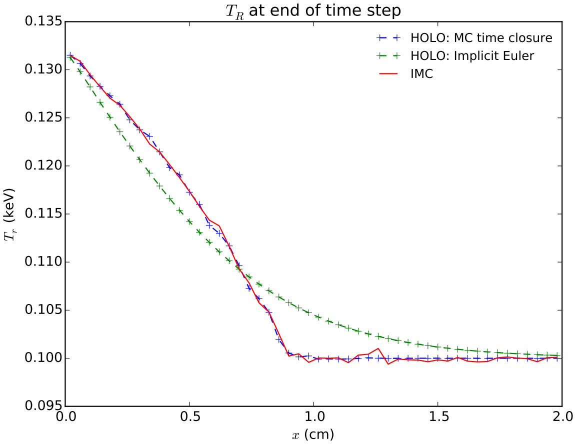
Sample and track in time
Tally error projection at t^{n+1}

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

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

The time-closure parameters preserve the accuracy of MC time integration

- Material is near-void, so temperature uncouples
  take 3 large time steps and compare T_R^{n+1}



A few other topics are under investigation

Negative intensities can occur in optically thick cells
Investigating artificial source with alternate trial space

Using HO solution to estimate spatial closure
by including face tallies

Source iteration with diffusion synthetic acceleration
for the LO equations

A HOLO Algorithm for Thermal Radiative Transfer

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

The LO system can resolve nonlinearities
with bounded angular consistency terms

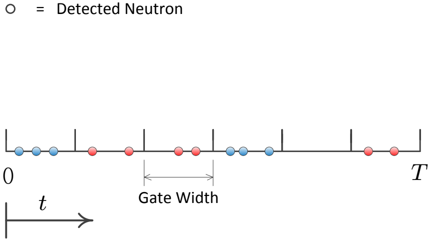
The next step is to extend to higher dimensions
main hurdle to overcome is infrastructure

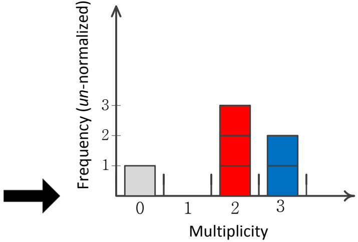
Simulations of Neutron Multiplicity Experiments with Perturbations to Nuclear Data

Simon Bolding and C.J. Solomon

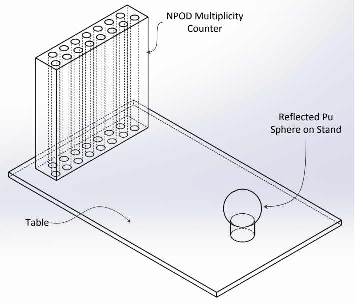
4 August 2016

Neutron multiplicity distributions provide passive multiplication information about a fissionable system





Multiplicity experiments were performed at LANL for validating subcritical simulations



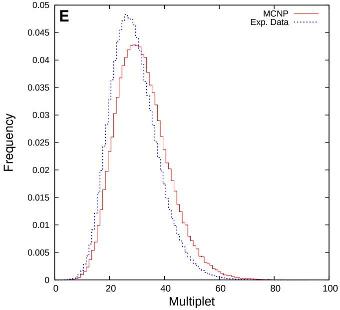
*Not to scale

Experimental Parameters

- 94% ^{239}Pu sphere
- 5 Different HDPE shells
  From none to 3.0 cm HDPE

Experiments repeated w/ ^{252}Cf

MCNP5 multiplicity simulations showed discrepancy for Pu but not for ^{252}Cf



Pu with 3.0-cm HDPE reflector

Previous work by Mattingly [2010]

- Caused by ^{239}**Pu** nuclear data
- Adjusted energy-integrated $\overline{\nu}$

ENDF adjusted $\overline{\nu}$ for ^{239}Pu
to match k_{eff} benchmarks

- $\overline{\nu}$ is $\sim 2\,\sigma$ above measured data for $E < 1.5$ MeV

Can we reduce discrepancy in multiplicity distributions without significantly altering k_{eff} ?

Perform energy-dependent perturbations of $\overline{\nu}(E)$ in ^{239}Pu
Random samples drawn from ENDF-VII.1 covariance data

Compare experimental and simulated multiplicity dist.
and a k_{eff} benchmark (Jezebel)

Compare $\overline{\nu}(E)$ results to energy-*independent* shifts of microscopic cross sections

We used LANL NDVV Python tools to generate energy-dependent $\overline{\nu}$ samples

1. Generate correlated samples of $\overline{\nu}(E)$
   - Assumed multivariate Gaussian
     with group-averaged covariances
2. Modify $\overline{\nu}(E)$ data in **ACE** file
3. Perform all MCNP simulations with modified ACE data

A cost function provides a measure of inaccuracy for each data realization

Reduced χ^2 values for the 5 multiplicity experiments and criticality benchmark

$$\chi^2_{\mathsf{red,mult},m} = \frac{1}{N_{bins} - 1} \sum_{i=1}^{N_{bins}} \frac{(P_i^{\mathrm{exp}} - P_i^{\mathrm{mcnp}})^2}{\sigma^2(P_i^{\mathrm{exp}}) + \sigma^2(P_i^{\mathrm{mcnp}})}$$

Equally weight χ^2 values in a cost function

the lower the score the higher the accuracy

$$\boxed{\mathrm{Cost} = \sum_{m=1}^{5} \chi^2_{\mathsf{red,mult},m} + \chi^2_{\mathsf{red},k_{\mathsf{eff}}}}$$

Multiplicity and k_{eff} simulations were performed for 500 unique realizations of $\overline{\nu}$ data

Trial	Cost	$\chi^2_{k_{\text{eff}}}$
$\overline{\nu}$ -1.14%	164.24	33.66
303	**197.07**	**4.18**
55	267.9	0.01
Original	426.86	0.27

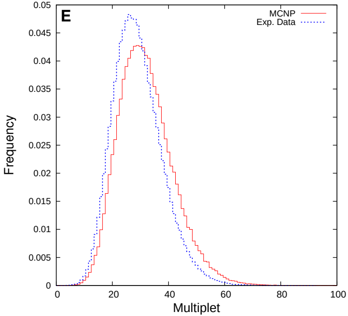
MCNP criticality test suite performed for best data
which includes 39 criticality benchmarks w/ ^{239}Pu :

Trial	*RMSD*
$\overline{\nu}$ -1.14%	1.23%
303	0.51%
Original	0.49%

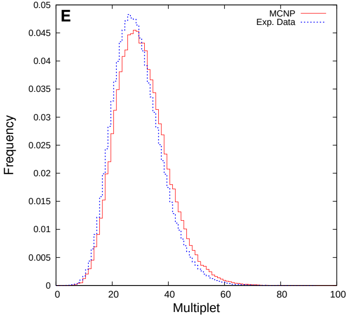
Energy-dependent $\overline{\nu}$ perturbations improved all 5 multiplicity distributions

- Plots for best data realization and 3.0 cm HDPE case

Original $\overline{\nu}$ Data

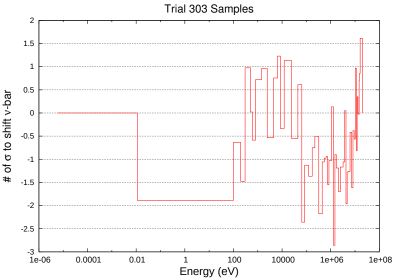


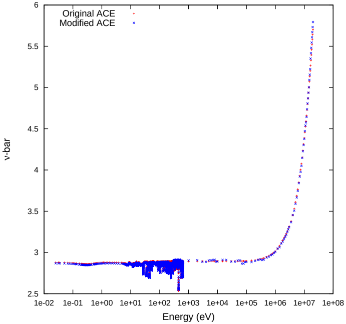
Trial 303: Lowest Cost



- Best data set reduced bias in 1st and 2nd moments, averaged over all 5 simulations, by $\sim 35\%$

The best $\overline{\nu}$ data (trial 303)





Fractional shifts to cross sections were made for comparison

Adjusted single cross sections uniformly at all energies
compensated with σ_{tot} or σ_{el}

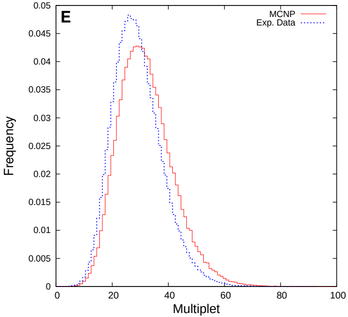
Scaling capture cross section was not effective
relative to variance in data

Scaling fission cross section 1.5% ($< 1\sigma$)
improved multiplicity distributions

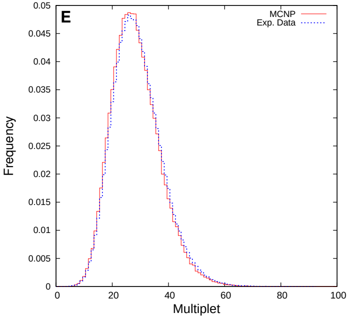
- Adjust elastic scattering (σ_{el}) to compensate change in σ_f, for $E > 1$ keV
- Better improvement that uniform scaling of $\overline{\nu}$

Adjusting the fission cross section showed good correction to multiplicity simulations

Original σ_f Data



σ_f decreased 1.5%



- High accuracy for all simulations: $\sum_{i=1}^{5} \chi^2_{red,mult,m} = 14.6$
- k_{eff} is not preserved: $\chi^2_{k_{\text{eff}}} = 22.6$

Simulations of Multiplicity Experiments with Nuclear Data Perturbations

Energy-dependent $\overline{\nu}$ perturbations reduced inaccuracies in multiplicity while preserving k_{eff}

- Majority of cross-correlation terms $\mathcal{O}(10^{-4})$ or less
- σ_f may need more investigation

Subcritical simulations should be considered in validation of nuclear data

Covariance sampling methodology was developed and demonstrated

- Ideally sample all cross sections and $\overline{\nu}$ simultaneously

Backup Slides

S.R. Bolding[1], C.J. Solomon[2]

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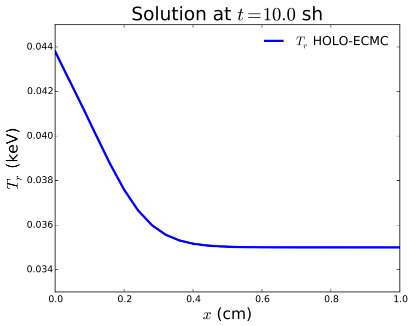
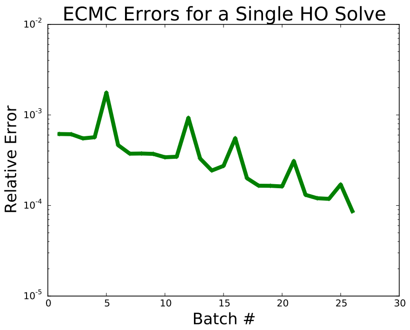
[2] *Los Alamos National Laboratory, Los Alamos, NM*

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

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

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

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

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

We can delay error stagnation

Investigating alternative positive projection of I

Solving LO System with Newton's Method

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

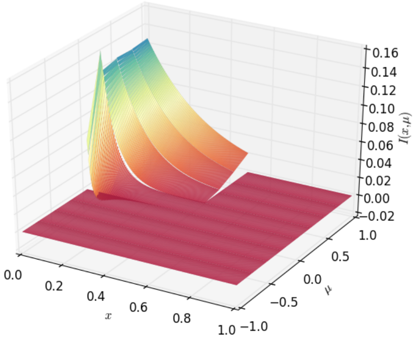
$$\left[\mathbf{D}(\mu^{\pm}) - \sigma_a^*(1-f^*)\right] \underline{\Phi}^{n+1} = f^* \underline{B}(T^*) + \frac{\underline{\Phi}^n}{c\Delta t}$$

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

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

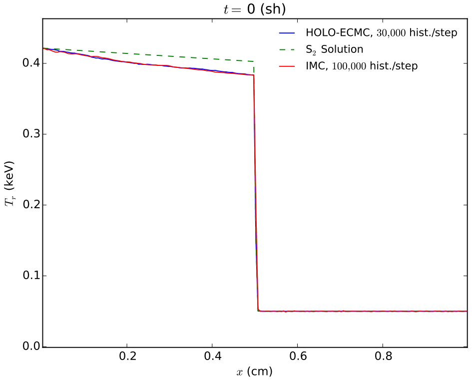
- Equation for T^{n+1} based on linearization that is conservative
- Converge T^{n+1} and $\langle \phi \rangle$ with Newton Iterations

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



Two Material Problem, comparison in optically thin region

- Plot of radiation temperature after 10 time steps



Backup slide with timing results

Derivation of LO System

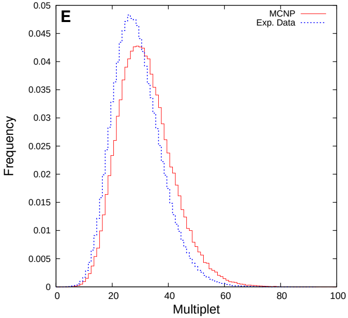
- Taking moments of TE yields 4 equations, per cell i, e.g.

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

- 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)

Energy-Integrated $\overline{\nu}$ Shift – 3.0 cm HDPE reflector

Original $\overline{\nu}$ Data



-1.14% $\overline{\nu}$ *Data*