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

Simon Bolding and Jim Morel

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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

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 $T(x, t)$

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

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

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

Overview of algorithm

Derivation of the LO equations

Exponentially Convergent MC High-Order Solver

Computational Results

Ongoing Research

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

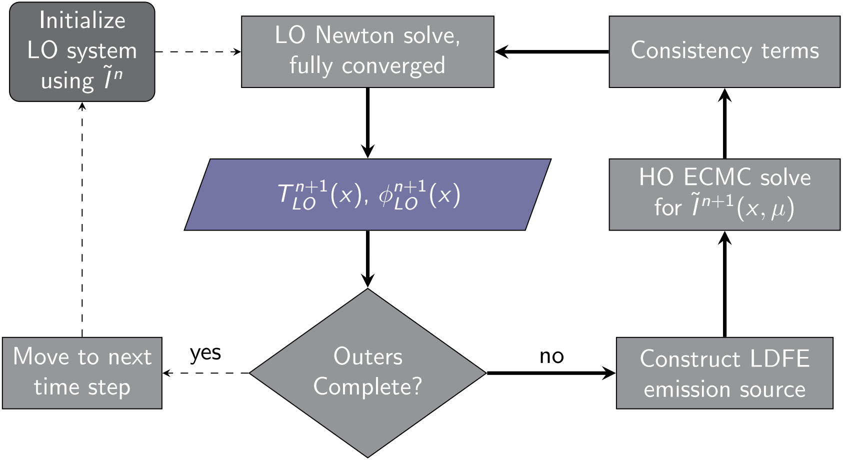
- **Output:** linear-discontinuous $\phi(x)$ and $T(x)$
  Construct LDFE scattering and emission source

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



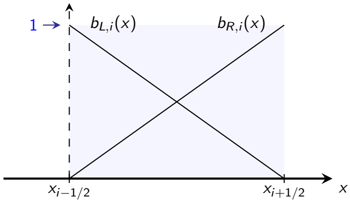
A HOLO Algorithm for Thermal Radiative Transfer

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

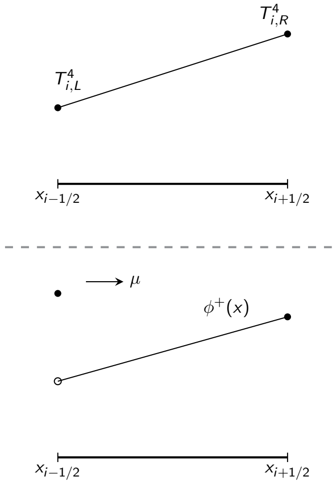
Ultimately, we get 4 radiation and 2 material equations
for each spatial element i

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

Use source-iteration with diffusion-synthetic acceleration (DSA) to solve LO equations

In higher dimensions, the scattering terms cannot be directly inverted easily

Use source iteration 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 with local balance equations over elements

Recast iterations as DSA-preconditioned Krylov method
to resolve convergence difficulties with inconsistencies

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 $I(x, \mu)$

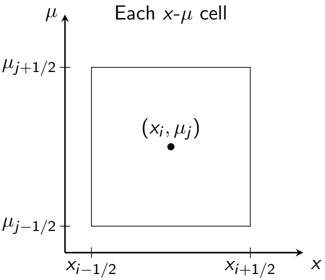
Can reduce solution error globally $\propto e^{-\alpha N}$
Adaptive *h*-refinement can help represent error

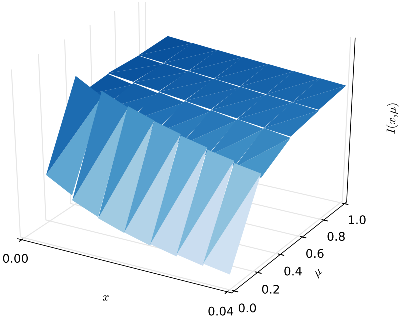
$I^n(x, \mu)$ often provides an *excellent* estimate of $I^{n+1}(x, \mu)$
No MC sampling for equilibrium regions

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

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

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

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 Monte Carlo simulation
- Update solution:

$$\begin{aligned}\tilde{I}^{n+1,(m+1)} &= \tilde{I}^{n+1,(m)} + \tilde{\epsilon}^{(m)} \\ &= \tilde{I}^{n+1,(m)} + \mathbf{L}^{-1}q - \mathbf{L}^{-1}\mathbf{L}\tilde{I}^{n+1,(m)}\end{aligned}$$

Our HO system allows for simple variance reduction methods

Histories stream without collision

along path s, weight reduces as $w(s) = w_0 e^{-\sigma_t s}$

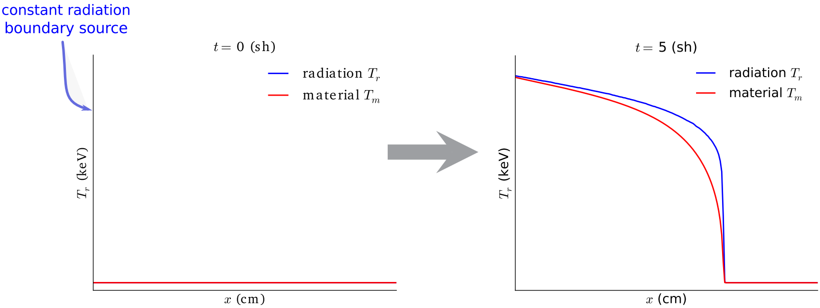
Use cell-wise systematic sampling for $|r^{(m)}|$ source

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

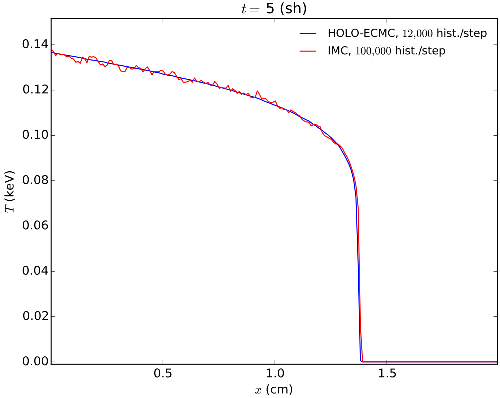
We will test our method with several standard **Marshak Wave** problems



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

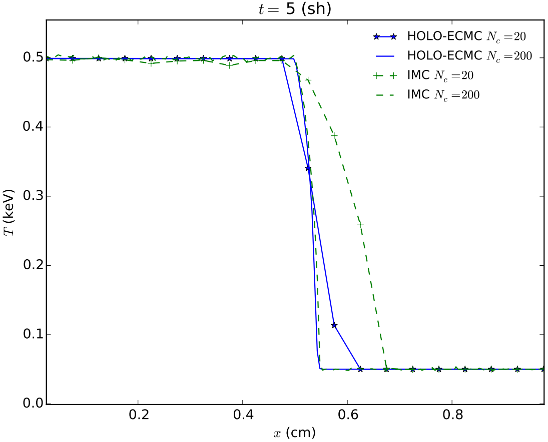
The HOLO method produces significantly less noise than IMC in a Marshak Wave test problem

- $\sigma_a \propto T^{-3}$
- Transient solution after 5 shakes
  200 x cells and 4 μ cells (for ECMC)

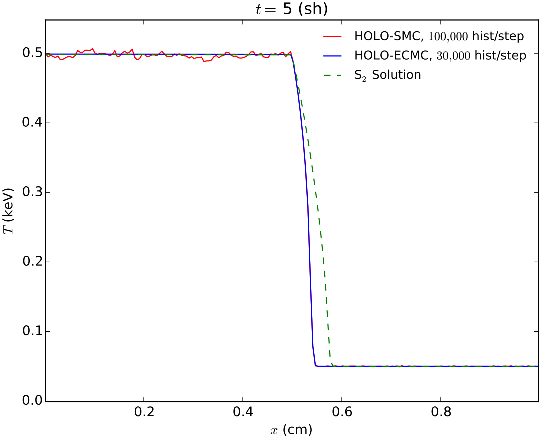


The LDFE representation has higher spatial accuracy than IMC linear reconstruction for two material problem

Problem features an optically thin (left) and optically thick (right) region. ECMC uses 8 μ cells



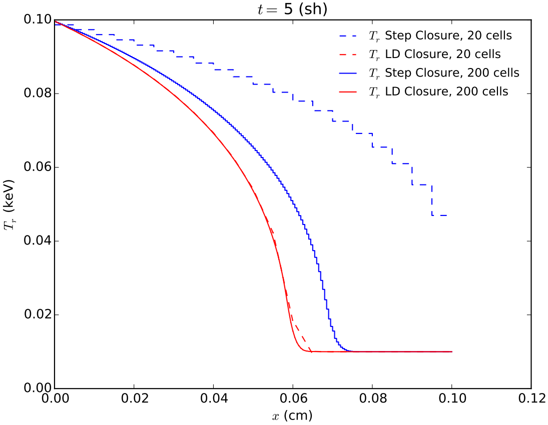
ECMC is more efficient than standard MC (SMC) as a HO solver



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

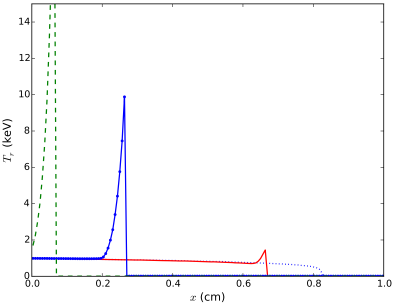


Our HOLO method preserves the maximum principle

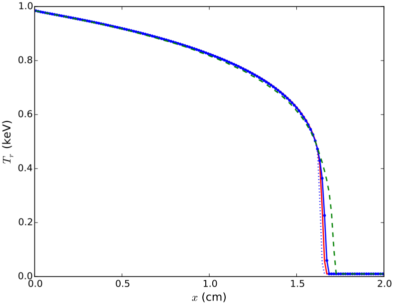
Comparison of material temperatures for different Δt

- $\sigma_a \propto T^{-3}$, c_v is small
- HOLO Newton Iterations required damping

IMC

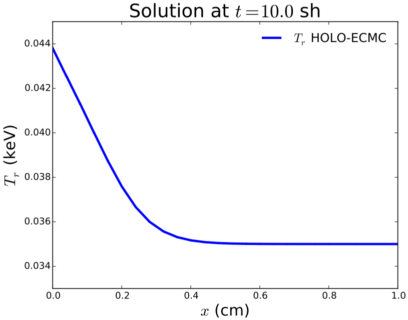


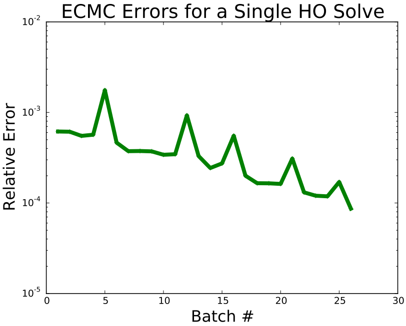
HOLO



DSA calculations

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





A HOLO Algorithm for Thermal Radiative Transfer

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

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

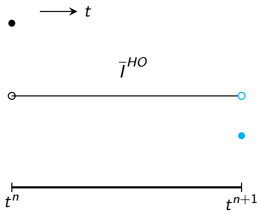
$\Rightarrow$

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

Could add source to LO equation
but it would affect energy conservation

Alternatively, add $\delta = -r^{(m)}_{\text{pos}}(x,\mu)$ to negative cells
I_{pos} must be recomputing based on balance

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



Include $\frac{1}{c}\frac{\partial}{\partial t}(\cdot)$ in **L**

with $T(x)$ still implicit

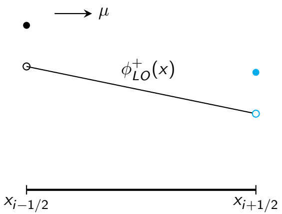
Sample and track in time

Tally $\tilde{\epsilon}(x,\mu)$ at t^{n+1}

In LO equations parameterize ϕ_{LO}^{n+1} using time-averaged quantities

$$\phi_R^{+,n+1} = 2\frac{\gamma^+_{i,HO}}{2}\langle\phi\rangle^+_{R,i} + \frac{\gamma^+_{i,HO} - 3}{2}\langle\phi\rangle^+_{L,i}$$

We will use a linear doubly-discontinuous (LDD) trial space to allow for a HO spatial closure



- $\tilde{I}_{HO}(x,\mu)$ will be linear in μ along face
  Error estimated with MC face tallies
- In LO equations use LDD for $\phi^{\pm}$
  The linear interior preserves the EDL
- Parameterize LO spatial closure to eliminate outflow:

$$\phi^+_{i+1/2} = \frac{3 + \gamma^+_{i,HO}}{2}\langle\phi\rangle^+_{R,i} + \frac{\gamma^+_{i,HO} - 3}{2}\langle\phi\rangle^+_{L,i}$$

There are several topics left to investigate:

1. Resolving issues with negative intensities
    - Accuracy of added source method
    - Consistency with LO solution
2. Using HO solution to estimate spatial closure
3. Source iterations with DSA for LO system
4. Implement damped Newton method to demonstrate maximum principle preservation in extreme problems
5. (Stretch goal) MC integration in time with consistent LO equations

Backup Slides

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Implementation specifics for results in the computational results section

- The LD representation of $I(x, \mu)$ is negative near the wave-front
  - Here, no correction is applied to the HO solution, and the LO solution uses lumped LD and S_2 equivalent terms in negative elements

- <u>For all results</u>
  1. Initial Δt of 0.001 sh (0.01 ns), linearly increased to 0.01 sh by 15% per step
  2. One HO solve per time step (predictor-corrector)
     - *each HO* solve has 3 ECMC batches
  3. $\sigma_s = 0$
  4. No mesh refinement in ECMC

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

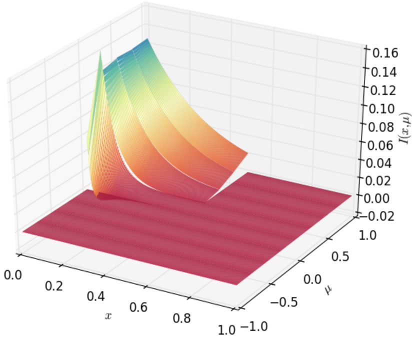
$$\left[\mathbf{D}(\mu^{\pm}) - \sigma_a^*(1-f^*)\right] \underline{\Phi}^{n+1} = f^* \underline{B}(T^*) + \frac{\underline{\Phi}^n}{c\Delta t}$$

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

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

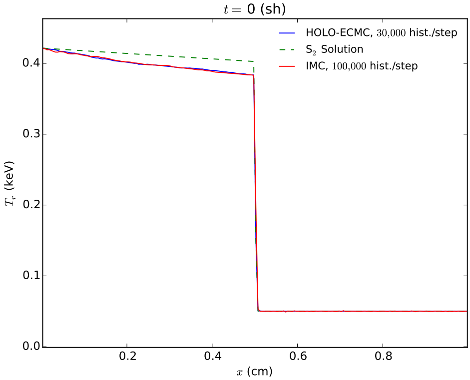
- Equation for T^{n+1} based on linearization that is conservative
- Converge T^{n+1} and $\langle\phi\rangle$ with Newton Iterations

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



Two Material Problem, comparison in optically thin region

- Plot of radiation temperature after 10 time steps



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)