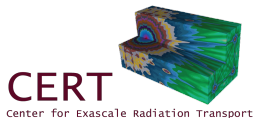


# A High-Order Low-Order Algorithm with Exponentially-Convergent Monte Carlo for Thermal Radiative Transfer

Simon Bolding and Jim Morel

4 August 2016



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  $T(x, t)$

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

Equations are **nonlinear** and may be tightly coupled

Absorption opacity ( $\sigma_a$ ) 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  $\Delta t$  for intensity

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

## Standard IMC

Large **statistical noise** possible

**Effective scattering** can make MC very expensive

Linearization can cause **non-physical** results (maximum principle violations)

Reconstruction of linear emission shape limits artificial energy propagation

## HOLo Method

ECMC is **very efficient** for TRT problems

MC solution has **no scattering**

Fully **implicit** time-discretization and LO solution **resolves nonlinearities**

Linear-discontinuous FE for  $T(x)$  preserving equilibrium diffusion limit

# A HOLO Algorithm for Thermal Radiative Transfer

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Overview of algorithm

Derivation of the LO equations

Exponentially Convergent MC High-Order Solver

Computational Results

Remaining Research

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# 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

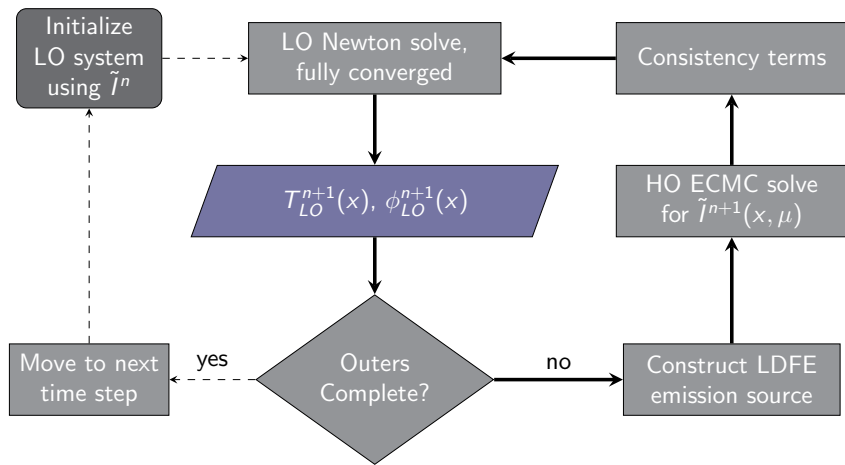
- ▶ Reduced dimensionality in angle  
allows for solution with Newton's method
- ▶ **Output:** linear-discontinuous  $\phi(x)$  and  $T(x)$   
Construct LDFE scattering and emission source

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



Overview of algorithm

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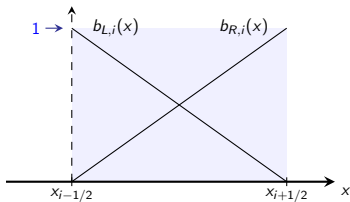
Exponentially Convergent MC High-Order Solver

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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
- ▶ FE basis functions are used for spatial moments



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

- ▶ Half-range integrals reduce angular dimensionality

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

Four moments of the transport equation  
are manipulated to form angular **consistency terms**

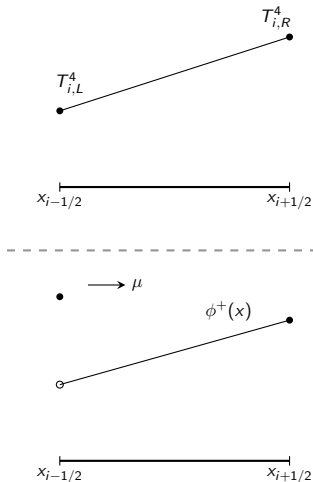
$$\begin{aligned}
 & -2 \mu_{i-1/2}^{n+1,+} \phi_{i-1/2}^{n+1,+} + \{\mu\}_{L,i}^{n+1,+} \langle \phi \rangle_{L,i}^{n+1,+} + \{\mu\}_{R,i}^{n+1,+} \langle \phi \rangle_{R,i}^{n+1,+} + \\
 & \left( \sigma_t^{n+1} + \frac{1}{c\Delta t} \right) h_i \langle \phi \rangle_{L,i}^{n+1,+} - \frac{\sigma_s h_i}{2}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

At this point, these equations are **exact**.

We performed algebra to form **consistency terms**:

$$\{\mu\}_{L,i}^{n+1,+} := \frac{\int_0^1 \int_{x_{i-1/2}}^{x_{i+1/2}} \mu b_{L,i}(x) I^{n+1}(x, \mu) dx d\mu}{\int_0^1 \int_{x_{i-1/2}}^{x_{i+1/2}} b_{L,i}(x) I^{n+1}(x, \mu) dx d\mu}$$

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



1. Assume  $T(x)$  and  $T^4(x)$  are LD
2.  $\tilde{I}_{\text{HO}}^{n+1}$  is used to evaluate consistency terms with high accuracy

3. Eliminate  $\phi_{i+1/2}^\pm$  with LD closure ensuring preservation of the EDL

$$\phi_{i+1/2}^+ = 2\langle\phi\rangle_{R,i}^+ - \langle\phi\rangle_{L,i}^+$$

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

# A HOLO Algorithm for Thermal Radiative Transfer

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# 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 is required to represent error

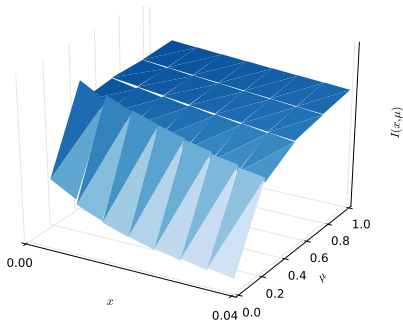
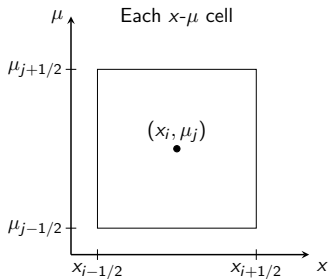
$I^n(x, \mu)$  often provides an *excellent* estimate of  $I^{n+1}(x, \mu)$

No MC sampling for equilibrium regions

We use a **projection**  $\tilde{I}(x, \mu)$  of the angular intensity onto a LDFFE 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

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

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:

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

# 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  $x-\mu$  cell  $\propto |r^{(m)}|$  in cell
- ▶ Set minimum  $n$  for cells  
except for cells in thermal equilibrium

# A HOLO Algorithm for Thermal Radiative Transfer

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Overview of algorithm

Derivation of the LO equations

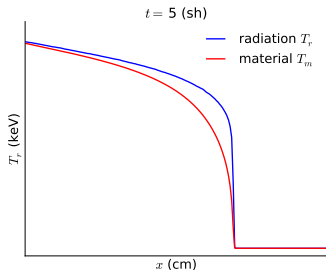
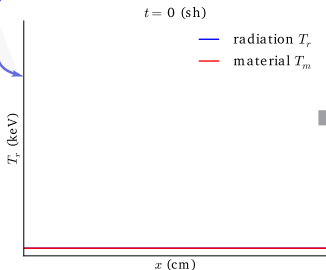
Exponentially Convergent MC High-Order Solver

Computational Results

Remaining Research

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

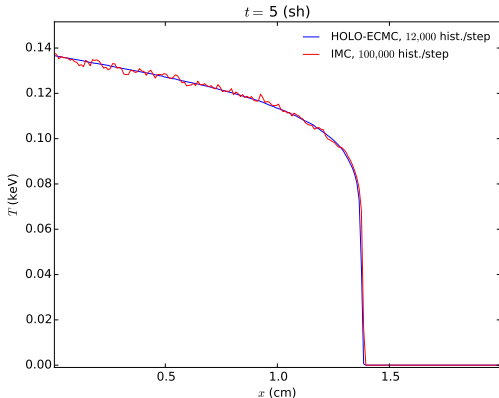
constant radiation  
boundary source



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

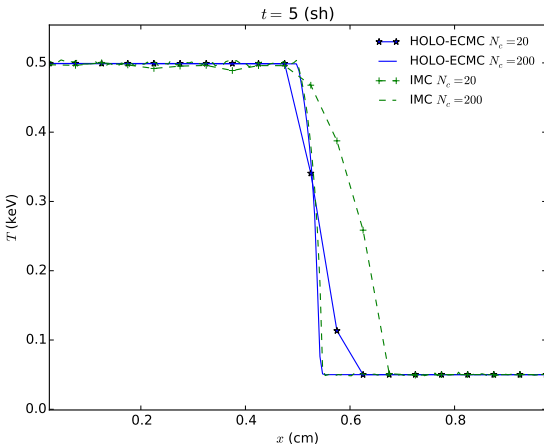
# The HOLO method produces significantly less noise than IMC for a Marshak Wave Test Problem

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

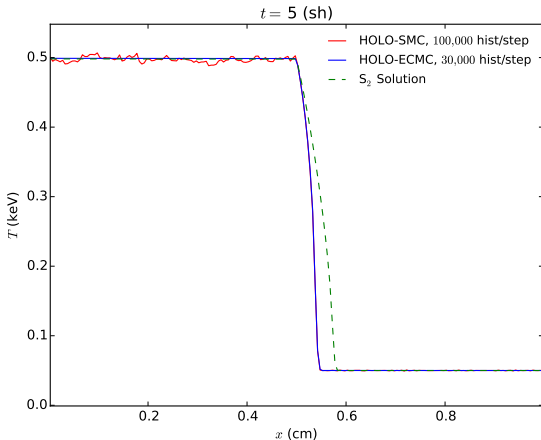


The LDFFE representation has higher spatial accuracy than IMC linear reconstruction for two material problem

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

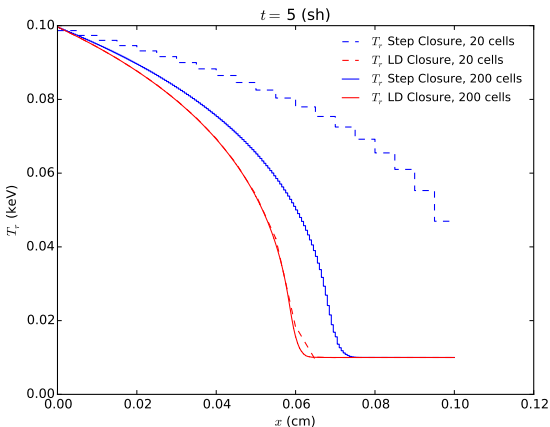


ECMC is more efficient than  
standard MC (SMC) as a HO solver



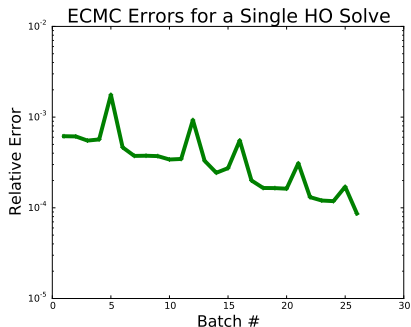
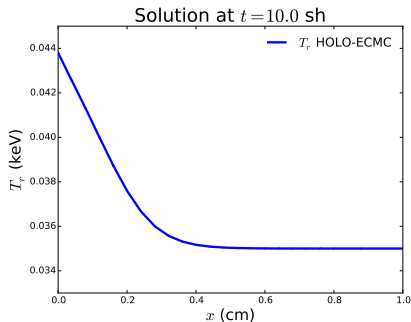
Different HO solvers: **ECMC** with 3 batches,  
standard MC (**SMC**), and an  $S_2$  solution

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





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



# A HOLO Algorithm for Thermal Radiative Transfer

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Overview of algorithm

Derivation of the LO equations

Exponentially Convergent MC High-Order Solver

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Remaining Research

We need a way to resolve issues when the LDFF 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 may be necessary  
E.g., lumping or preserving balance with floored  $\phi(x)$

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

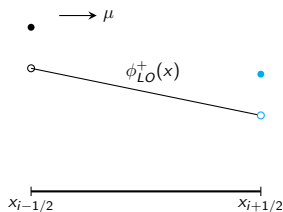
Produce  $\tilde{l}_{pos}$  by scaling  $x - \mu$  moments equally,  
to estimate source for the next iteration

$$\begin{array}{l} \mathbf{L} \tilde{l}^{(m)} = q - r^{(m)} \\ \mathbf{L} \tilde{l}_{pos}^{(m)} = q - r^{(m)} + \delta^{(m+1)} \end{array} \quad \longrightarrow \quad \begin{array}{l} \delta^{(m+1)} = \mathbf{L} \left( \tilde{l}^{(m)} - \tilde{l}_{pos}^{(m)} \right) \\ q \rightarrow q + \delta^{(m+1)} \end{array}$$

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

**Alternatively**, add  $\delta = -r_{pos}^{(m)}(x, \mu)$  to negative cells  
 $l_{pos}$  must be recomputing based on balance

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  $\mu$  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:

$$\phi_{i+1/2}^+ = \frac{3 + \gamma_{i,HO}^+}{2} \langle \phi \rangle_{R,i}^+ + \frac{\gamma_{i,HO}^+ - 3}{2} \langle \phi \rangle_{L,i}^+$$

We will use source-iteration with diffusion-synthetic acceleration (DSA) to solve LO system

In higher dimensions, the scattering terms in LO system cannot be directly inverted efficiently

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

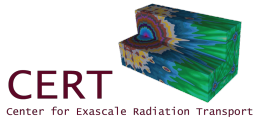
Inconsistencies may cause difficulties in convergence  
Will resolve with DSA-preconditioned Krylov methods

## 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

Simon Bolding and Jim Morel





## 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
- ▶ For all results
  1. Initial  $\Delta t$  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:

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

- Modified system

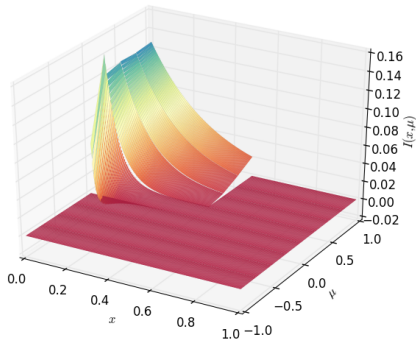
$$[\mathbf{D}(\mu^\pm) - \sigma_a^*(1 - f^*)] \underline{\Phi}^{n+1} = f^* \underline{B}(T^*) + \frac{\underline{\Phi}^n}{c\Delta t}$$

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

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

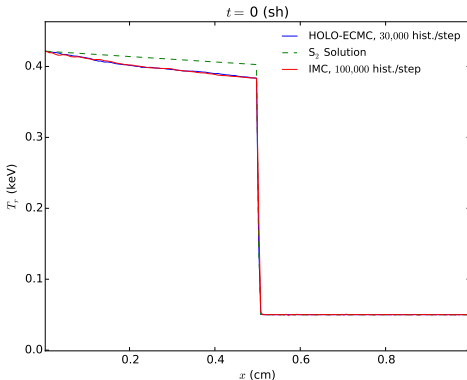
- Equation for  $T^{n+1}$  based on linearization that is conservative
- Converge  $T^{n+1}$  and  $\langle \phi \rangle$  with Newton Iterations

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.

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

- 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)