Moment-Based Multiscale Solution Approach for Thermal Radiation Transport

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Motivation for Moment-Based Multiscale Solution Approach

- Multi-temporal and spatial scale phenomena are common.
- An efficient *scale-bridging algorithm* is a key for accurately modeling these phenomena.
- Accurate solution of the fine-scale (i.e., transport equation) problem is desired. However, the problem can soon become intractable.
- Many problems exhibit both “continuum (diffusion)” and “kinetic (transport)” regimes. → Unified treatment in both regimes are desired, but difficult.
Moment-Based HO and LO Grey TRT Problems

Some Definitions

- **High-Order (HO) problem**: a fine-scale kinetic equation, i.e.,

\[
\frac{1}{c} \frac{\partial I}{\partial t} + \hat{\Omega} \cdot \nabla I + \sigma I = \frac{ac}{4\pi} \sigma T^4 + \frac{Q}{4\pi} \tag{1}
\]

\[
\rho C_v \frac{\partial T}{\partial t} = \int d\Omega \sigma \left( I - \frac{ac}{4\pi} T^4 \right) \tag{2}
\]

- **Low-Order (LO) problem**: engineering-scale angularly integrated moment equations, i.e.,

\[
0\text{th} \quad \frac{\partial E}{\partial t} + \nabla \cdot \vec{F} + c\sigma E = ac\sigma T^4 + Q \tag{3}
\]

\[
1\text{st} \quad \frac{\partial \vec{F}}{\partial t} + c^2 \nabla \cdot \mathcal{E} E + c\sigma \vec{F} = 0 \tag{4}
\]

- where \( E = \frac{1}{c} \int d\Omega \ I, \ \vec{F} = \int d\Omega \ \hat{\Omega} \ I, \) and \( \mathcal{E}_{\alpha\beta} = \frac{\int d\Omega \ \Omega_\alpha \ \Omega_\beta \ I}{\int d\Omega \ I} \)
Our moment-based approach (Quasi-diffusion\textsuperscript{1}) is not a geometric hybrid, rather it is similar to multigrid → Smoothing more isotropic physics (e.g., scattering-emission) using the LO problem.

Pros:

- **Elimination of angular dependence** → LO problem size is independent of fidelity of angular discretization
- **Implicit treatment of absorption-emission physics** → providing acceleration of the HO solution.
- **Availability of both deterministic and Monte Carlo HO solver** → multiphysics coupling takes place in LO problem.

Cons:

- Must solve nonlinear system.
- Prone to additional discretization errors (e.g., mismatch between HO and LO discretizations).

\textsuperscript{1}V.Ya.Gol’din (1967) *USSR Computational Mathematics and Physics* 4, 136–149
Absorption-emission process is strongly (nonlinearly) coupled → stiff physics coupling

Fleck-Cummings linearization

\[
\frac{1}{c} \frac{\partial I}{\partial t} + \hat{\Omega} \cdot \nabla I + \sigma I = \sigma_{s,\text{eff}} E + \frac{Q}{4\pi} \quad (7)
\]

In an optically thick medium, a large number of effective scatters occur → source iteration converges slowly

In an optically thin medium, transport effects become significant → significant errors in diffusion approximation (space and time).

A developed algorithm should be effective in both diffusive and transport regimes:

- IMC+IMD
- DDMC
- QD

As a true acceleration method, we further seek “consistency” between HO and LO solutions.

We will introduce a similar concept to “Nonlinear Diffusion Acceleration (NDA)” to bring consistency (i.e., $E^{HO} = E^{LO}$).

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Algorithm Overview

A time step:

1. solve HO problem with fixed emission source and opacity (e.g., transport sweep) to get $I$.
2. compute Eddington tensor, $\mathcal{E}$, consistency term, $\gamma$, and boundary conditions, $\vec{F}_{\text{in/out}}$.
3. solve LO problem (coupled radiation energy, $E$,-material temperature, $T$, equations) with the Newton-Krylov method.

- Currently, no outer iterations within a time step.
- Use same spatial mesh for HO and LO problems.
- Advanced time-stepping algorithms (e.g., predictor-corrector) are possible → a second-order time accurate solution$^8$.

Time Discretization/Linearization

▶ HO problem: solved via a transport sweep.

\[
\frac{1}{c} \frac{I^{n+1} - I^n}{\Delta t} + \hat{\Omega} \cdot \nabla I^{n+1} + \sigma^n I^{n+1} = \left(\frac{ac}{4\pi} \sigma T^4\right)^n + \frac{Q}{4\pi}
\]  

\[
\mathcal{E}_{\alpha,\beta}^{*} = \frac{\int d\Omega \Omega_{\alpha} \Omega_{\beta} I^{n+1}}{\int d\Omega I^{n+1}}
\]  

▶ LO problem: solved via Newton-Krylov iteration.

\[
\frac{E^{n+1} - E^n}{\Delta t} + \nabla \cdot \vec{F}^{n+1} + c\sigma^n E^{n+1} = \sigma^n \left(acT^4\right)^{n+1} + Q
\]  

\[
\frac{\vec{F}^{n+1} - \vec{F}^n}{\Delta t} + c^2 \nabla \cdot \mathcal{E}^{*} E^{n+1} + c\sigma^n \vec{F}^{n+1} = 0
\]  

\[
\rho C_v \frac{T^{n+1} - T^n}{\Delta t} = \sigma^n \left(I^{n+1} - (acT^4)^{n+1}\right)
\]

▶ HO and LO problems may have different truncation errors → mismatch in resulting solution (will be shown later)

▶ add “Consistency” term to LO problem to enforce same local truncation errors.
Consider mono-energetic transport equation with a constant opacity and source term in a 1D slab:

\[ \mu \frac{\partial I}{\partial x} + \sigma I = S. \] (13)

which has the following analytical solution (i.e., step characteristics):

\[ I(x, \mu) = I_0 e^{-\sigma x/\mu} + \frac{S}{\sigma} (1 - e^{-\sigma x/\mu}) \] (14)

Therefore, we can obtain analytical solution for, \( E^{HO} \), \( F^{HO} \)

But LO cell face flux is:

\[ F_{i+1/2}^{LO} = -\frac{1}{\sigma} \frac{\mathcal{E}E_{i+1} - \mathcal{E}E_i}{\Delta x} \] (15)
Consistency Term (example)

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- Truncation error (T.E.) estimate:

\[ \text{T.E.} = F_{i+1/2}^{HO} - F_{i+1/2}^{LO} = F_{i+1/2}^{HO} + \frac{1}{\sigma} \frac{\varepsilon E_{i+1}^{HO} - \varepsilon E_i^{HO}}{\Delta x} \]  \hspace{1cm} (16)

- We can compute a mismatch in the truncation error (\(\Delta \text{T.E.}\)) with

\[ \Delta \text{T.E.} \equiv \text{T.E}^{HO} - \text{T.E}^{LO} = F^{HO} + \frac{1}{\sigma} \frac{\partial \varepsilon E^{HO}}{\partial x} \bigg|_{LO} \]  \hspace{1cm} (17)

where \(\bigg|_{LO}\) denotes evaluating the derivative with the spatial discretization used in LO problem.

- We then write \(\Delta \text{T.E.}\) as

\[ \Delta \text{T.E.} = \gamma E^{HO} \rightarrow \gamma = \frac{F^{HO} + \frac{1}{\sigma} \frac{\partial \varepsilon E^{HO}}{\partial x} \bigg|_{LO}}{E^{HO}} \]
Rewrite 1st moment of LO problem along the interface between cell $i$ and $j$, $(\vec{n}_{i,j} \cdot \vec{F}) = F_{i,j}^+ - F_{i,j}^-$

$$F_{i,j}^{+,n+1} (1 + c \Delta t \sigma) - F_{i,j}^{+,n} + c^2 \Delta t \frac{\vec{n}_{i,j}}{2} \cdot (\nabla \cdot \mathcal{E}E)|_{i,j} + c \gamma_{i,j}^+ E_i = 0 \quad (18)$$

$$F_{i,j}^{-,n+1} (1 + c \Delta t \sigma) - F_{i,j}^{-,n} + c^2 \Delta t \frac{\vec{n}_{j,i}}{2} \cdot (\nabla \cdot \mathcal{E}E)|_{i,j} + c \gamma_{i,j}^- E_j = 0 \quad (19)$$

We compute two correction factors, $\gamma^\pm$, by substituting HO solution into the above equation.

We use QD (not altering physics) for closure and let the consistency term pick up only discretization mismatch (other LO formulations are possible).
Nonlinear elimination technique reduces the LO system from \( \{E, F, T\} \) to \( \{E\} \).

A stiff ODE is eliminated from outer Newton iterations \( \rightarrow \) trade-off between number of Newton iterations and complexity of nonlinear residual evaluation.

*The number of governing equations does not increase with dimension (complexity of evaluating flux term may increase.)*

Resulting matrix for radiation energy \( \tilde{J}_{E,E} \) is equivalent to advection-diffusion equation \( \rightarrow \) readily inverted via multigrid preconditioned GMRES.
Nonlinear Elimination of Flux $F$ and Temperature $T$

in LO Solver 2 of 2

- (After nonlinear elimination of $F$ and $T$,) resulting LO matrix problem becomes

\[
\tilde{J}_{E,E}\delta E = -\tilde{F}_E
\]

- Jacobian-free Newton-Krylov (JFNK) method merely requires evaluation of $\tilde{F}_E = \frac{\partial E}{\partial t} + \nabla \cdot \vec{F} + c\sigma E - ac\sigma T^4 - Q$.

- We compute $\tilde{F}_E$ with the following steps:

1. **solve nonlinear ODE**, $c_v \frac{\partial T}{\partial t} = \int d\Omega \sigma \left( I - \frac{ac}{4\pi} T^4 \right)$, for $T^{n+1}$ with given $E^*$ and $T^n$.
2. **evaluate the face current (flux) $F$** using

   \[
   F^{\pm,n+1}_{i,j} \left( 1 + c\Delta t\sigma \right) - F^{\pm,n}_{i,j} \pm c^2\Delta t \frac{\vec{n}_{i,j}}{2} \cdot (\nabla \cdot \vec{E}E) \big|_{i,j} + c\gamma^{\pm}_{i,j} E^\pm = 0 \text{ and } E^*,
   \]
3. **evaluate nonlinear residual**

   \[
   \tilde{F}_E = \frac{\partial E}{\partial t} + \nabla \cdot \vec{F} + c\sigma E - ac\sigma T^4 - Q.
   \]
Simplification of Eddington tensor and consistency term:

- set $\mathcal{E}_{xy} = 0, \gamma = 0$
- then

\[
\frac{F_{n+1}^{\alpha} - F_n^{\alpha}}{\Delta t} + c^2 \frac{\partial \mathcal{E}_{\alpha\alpha}}{\partial \alpha} E + c\sigma F_{n+1}^{\alpha} = 0 \tag{21}
\]

\[
F_{n+1}^{\alpha} = \frac{-c^2 \frac{\partial \mathcal{E}_{\alpha\alpha}}{\partial \alpha} E + F_n^{\alpha}}{\sigma + \frac{1}{c\Delta t}} \tag{22}
\]

- substitute into the 0th moment equation and gather terms to get:

\[
- \nabla \cdot \left( \tilde{D} \nabla \cdot \mathcal{E} E^{n+1} \right) + \left( c\sigma + \frac{1}{\Delta t} \right) E^{n+1} = a c\sigma T^4 + \tilde{Q}(E^n, \tilde{F}^n) \tag{23}
\]
Fleck-Cummings linearization:

- Let $\Theta = acT^4$, $\beta = \frac{4acT^3}{\rho C_v}$, and $\frac{\partial \Theta}{\partial T} = 4acT^3$.
- Discretize material energy equation in time and linearize

\[
\frac{\Theta^{n+1} - \Theta^n}{\beta^* \Delta t} = \sigma E^{n+1} - \sigma \Theta^{n+1}
\]  
(24)

- Substitute $\Theta$ in the 0th moment equation to get

\[
-\nabla \cdot \tilde{D} \nabla \cdot \mathcal{E} E^{n+1} + \tilde{\sigma} (1 - \frac{\sigma \beta^* \Delta t}{1 + \sigma \beta^* \Delta t}) E^{n+1} = S
\]  
(25)
Finally, we have the following operator for preconditioning.

\[ \mathbb{M}_{E,E} = -\nabla \cdot \tilde{D} \cdot \nabla \cdot \mathcal{E} + \sigma_{\text{eff},a} \]  

(26)

where \( \sigma_{\text{eff},a} \) is the “effective absorption” cross section, including time absorption and effective scattering.

We recompute the preconditioning operator each Newton step in order to use up-to-date \( \beta \).

There are other choices for the preconditioning matrix:

- P1 approximation
- Factor, \( \beta \), computed from the previous time step solution.

The preconditioning matrix has a form of a discrete elliptic operator \( \rightarrow \) efficiently inverted via multigrid sweeps.
1D Grey Marshak Wave

- $0 < x < 2cm$
- $0 < t < 5e - 8sec$
- $\rho = 1.0[g/cc], \ C_v = 1.3784e11[erg/eV - g]$
- $T_0 = 0.025eV$, incoming temperature BC at right face = 150eV
- $a = 137.20172[erg/cc - eV^4], \ c = 2.998e10[cm/s]$
- $\sigma = 0.001\left(\frac{1000}{T}\right)^3$
- HO: $S_{16}$, Linear Discontinuous Galerkin spatial discretization.
- LO: Finite Volume
Wave front location is different.

Consistency term adds more energy to cold region → smaller opacity at wave front.
Two Region Problem
1 of 2 (problem setup)

- thin region: $0 < x < 0.5cm$
- thick region: $0.5 < x < 1cm$
- $\sigma_1 = 0.2, \sigma_2 = 2000$
- $C_{v1} = C_{v2} = 1e12$
- $\rho_1 = 0.01, \rho_2 = 10.0$
- $T_0 = 50eV$
- $T_{BC} = 500eV @ x = 0$
- HO: $S_{16}$ LDG.
- LO: Finite Volume
Simple finite difference approximation is not adequate to approximate abrupt solution change near material interface.

Too much energy flows into LO system.
Two Region Problem

mesh refinement brings LO and HO solution together
Monte Carlo HO Result

1 of 2 (small number of time steps)

- 20 time steps (t=1e-10sec)
- Consistency term brings HO and LO solution together even with HO MC solution
- Inconsistent formulation has unphysical radiation temperature.
Monte Carlo HO Result

2 of 2 (more time steps)

- 200 time steps (t=1e-9sec)
- Consistent formulation requires more particles per cycle.
- Noise is amplified because of taking the difference of solution.

\[ \gamma = \frac{F^{HO} + \frac{1}{\sigma} \frac{\partial E^{HO}}{\partial x} |_{LO}}{E^{HO}} \]
2D result

TopHat problem

- t=1e-9sec
- S16 linear DG
- inconsistent formulation yields in unphysical radiation temperature. (>\(T_{in}\))
Conclusions/Future Work

▶ Conclusions
  ▶ Moment-based approach with consistency term can result in an efficient solution algorithm for transport problem.
  ▶ We have combined two concepts:
    ▶ Quasi-diffusion\(^9\)
    ▶ Nonlinear diffusion acceleration \(^{10}\)

▶ Future Work
  ▶ potential for 2nd order time accurate solution (time centering the Eddington tensor and opacity)\(^{11}\).
  ▶ multifrequency HO with grey LO problem.
  ▶ advanced Monte Carlo HO solver (IMC, ECMC)

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References


