Second-Order Discretization in Space and Time for Grey S_2-Radiation Hydrodynamics

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CLASS seminar

Outline

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1. Overview
2. The MUSCL-Hancock Method
3. Discretizations for TRT Equations
4. The algorithm
5. Results
6. Conclusions and Future Work

What is radiation hydrodynamics?

- Thermal radiative transfer (TRT) coupled to material hydrodynamics
  - Inertial confinement fusion (NIF) and astrophysics calculations

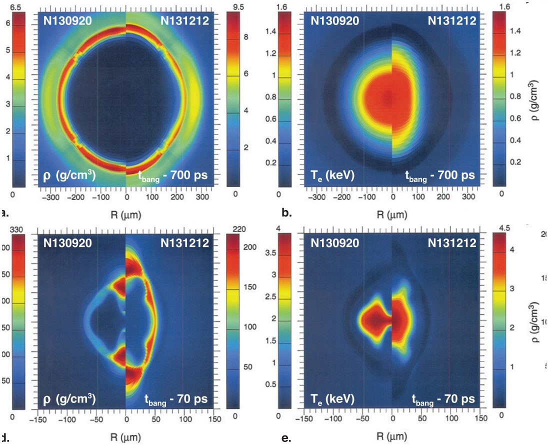


Figure : Comparison of HYDRA simulations for collapses of 2 NIF hohlraum designs, from Meezan et. al., 2015

We have implemented and tested a 2nd order solution method

- Previous work by Edwards and Morel for an algorithm that is second-order in space and time
  - **Hydrodynamics** is solved with a MUSCL-Hancock (MH) method predictor-corrector in time
  - **Radiation diffusion** is solved with linear discontinuous finite elements in space (LDFE) and a modified form of TRBDF2 in time
- Resolved issues with mixing of different spatial discretizations for the hydrodynamic and radiation variables
- Used approximate radiation hydrodynamics equations that produce the correct equilibrium diffusion limit solution to $\mathcal{O}(u/c)$

We have extended the method to S_2 equations

- S_2 allows for conservation of momentum
- Can be generalized to S_n equations, but would also be well suited for a high-order low-order approach

The non-relativistic radiation hydrodynamics equations

- For hydro, we have the 1D Euler Equations with source terms from interaction and emission of radiation (grey)

$$\boxed{\frac{\partial}{\partial t}\mathbf{U} + \frac{\partial}{\partial x}F(\mathbf{U}) = \mathbf{Q}(\mathbf{U})} \tag{1}$$

$$\mathbf{U} = \begin{pmatrix} \rho \\ \rho u \\ E \end{pmatrix}, \quad F(\mathbf{U}) = \begin{pmatrix} \rho u \\ \rho u^2 + p \\ u\,(E+p) \end{pmatrix}, \quad Q(\mathbf{U}) = \begin{pmatrix} 0 \\ Q_{\text{mom}} \\ Q_{\text{erg}} \end{pmatrix}$$

- The coupling terms are

$$Q_{\text{mom}} = \frac{\sigma_t}{c}\mathcal{F}_0, \qquad Q_{\text{erg}} = -\sigma_a c\left(aT^4 - \mathcal{E}\right) + \frac{\sigma_t u}{c}\mathcal{F}_0$$

- There is an equation of state to relate internal energy e and T
- The Euler equations are typically solved with explicit time discretizations that require a time step limit (CFL)

The S_2 equations for radiation hydrodynamics

- The radiation transport equation contains source and loss terms from interaction with material
- To get S_2 equations, we collocate to $\mu = \pm\frac{1}{\sqrt{3}}$ to get equations for half-range intensities $I^{\pm}$

$$\frac{1}{c}\frac{\partial I^+(x,t)}{\partial t} + \frac{1}{\sqrt{3}}\frac{\partial I^+}{\partial x} + \sigma_t I^+ = \frac{\sigma_s}{4\pi}c\mathcal{E} + \frac{\sigma_a}{4\pi}acT^4 - \frac{\sigma_t u}{4\pi c}\mathcal{F}_0 + \frac{\sigma_t}{\sqrt{3}\pi}\mathcal{E}u,$$

$$\frac{1}{c}\frac{\partial I^-(x,t)}{\partial t} - \frac{1}{\sqrt{3}}\frac{\partial I^-}{\partial x} + \sigma_t I^- = \frac{\sigma_s}{4\pi}c\mathcal{E} + \frac{\sigma_a}{4\pi}acT^4 - \frac{\sigma_t u}{4\pi c}\mathcal{F}_0 - \frac{\sigma_t}{\sqrt{3}\pi}\mathcal{E}u,$$

- with

$$\mathcal{E} = \frac{1}{c}2\pi\int_{-1}^{1} I(\mu)\,\mathrm{d}\mu, \qquad \mathcal{F} = 2\pi\int_{-1}^{1}\mu\, I(\mu)\,\mathrm{d}\mu, \qquad \mathcal{F}_0 = \mathcal{F} - \frac{4}{3}\mathcal{E}u$$

- These equations are solved using implicit time discretizations
- Angular moments of the S_2 equations gives the radiation balance and momentum equations, with correct $-Q_{\text{erg}}$ and $-Q_{\text{mom}}$

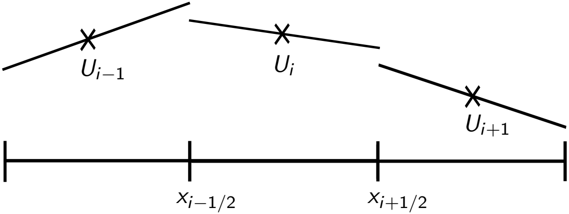
Solution to the radiation hydrodynamics equations

- Operator splitting in time of the Euler equations and thermal radiative transfer equations with momentum deposition
  - First, MH solver advects discrete hydro states from t^n to t^*
  - Then, a simultaneous solve for implicit radiation and hydro states from t^* to t^{n+1}
- **For hydrodynamics**, the spatial mesh is fixed and mass flows between cells (Eulerian)
- Within a **radiation solve**,
  - An outer fixed-point iteration is used to update momentum from radiation deposition
  - The radiation intensityand internal energy have to be solved with a Newton's method due to non-linear emission term $\sigma_a acT^4$
- Ensure total energy, momentum, and mass conservation

Outline

The MUSCL Hancock method is second-order accurate in x & t

- The MUSCL Hancock method uses a reconstructed linear shape in space, with slope limiting



- Explicit predictor-corrector steps are taken in time
- For the predictor step interior $F(\mathbf{U})$ is used on the faces. For the corrector step, an approximate Riemann solver is used for $F_{i\pm1/2}(\mathbf{U})$.

Step 1:

$$\tilde{\mathbf{U}}_i^{n+1/2} - \mathbf{U}_i^n = -\frac{\Delta t}{2\Delta x}\left[F(\mathbf{U}_{i,R}^n) - F(\mathbf{U}_{i,L}^n)\right]$$

Step 2:

$$\mathbf{U}^{n+1} - \mathbf{U}^n = -\frac{\Delta t}{\Delta x}\left[F(\tilde{\mathbf{U}}_{i+1/2}^{n+1/2}) - F(\tilde{\mathbf{U}}_{i-1/2}^{n+1/2})\right]$$

Outline

Time discretization for the S_2, energy, and momentum solve

- We use a combination of Crank-Nicholson (CN) over half a time step, followed by a modified version of BDF2
- The BDF2 step takes place over a second half time step, rather than the over the full time step.
- This is done to conserve total energy and momentum over the full time step, in conjuction with two MH predictor-corrector steps.
- As an example, consider $\frac{d\mathbf{Y}}{dt} = f(\mathbf{Y})$. Our algorithm uses

$$\frac{(\mathbf{Y}^{n+1/2} - \mathbf{Y}^{n})}{\frac{\Delta t}{2}} = \frac{1}{2}\left[f(\mathbf{Y}^{n+1/2}) + f(\mathbf{Y}^{n})\right]$$

$$\frac{(\mathbf{Y}^{n+1} - \mathbf{Y}^{n+1/2})}{\frac{\Delta t}{2}} = \frac{2}{3}f(\mathbf{Y}^{n+1}) + \frac{1}{6}f(\mathbf{Y}^{n+1/2}) + \frac{1}{6}f(\mathbf{Y}^{n})$$

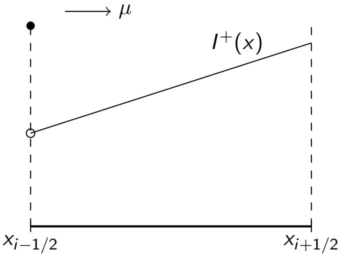
LD Galerkin Spatial Discreziation for TRT

- Within a Newton step, the material energy equation can be linearized and eliminated, producing fixed source S_2 equations

$$\pm\frac{1}{\sqrt{3}}\frac{\partial I^{\pm}}{\partial x} + \hat{\sigma}_t I^{\pm} - \frac{\hat{\sigma}_s E c}{4\pi} = \hat{q} \tag{2}$$

  where $\hat{\cdot}$ quantities depend on the time discretization and material energy linearization

- We use a lumped LDFE in space with upwinding to define I on faces



- Fully discrete system is formed with spatial unknowns at the left and right edges of a cell. The system can be inverted directly for S_2

Spatial discretization of material variables in radiation solve

- S_2 equations requires LD values of ρ, u, and e at edges of a cell
  - Use explicit MH slopes to get edge values of ρ and u for kinetic energy
  - The internal energy e is updated at edges based on new $\mathcal{E}$
  - We save LD e slopes between radiation solves to construct e^* at edges
- Need to update hydro energy and momentum based on radiation deposition
  - *We only change cell averages* for the material momentum and total energy updates
  - The MH slopes are unaffected and reconstructed each hydro solve

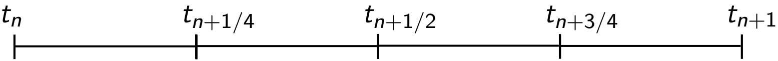
Non-linear iteration scheme for each implicit solve

- Herein, a "nonlinear solve" refers to a simultaneous solve of the S_2 equations, radiation momentum deposition, and new total material energy
- FOR each nonlinear iteration
    1. Update cell-averaged material momentum from radiation deposition
    2. Using Newtons method, we eliminate the material energy equation and solve for new LD values of $I^{\pm}$
    3. Update material internal energy e based on new $\mathcal{E}$
    4. Update cell-averaged total material energy E
- Repeat iterations until convergence
- $\mathcal{F}_0$ terms are lagged for entire iteration
- We conserve momentum to the tolerance of outer iteration

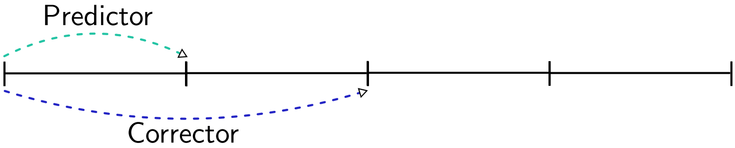
$$\frac{1}{c^2}\frac{\partial \mathcal{F}^{k+1}}{\partial t} + \frac{1}{3}\frac{\partial \mathcal{E}^{k+1}}{\partial x} = -\left(\sigma_t \mathcal{F}^{k+1} - \frac{4}{3}(\mathcal{E}u)^k\right)$$

Outline

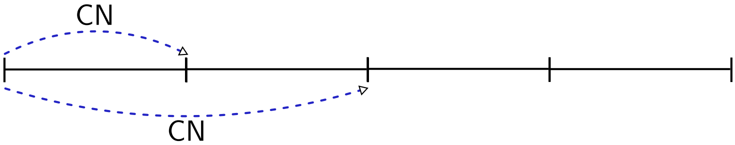
Time stepping algorithm, first half of time step



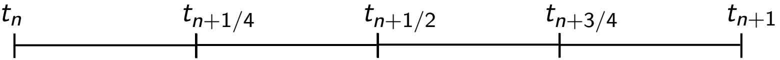
- MUSCL-Hancock steps



- Nonlinear solves of TRT equations



Time stepping algorithm, second half of time step



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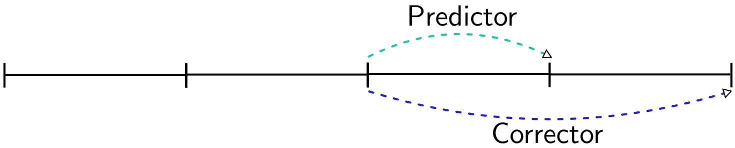
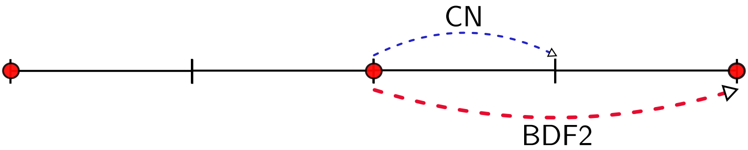


- Nonlinear solves of TRT equations



Why all the steps?! This seems expensive. . .

- In a TRBDF2 scheme, we need a second order accurate estimate of solution at $t_{n+1/2}$

$$\frac{(\mathbf{U}^{n+1} - \mathbf{U}^{n+1/2})}{\frac{\Delta t}{2}} = \frac{2}{3} f(\mathbf{U}^{n+1}) + \frac{1}{6} f(\mathbf{U}^{n+1/2}) + \frac{1}{6} f(\mathbf{U}^{n})$$

- If we used a MH predictor to $t_{n+1/2}$, then the hydro variables would only be first order accurate
- The 4 nonlinear solves are not that bad. . . The maximum allowable size of Δt based on CFL limit is now twice as big.
- For the same total number of hydro steps, we do the same amount of work as a two step method, but are second order accurate

Outline

Method of Manufactured Solutions

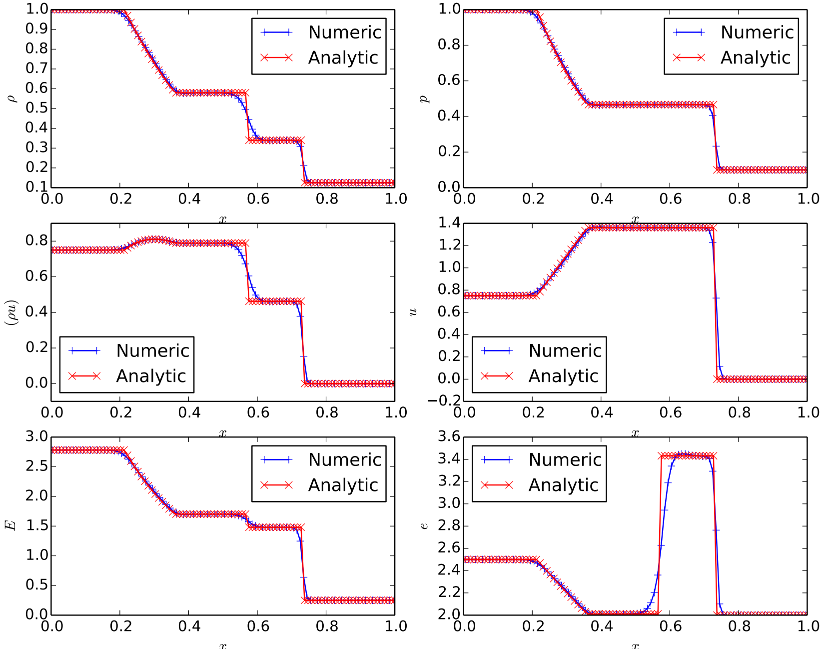
- Add effective source equation
- saem for radiation
- Adds in a mass term. blah blah
- Use same temporal discretization for sources, but quadruature for high accuracy spatial integration of sources
- Can be automated relatively easily with **Sympy**

Before and after of schock solution

- Shock is a discontinuity in the solution
-

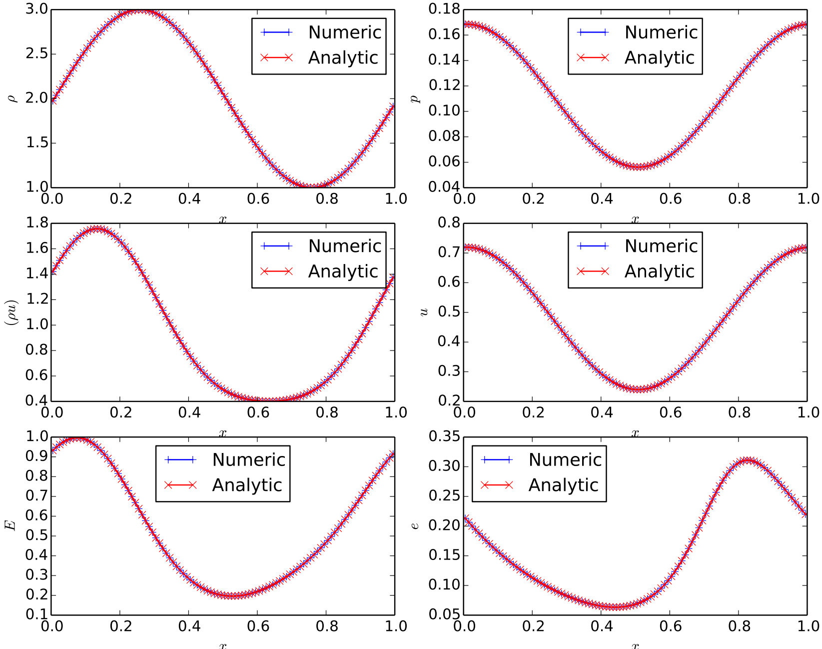
Results

Pure Hydrodynamics: Shock Tube Problem Solutions with van Leer Slope Limiter



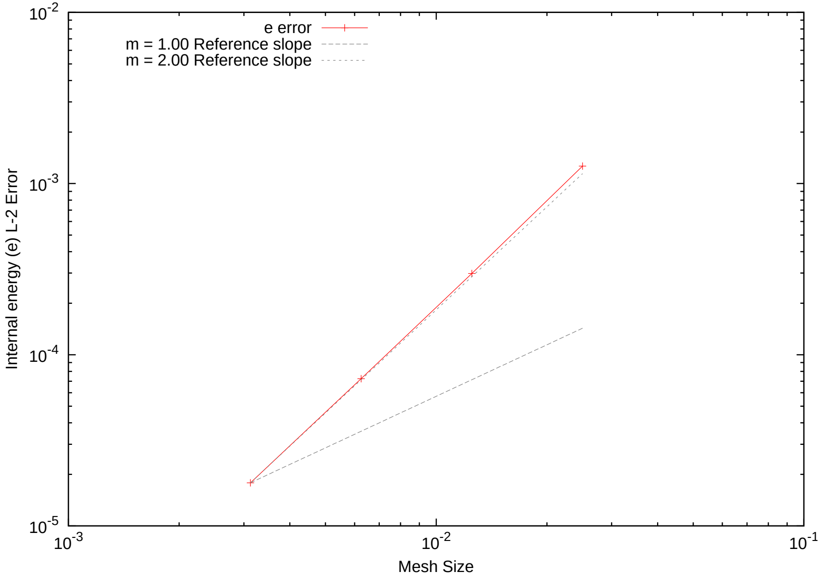
Results

Diffusion-Limit MMS Problem Solutions



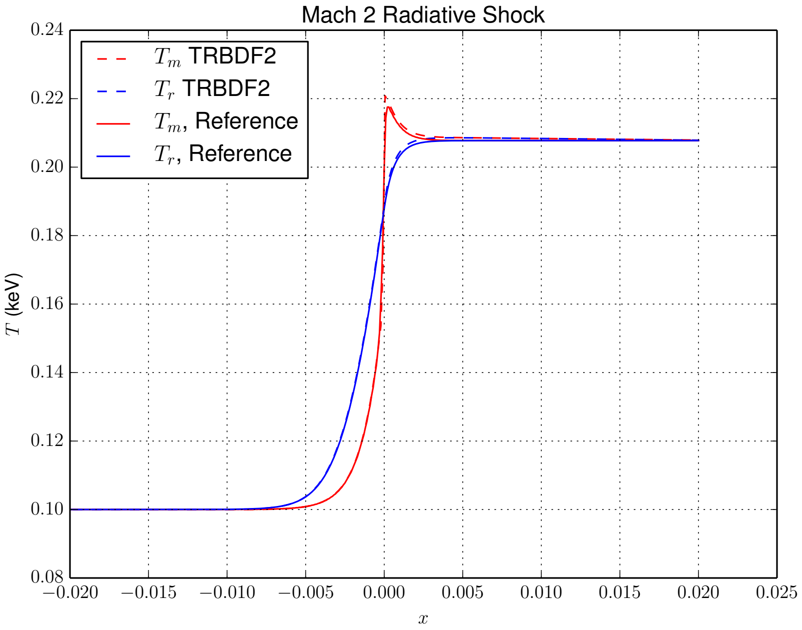
Results

Convergence Rate for Diffusion-Limit MMS Problem



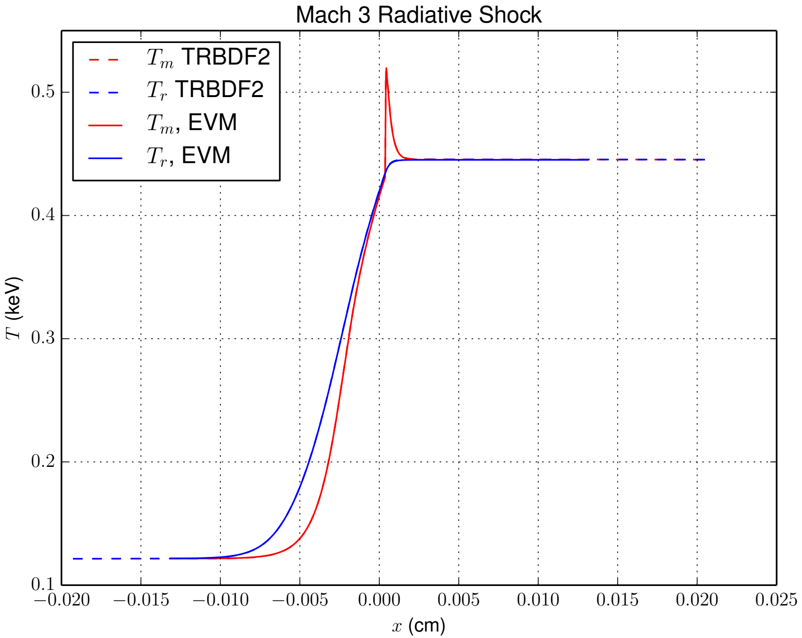
Results

Mach 2 Radiation-Hydrodynamics Shock



Results

Mach 3 Radiation-Hydrodynamics Shock, 1000 cells



Outline

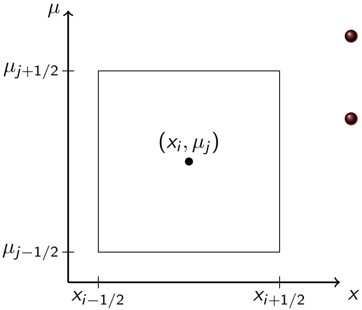
Conclusions

Demonstrated second order accuracy using manufactured solutions
Able to obtain accurate solutions in the EDL
When radiaiton or material motion become insignificant, you get back the respective algorithms

Future Work

Coupling to a high-order system using hybrid-"S_2-like" equations.
Exploring slope limiting and EDL, what is going wrong there
Different way to use internal energy slopes Stability of nonlinear iteration scheme.

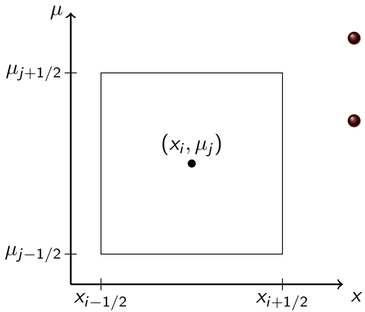
Space-Angle LDFE Mesh



- $\tilde{\psi}(x,\mu)$ is linear over each cell, preserving 0^{th} and 1^{st} moment in x and μ
- Use path-length estimators of flux to approximate moments e.g.

$$\langle\psi\rangle_{\mu,ij} = \frac{6}{h_\mu^2 h_x}\iint_{\mathcal{D}} (\mu - \mu_i)\psi(x,\mu)\mathrm{d}x\mathrm{d}\mu$$

Space-Angle LDFE Mesh



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$$\langle\psi\rangle_{\mu,ij} = \frac{6}{h_\mu^2 h_x}\iint_{\mathcal{D}}(\mu-\mu_i)\psi(x,\mu)\mathrm{d}x\mathrm{d}\mu$$

- Use standard LD and upwinding to get face terms

Questions?

Second-Order Discretization in Space and Time for Grey S_2-Radiation Hydrodynamics

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The full equations

- Material balance equations

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho u) = 0$$
$$\frac{\partial}{\partial t}(\rho u) + \frac{\partial}{\partial x}\left(\rho u^2 + p\right) = \frac{\sigma_t}{c}\mathcal{F}_0$$
$$\frac{\partial E}{\partial t} + \frac{\partial}{\partial x}\left[(E + p)\, u\right] = -\sigma_a c\left(aT^4 - \mathcal{E}\right) + \frac{\sigma_t u}{c}\mathcal{F}_0$$

- Radiation transport equation, collocated to $\mu = \pm\frac{1}{\sqrt{3}}$

$$\frac{1}{c}\frac{\partial \psi^\pm}{\partial t} \pm \frac{1}{\sqrt{3}}\frac{\partial \psi^\pm}{\partial x} + \sigma_t \psi^\pm = \frac{\sigma_s}{4\pi}c\mathcal{E} + \frac{\sigma_a}{4\pi}acT^4 - \frac{\sigma_t u}{4\pi c}\mathcal{F}_0 \pm \frac{\sigma_t}{\sqrt{3}\pi}\mathcal{E}u$$