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

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CLASS seminar

Outline

1. Overview
2. Solution to Euler Equations
3. Solution to TRT Equations
4. The algorithm
5. Results
6. Conclusions and Future Work

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What is radiation hydrodynamics?

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

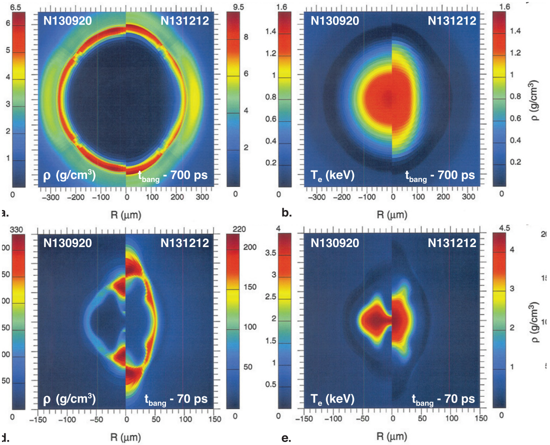

Figure : Comparison of HYDRA simulations for collapses of 2 NIF hohlraum designs, from Meezan et. al., 2015

We have implemented and tested a 2^{nd} 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 method predictor-corrector in time
- **Radiation diffusion** is solved with linear discontinuous finite elements in space and a conservative form of TRBDF2 in time
- Resolves issues with mixing of implicit and explicit time discretizations, as well as different spatial discretizations
- 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)

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

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

- 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

- Combining equations from last two slides gives full rad-hydro equations
- Operator splitting in time is used to separate the Euler equations from thermal radiative transfer equations.
  - In our notation Euler equations will advect hydro variables from U to U^*,
- For hydrodynamics, we use a Eularian mesh where the mesh is fixed and mass flows between cells
- The radiation and internal energy have to be solved with a Newton's method due to non-linear emission term $\sigma_a acT^4$
- An outer fixed point method is used to compute for comoving frame flux term $\mathcal{F}_0$, which is a function of u
- Want to conserve balance of total energy, momentum, and mass

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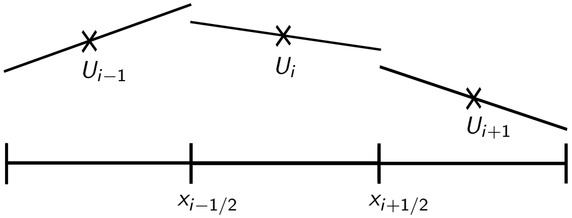
The MUSCL Hancock method is second-order accurate in x & t

- The MUSCL Hancock method uses slope-limited reconstruction in space and explicit predictor-corrector steps 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 $F_{i\pm 1/2}(\mathbf{U})$.

- The time from t_n to t_{n+1} is

  Step 1:

$$U_i^* = U_i^n - \frac{\Delta t}{2\Delta x}\left[F(\mathbf{U}_{i,R}^n) - F(\mathbf{U}_{i,L}^n)\right]$$

  Step 2:

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

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Time stepping for the radiation and total energy solves

- We use a combination of Crank-Nicholson (CN) and 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 the two explicit hydro steps.
- As an example, consider $\frac{d\mathbf{Y}}{dt} = f(\mathbf{Y})$. Our algorithm uses

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

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

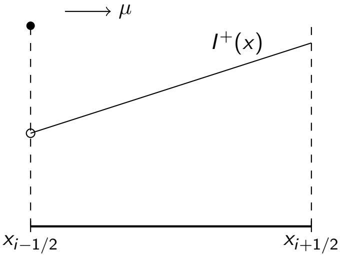
Linear Discontinuous Galerkin Spatial Discreziation for TRT

- Within a Newton step, the material energy equation can be eliminate, leaving the equations for the radiation as a fixed source problem

$$\pm\frac{1}{\sqrt{3}}\frac{\partial I^{\pm}}{\partial x}+\hat{\sigma}_t I^{\pm}-\frac{\hat{\sigma}_s Ec}{4\pi}=\hat{Q} \qquad (2)$$

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

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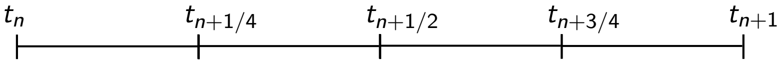
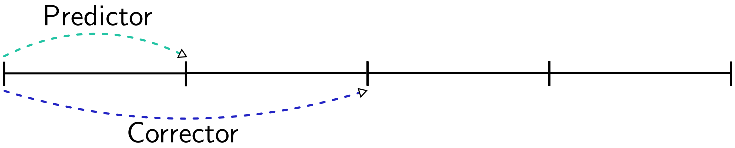
Non-linear iteration scheme for each implicit solve

- Herein "non-linear solve" refers to a simultaneous solve of the equations for S_2 equations, radiation momentum deposition, and new total material energy
- Algorithm
  1. Update material momentum from radiation deposition
  2. Using Newtons method, we eliminate the material energy equation and solve for a new $I^{\pm}$, and thus $\mathcal{E}$
  3. Update material internal energy equation based on new $\mathcal{E}$
- Energy and momentum updates use lagged $\mathcal{F}_0$
- *Initial* numerical tests indicate the momentum update may be unstable if $E/\rho u^2$ or u/c are too large
- We only conserve momentum to the tolerance of outer iteration

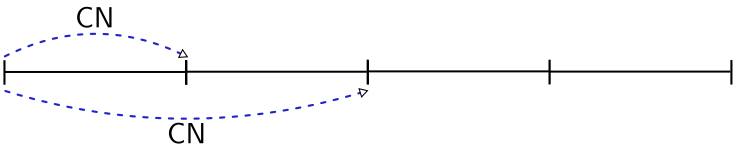
Time stepping algorithm, first half of time step



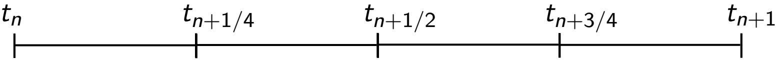
- Euler equations MH steps



- Nonlinear solve for $I^{\pm}$, e, and momentum deposition



Time stepping algorithm, second half of time step



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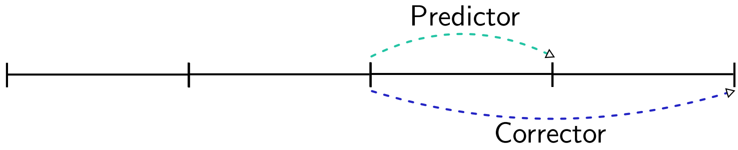

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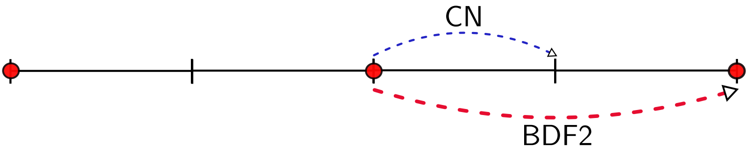

Why all the steps?! This seems expensive. . .

- 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

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Method of Manufactured Solutions

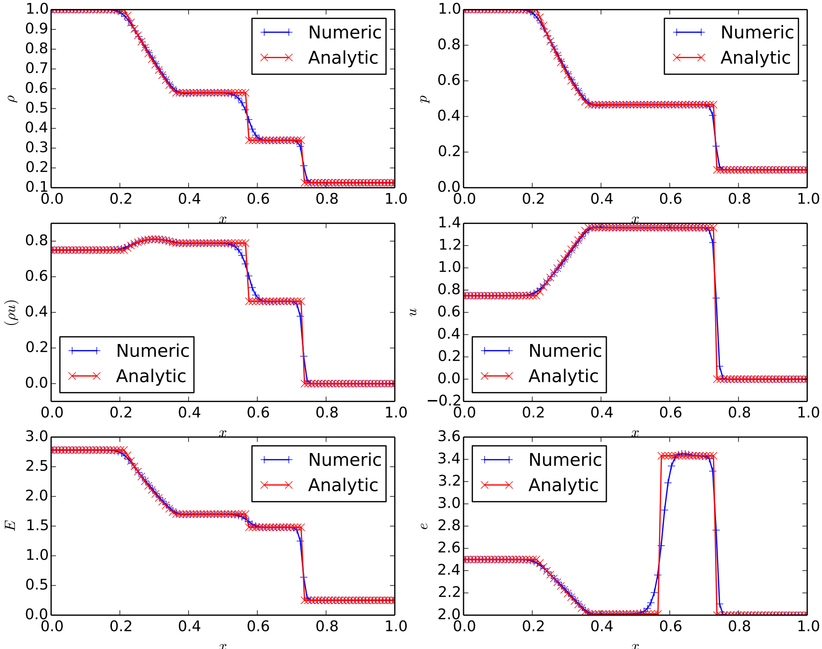
- Add effective source equation
- saem for radiation
- Adds in a mass term. blah blah
- Use same temporal discretization for sources, but quadruature for high accuracy spatial integration of sources
- Can be automated relatively easily with **Sympy**

Before and after of schock solution

- Shock is a discontinuity in the solution
-

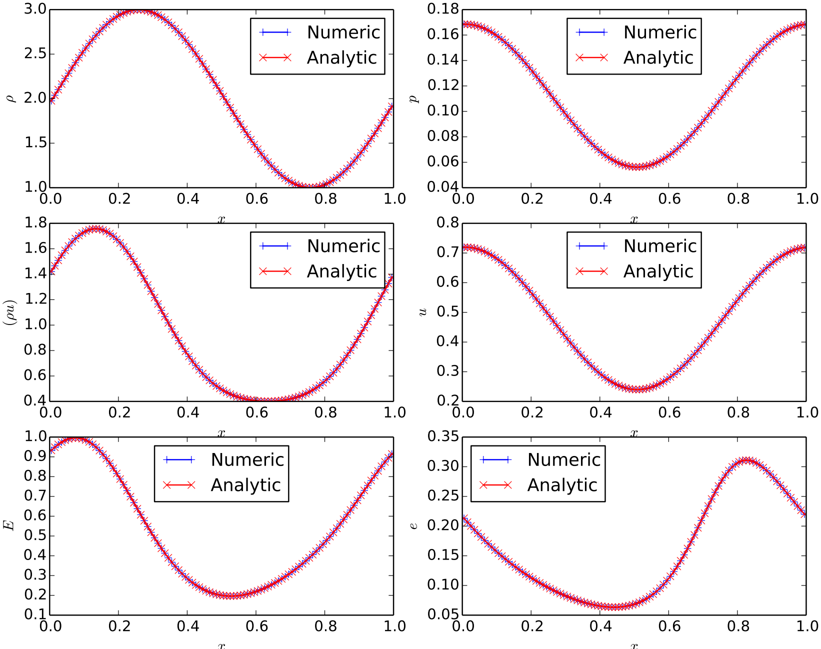
Results

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



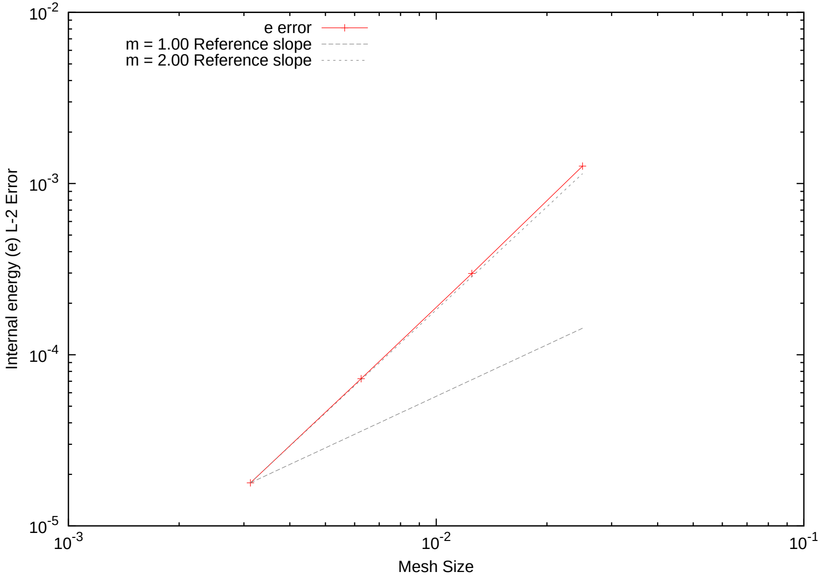
Results

Diffusion-Limit MMS Problem Solutions



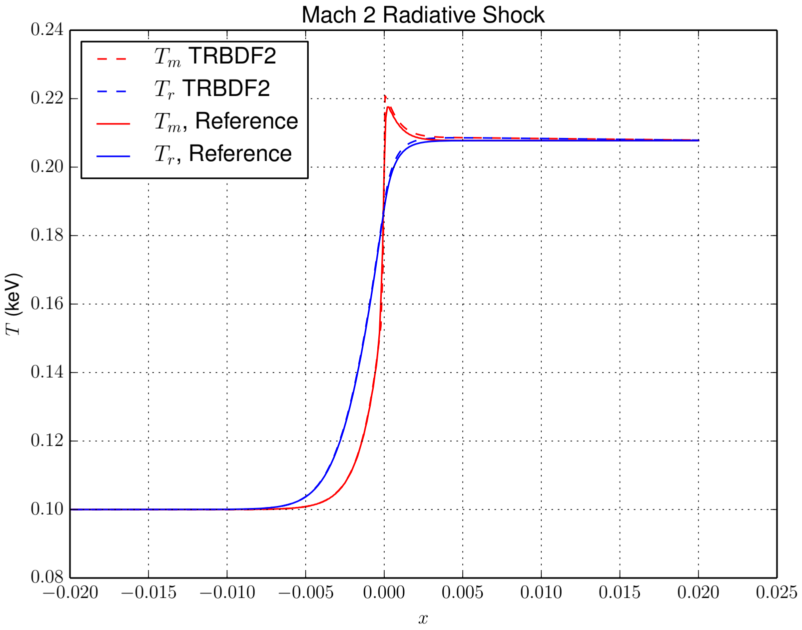
Results

Convergence Rate for Diffusion-Limit MMS Problem



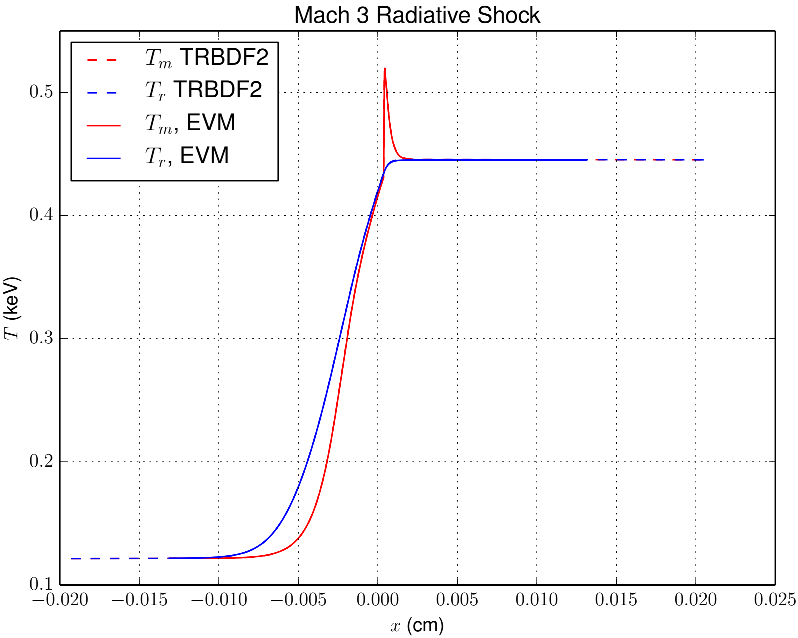
Results

Mach 2 Radiation-Hydrodynamics Shock



Results

Mach 3 Radiation-Hydrodynamics Shock, 1000 cells



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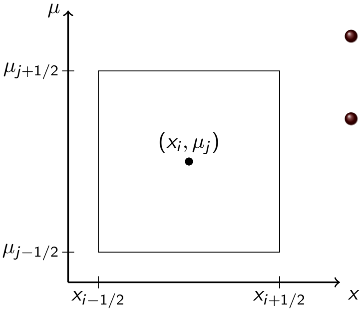
Conclusions

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

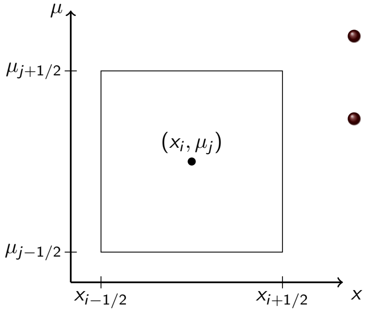
Space-Angle LDFE Mesh



- $\tilde{\psi}(x,\mu)$ 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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- Use standard LD and upwinding to get face terms

Questions?

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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 $\mu = \pm\frac{1}{\sqrt{3}}$

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