An anisotropic diffusion approximation to nonlinear radiation transport

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Outline

Thermal radiative transfer

- TRT is the dominant heat transfer process in very hot materials
- Photons born isotropically via black body emission ($q_{\text{rad}} \propto \sigma T^4$)
- Cold material heats up and becomes relatively transparent ($\sigma \propto T^{-3}$)

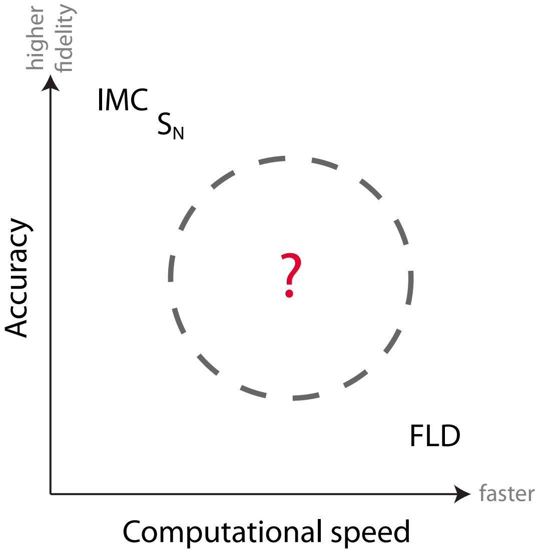
Difficulties in solving:

- High dimensionality of solution phase space $(\boldsymbol{x}, \boldsymbol{\Omega}, h\nu, t)$
- Highly nonlinear coupled partial differential equations for radiation field $\psi(\boldsymbol{x}, \boldsymbol{\Omega}, h\nu, t)$ and material energy

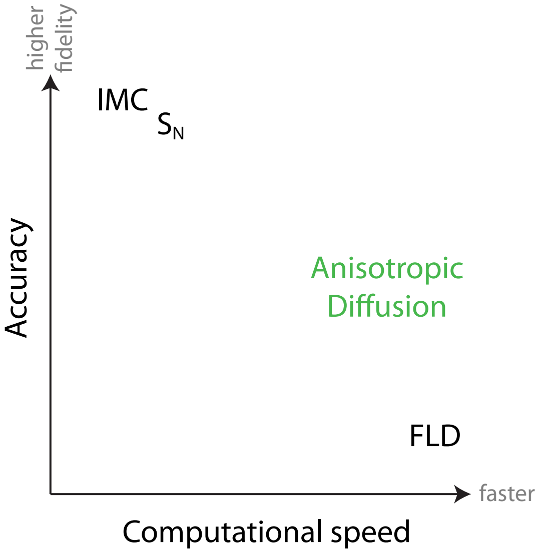
Particular application of this work: CRASH project

- Center for RAdiative Shock Hydrodynamics program: "Assessment of Predictive Capability"
- Simulate laser-driven shock in a xenon-filled tube
- Uncertainty quantification: hundreds of solution instances needed

Motivation


higher
fidelity
IMC
S_N
?
FLD
Accuracy
faster
Computational speed

Motivation


higher fidelity
IMC
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Accuracy
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Gray TRT equations

Common approximations for radiation transport methods development:

- work in a fixed medium, disregarding material advection;
- assume local thermodynamic equilibrium (LTE), which uses a single material temperature;
- neglect thermal conduction in material;
- average over all photon energies $h\nu$ (gray).

Radiation transfer equation, angular flux $\psi(\boldsymbol{x}, \boldsymbol{\Omega}, t)$:

$$\frac{1}{c}\frac{\partial \psi}{\partial t} + \boldsymbol{\Omega} \cdot \boldsymbol{\nabla} \psi + \sigma \psi = \frac{\sigma c a T^4}{4\pi} + \frac{cQ}{4\pi} \tag{1a}$$

Material energy balance equation:

$$\frac{1}{c_v}\frac{\partial T}{\partial t} = \sigma \int_{4\pi} \psi \, \mathrm{d}\Omega - \sigma c a T^4 \tag{1b}$$

Anisotropic diffusion

Previous work:

- Steady-state infinite medium VHTR-like problem with analytically calculated coefficients [1]
- Non-local tensor diffusion [2] for steady-state radiative transfer, no further development or analysis in literature

Current work:

- Formulates boundary conditions and time-dependent terms
- Uses transport-calculated anisotropic diffusion tensors
- Applies to nonlinear, time-dependent problems with isotropic sources

Potential applications:

- Extends diffusion theory to new regimes of applicability
- Variance reduction with shielding problems that have voids

Outline

1. Define the anisotropic angular flux as $\Psi = \psi - \frac{1}{4\pi}\phi$.
2. From the radiation transport equation and conservation equation, we get a differential transport equation for Ψ. Transform to an *integral* transport equation for Ψ.
3. Assume $\psi = O(1)$, $\frac{1}{c}\frac{\partial}{\partial t} = O(\epsilon^2)$, $\boldsymbol{\nabla} = O(\epsilon)$, $\int_{4\pi} \boldsymbol{\Omega}(\cdot)\, \mathrm{d}\Omega = O(\epsilon)$.
4. Use Taylor series to approximate nonlocal unknowns with local unknowns, discarding small terms. This yields

$$\Psi(\boldsymbol{x}, \boldsymbol{\Omega}) \approx -f(\boldsymbol{x}, \boldsymbol{\Omega})\boldsymbol{\Omega} \cdot \boldsymbol{\nabla}\phi\,.$$

5. Take the first angular moment of Ψ to get $\boldsymbol{J} = -\mathbf{D} \cdot \boldsymbol{\nabla}\phi$
6. Substitute $\boldsymbol{J}$ into the time-dependent particle conservation equation to get time-dependent anisotropic diffusion.

Transport equation (interior)

Inside a time step, with "frozen" cross section:

$$\frac{1}{c}\frac{\partial\psi}{\partial t}(\boldsymbol{x},\boldsymbol{\Omega},t)+\boldsymbol{\Omega}\cdot\boldsymbol{\nabla}\psi(\boldsymbol{x},\boldsymbol{\Omega},t)+\sigma^*(\boldsymbol{x})\psi(\boldsymbol{x},\boldsymbol{\Omega},t)$$
$$=\frac{1}{4\pi}\sigma^*(\boldsymbol{x})ac[T(\boldsymbol{x},t)]^4+\frac{1}{4\pi}q_r(\boldsymbol{x},t)\equiv\frac{1}{4\pi}Q(\boldsymbol{x},t)\,,$$
$$x\in V,\ 0\le t<\Delta_t,\ \boldsymbol{\Omega}\in 4\pi, \quad (2)$$

with a boundary condition and initial condition.
Operating on Eq. (2) by $\int_{4\pi}(\cdot)\,\mathrm{d}\Omega$ gives the conservation equation:

$$\frac{1}{c}\frac{\partial\phi}{\partial t}(\boldsymbol{x},t)+\boldsymbol{\nabla}\cdot\boldsymbol{J}(\boldsymbol{x},t)+\sigma^*\phi(\boldsymbol{x},t)=Q(\boldsymbol{x},t)\,. \quad (3)$$

Add $\boldsymbol{\Omega}\cdot\boldsymbol{\nabla}\phi$ to both sides of Eq. (3) and multiply by $\frac{1}{4\pi}$:

$$\frac{1}{4\pi}\frac{1}{c}\frac{\partial\phi}{\partial t}+\frac{1}{4\pi}\boldsymbol{\Omega}\cdot\boldsymbol{\nabla}\phi+\frac{1}{4\pi}\sigma^*\phi=\frac{1}{4\pi}Q(\boldsymbol{x},t)+\frac{1}{4\pi}\boldsymbol{\Omega}\cdot\boldsymbol{\nabla}\phi-\frac{1}{4\pi}\boldsymbol{\nabla}\cdot\boldsymbol{J} \quad (4)$$

Anisotropic angular flux equation

Define "anisotropic angular flux":

$$\Psi(\boldsymbol{x}, \boldsymbol{\Omega}) \equiv \psi(\boldsymbol{x}, \boldsymbol{\Omega}) - \frac{1}{4\pi}\phi(\boldsymbol{x})\,. \tag{5}$$

(This satisfies $\int_{4\pi} \Psi = 0$ and $\int_{4\pi} \boldsymbol{\Omega}\Psi = \boldsymbol{J}$.)
Subtract Eq. (4) from Eq. (2); the isotropic source cancels:

$$\frac{1}{c}\frac{\partial}{\partial t}\left[\psi - \frac{\phi}{4\pi}\right] + \boldsymbol{\Omega}\cdot\boldsymbol{\nabla}\left[\psi - \frac{\phi}{4\pi}\right] + \sigma^*(\boldsymbol{x})\left[\psi - \frac{\phi}{4\pi}\right] = \frac{1}{4\pi}\boldsymbol{\nabla}\cdot\boldsymbol{J} - \frac{1}{4\pi}\boldsymbol{\Omega}\cdot\boldsymbol{\nabla}\phi$$

Transport equation for Ψ:

$$\frac{1}{c}\frac{\partial}{\partial t}\Psi + \boldsymbol{\Omega}\cdot\boldsymbol{\nabla}\Psi + \sigma^*(\boldsymbol{x})\Psi = \frac{1}{4\pi}\boldsymbol{\nabla}\cdot\boldsymbol{J} - \frac{1}{4\pi}\boldsymbol{\Omega}\cdot\boldsymbol{\nabla}\phi \equiv \hat{Q}(\boldsymbol{x}, \boldsymbol{\Omega}, t)$$

The exact solutions for ψ, ϕ, $\boldsymbol{J}$ satisfy this equation: no approximations.

Integral transport equation

Streaming path from $(\boldsymbol{x}, t)$ backward along $-\boldsymbol{\Omega}$, accumulate sources and attenuate:

$$\Psi(\boldsymbol{x}, \boldsymbol{\Omega}, t) = \Psi^i(\boldsymbol{x} - ct\boldsymbol{\Omega}, \boldsymbol{\Omega})\, \mathrm{e}^{-\tau(\boldsymbol{x}, \boldsymbol{x} - ct\boldsymbol{\Omega})} + \int_0^\infty \left[\hat{Q}(\boldsymbol{x} - s\boldsymbol{\Omega}, \boldsymbol{\Omega}, t - s/c)\right] \mathrm{e}^{-\tau(\boldsymbol{x}, \boldsymbol{x} - s\boldsymbol{\Omega})}\, \mathrm{d}s\,. \tag{6a}$$

$$\equiv \mathcal{L}_i^{-1}\left[\Psi^i\right] + \mathcal{L}_v^{-1}\left[\hat{Q}\right] \tag{6b}$$

where we have defined the optical thickness is

$$\tau(\boldsymbol{x}, \boldsymbol{x}') = \int_0^{\|\boldsymbol{x} - \boldsymbol{x}'\|} \sigma^*(\boldsymbol{x} - s\boldsymbol{\Omega})\, \mathrm{d}s\,. \tag{6c}$$

These are nonlocal unknowns; we will approximate them with local unknowns.

Time for some approximations

Asymptotic ansatz: assume weak spatial gradients, mildly anisotropic angular flux, very small time derivative:

$$\psi = O(1), \qquad \boldsymbol{\nabla}\psi = O(\epsilon) \qquad \int_{4\pi} \boldsymbol{\Omega}\psi \, \mathrm{d}\Omega = O(\epsilon) \qquad \frac{1}{c}\frac{\partial}{\partial t} = O(\epsilon^2)$$

Our first approximation: $\mathcal{L}_i^{-1}[\cdot] = O(\epsilon^2)$ and $\boldsymbol{\nabla} \cdot \boldsymbol{J} = O(\epsilon^2)$:

$$\Psi = \mathcal{L}_i^{-1}\left[\Psi^i\right] + \mathcal{L}_v^{-1}\left[\frac{1}{4\pi}\boldsymbol{\nabla} \cdot \boldsymbol{J}\right] - \mathcal{L}_v^{-1}\left[\frac{1}{4\pi}\boldsymbol{\Omega} \cdot \boldsymbol{\nabla}\phi\right]$$

$$\Psi \approx -\mathcal{L}_v^{-1}\left[\frac{1}{4\pi}\boldsymbol{\Omega} \cdot \boldsymbol{\nabla}\phi\right] + O(\epsilon^2)$$

Taylor series expansion:

$$\phi(\boldsymbol{x} - s\boldsymbol{\Omega}, t - s/c) \sim \phi(\boldsymbol{x}, t) - s\left(\frac{1}{c}\frac{\partial}{\partial t} + \boldsymbol{\Omega} \cdot \boldsymbol{\nabla}\right)\phi(\boldsymbol{x}, t) + O(\epsilon^2)$$

$$\phi(\boldsymbol{x} - s\boldsymbol{\Omega}, t - s/c) = \phi(\boldsymbol{x}, t) + O(\epsilon) \tag{7}$$

Taylor series applied

If ϕ is smooth like the ansatz hypothesizes, the volumetric term becomes:

$$\begin{aligned} -\mathcal{L}_v^{-1}\left[\frac{1}{4\pi}\boldsymbol{\Omega}\cdot\boldsymbol{\nabla}\phi\right] &= -\int_0^\infty \left[\frac{1}{4\pi}\boldsymbol{\Omega}\cdot\boldsymbol{\nabla}\phi\right]_{(\boldsymbol{x}-s\boldsymbol{\Omega},t-s/c)} \mathrm{e}^{-\tau(\boldsymbol{x},\boldsymbol{x}-s\boldsymbol{\Omega})}\,\mathrm{d}s \\ &\sim -\int_0^\infty \left[\frac{1}{4\pi}\right]\mathrm{e}^{-\tau(\boldsymbol{x},\boldsymbol{x}-s\boldsymbol{\Omega})}\,\mathrm{d}s\boldsymbol{\Omega}\cdot\boldsymbol{\nabla}\phi(\boldsymbol{x},t) + O(\epsilon^2) \\ &= -\mathcal{L}_v^{-1}\left[\frac{1}{4\pi}\right]\boldsymbol{\Omega}\cdot\boldsymbol{\nabla}\phi(\boldsymbol{x},t)\,. \end{aligned} \quad (8)$$

Thus,

$$\Psi(\boldsymbol{x},\boldsymbol{\Omega},t) \approx -\left[\mathcal{L}_v^{-1}\left[\frac{1}{4\pi}\right]\right]\boldsymbol{\Omega}\cdot\boldsymbol{\nabla}\phi(\boldsymbol{x},t) \equiv -f(\boldsymbol{x},\boldsymbol{\Omega})\boldsymbol{\Omega}\cdot\boldsymbol{\nabla}\phi(\boldsymbol{x},t) \quad (9)$$

An analogy to Fick's law

To get an expression for the current use the identity $\boldsymbol{J} = \int_{4\pi} \boldsymbol{\Omega}\Psi \, \mathrm{d}\Omega$, which gives

$$\begin{aligned}\boldsymbol{J}(\boldsymbol{x},t) &= \int_{4\pi} \boldsymbol{\Omega}\left\{-f\boldsymbol{\Omega}\cdot\boldsymbol{\nabla}\phi(\boldsymbol{x},t)\right\}\mathrm{d}\Omega \\ &= -\left[\int_{4\pi}\boldsymbol{\Omega}\boldsymbol{\Omega}f\,\mathrm{d}\Omega\right]\cdot\boldsymbol{\nabla}\phi(\boldsymbol{x},t) \\ &\equiv -\mathbf{D}\cdot\boldsymbol{\nabla}\phi\,.\end{aligned}$$

Substitute into radiation energy conservation equation:

$$\frac{1}{c}\frac{\partial\phi}{\partial t} + \boldsymbol{\nabla}\cdot\boldsymbol{J} + \sigma^*\phi = \sigma acT^4 + cQ$$

Couple with the material energy balance equation:

$$\frac{1}{c_v}\frac{\partial T}{\partial t} = \sigma^*\phi - \sigma^* acT^4$$

Approximate the red terms semi-implicitly.

The transport problem used to calculate $\mathbf{D}$ is

$$\boldsymbol{\Omega} \cdot \boldsymbol{\nabla} f + \sigma^* f = \frac{1}{4\pi}\,, \boldsymbol{x} \in V,\ \boldsymbol{\Omega} \in 4\pi\,,$$

with boundary condition

$$f(\boldsymbol{x}, \boldsymbol{\Omega}) = f(\boldsymbol{x}, -\boldsymbol{\Omega})\,, \boldsymbol{x} \in \partial V,\ \boldsymbol{\Omega} \cdot \boldsymbol{n} < 0\,.$$

- Takes only one transport sweep to solve if the boundaries are many mean free paths apart
- Only needs to be calculated once per time step (because of changing σ^*) in a nonlinear problem
- Requires no storage of the angular flux, just accumulation of second moment, $D_{ij} = \int_{4\pi} \Omega_i \Omega_j f \, \mathrm{d}\Omega$
- Has the solution $f = 1/4\pi\sigma$ if σ is a constant. Then, $\int_{4\pi} \boldsymbol{\Omega}\boldsymbol{\Omega} f \, \mathrm{d}\Omega = \mathbf{I}/3\sigma$.

Properties of anisotropic diffusion

The anisotropic diffusion tensor $\mathbf{D}(\boldsymbol{x}, t)$:

- Does not "blow up" in void regions
- Has a greater "action" along the direction of a voided channel than across it
- Reduces to $\mathbf{I}/3\sigma$ for a homogeneous medium, which gives standard diffusion solution (and boundary conditions reduce to transport-corrected diffusion BCs)
- Is symmetric positive definite, guaranteeing a positive solution for ϕ.
- Is continuous in $\boldsymbol{x}$, so the approximate AD-calculated ϕ has continuous first derivatives (i.e., ϕ is smooth like our ansatz requires)

Outline

Compared methods

- Implicit Monte Carlo (IMC) [3] implemented with variance reduction methods, 10^7 particles per time step
- Flux-limited diffusion (FLD) with Larsen limiter [4], with semi-implicit treatment of diffusion coefficient and radiation:

$$\boldsymbol{J}^{n+1} = -D^n \boldsymbol{\nabla}\phi^{n+1} = -\left[(3\sigma^n)^2 + \left(\frac{\|\boldsymbol{\nabla}\phi^n\|}{\phi^n}\right)^2\right]^{-1/2} \boldsymbol{\nabla}\phi^{n+1}$$

- Anisotropic diffusion, with semi-implicit treatment of nonlinearities:

$$\boldsymbol{J}^{n+1} = -\mathbf{D}^n \cdot \boldsymbol{\nabla}\phi^{n+1}$$

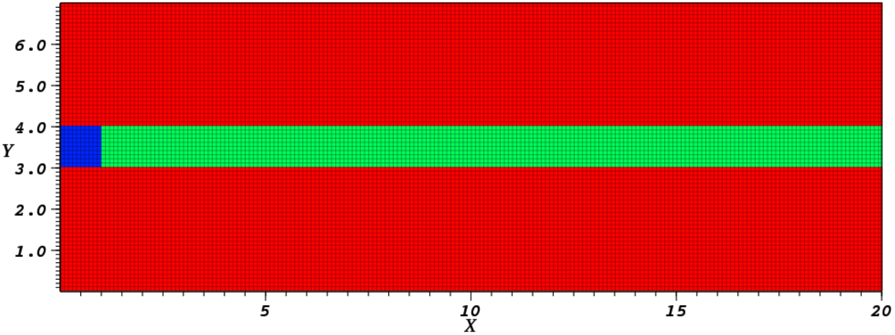
- Flux-limited anisotropic diffusion:

$$\boldsymbol{J}^{n+1} = -\mathbf{D}^n \cdot \boldsymbol{\nabla}\phi^{n+1} \times \max\left(1, \left\|\mathbf{D}^n \cdot \frac{\boldsymbol{\nabla}\phi^n}{\phi^n}\right\|\right)^{-1}$$

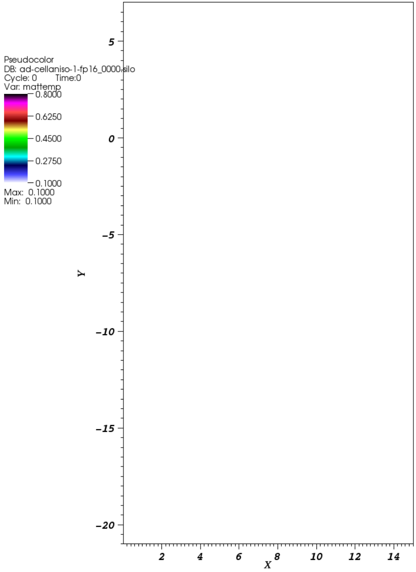
Problem description

Flatland geometry!
Uniform spatial grid: $\Delta_x = 0.1$
Piecewise linear time grid: $\Delta_t = 0.1$ for $t \geq 1$
Reflecting bndy on left, others vacuum

Source: $c_v = 0.5$, $\sigma = 0.5$; $Q = 1$ for $0 \leq t \leq 1$, $Q = 0$ for $t > 1$.
Diffusive: $c_v = 0.1$, $\sigma = T^{-3}$
Channel: $c_v = 0.1$, $\sigma = 0.01T^{-3}$
Initial condition: $T = T_{\text{rad}} = 0.1$



Time evolution of material temperature



IMC

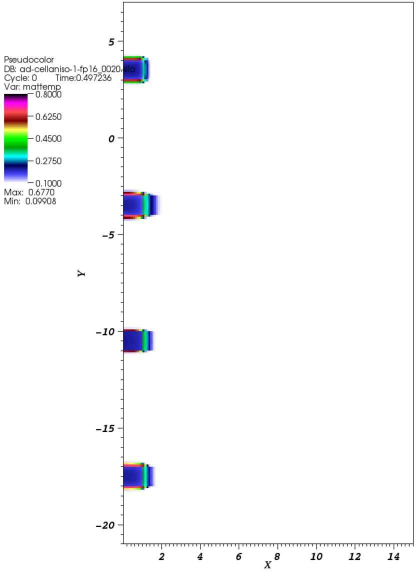
AD

FLD

FLAD

$t = 0$

Time evolution of material temperature



IMC

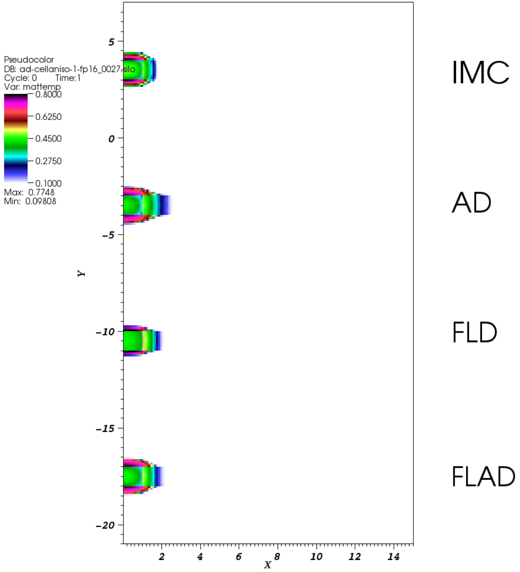
AD

FLD

FLAD

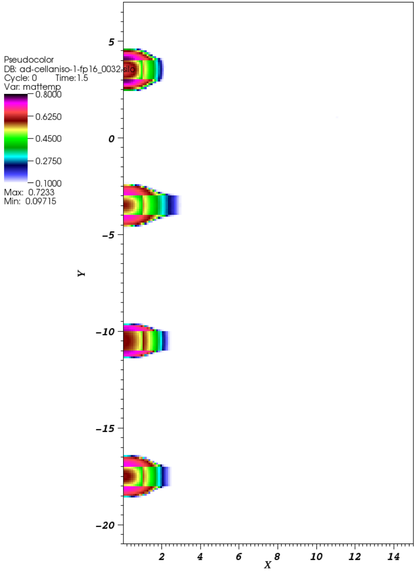
$t = 0.5$

Time evolution of material temperature



$t = 1.0$

Time evolution of material temperature



IMC

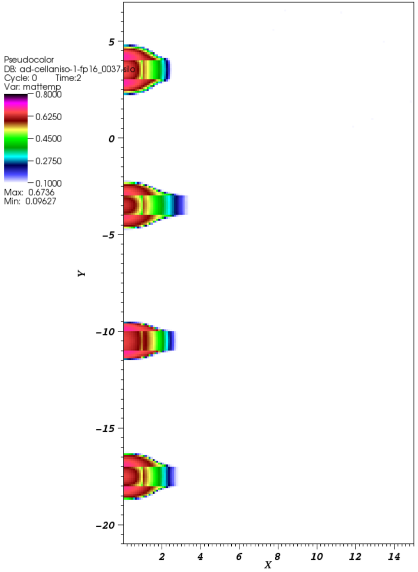
AD

FLD

FLAD

$t = 1.5$

Time evolution of material temperature



IMC

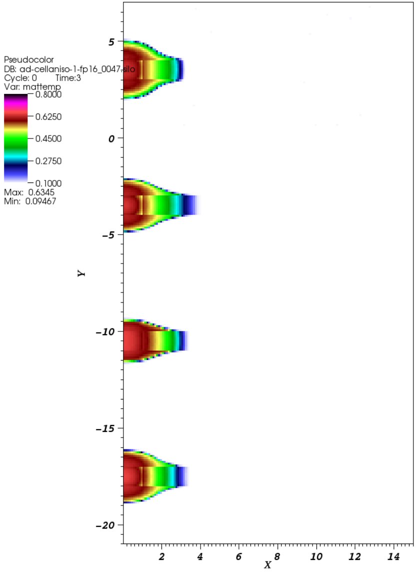
AD

FLD

FLAD

$t = 2$

Time evolution of material temperature



IMC

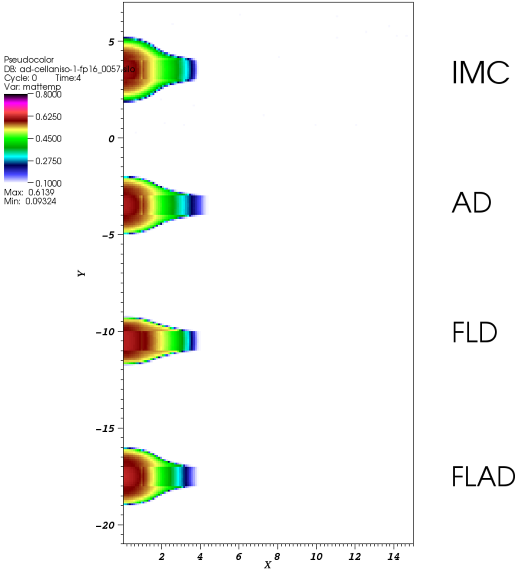
AD

FLD

FLAD

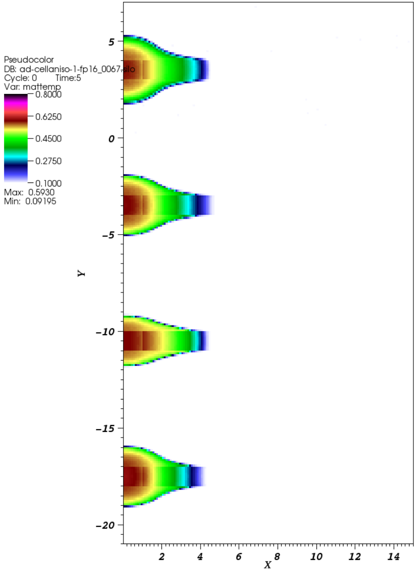
$t = 3$

Time evolution of material temperature



$t = 4$

Time evolution of material temperature



IMC

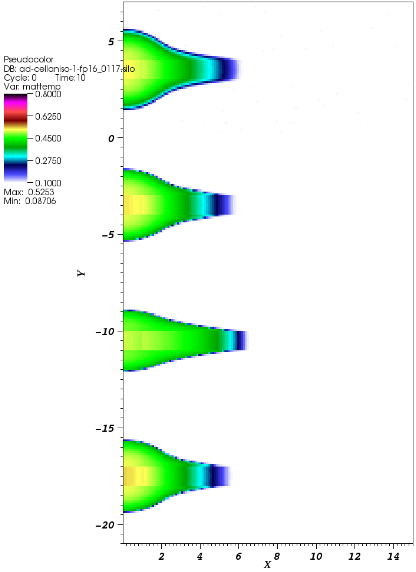
AD

FLD

FLAD

$t = 5$

Time evolution of material temperature



IMC

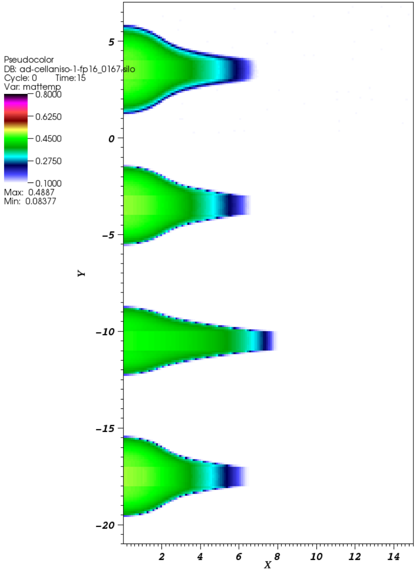
AD

FLD

FLAD

$t = 10$

Time evolution of material temperature



IMC

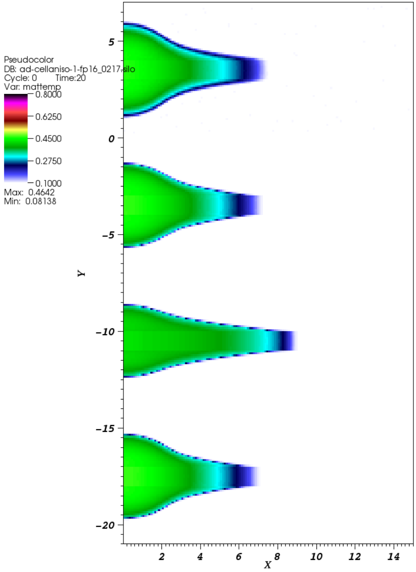
AD

FLD

FLAD

$t = 15$

Time evolution of material temperature



IMC

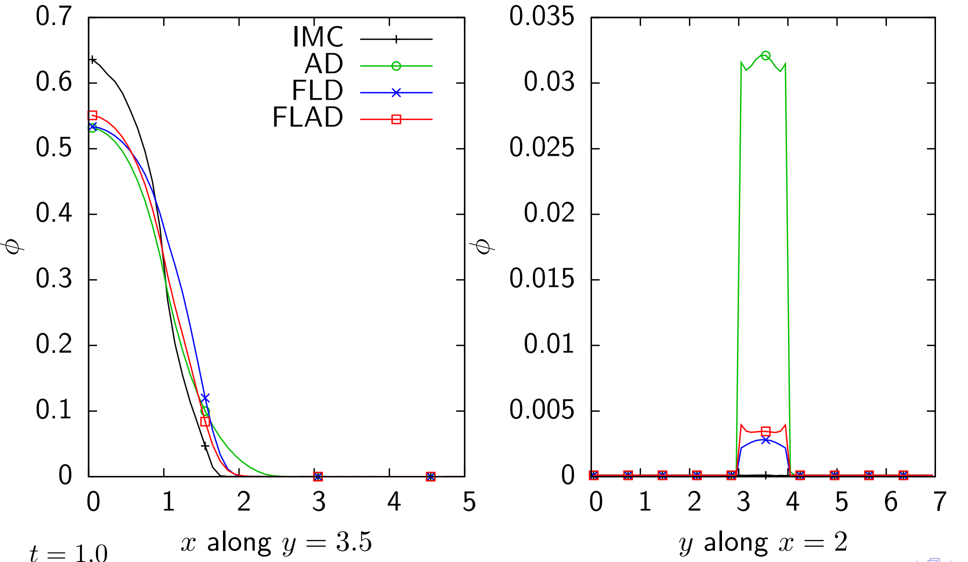
AD

FLD

FLAD

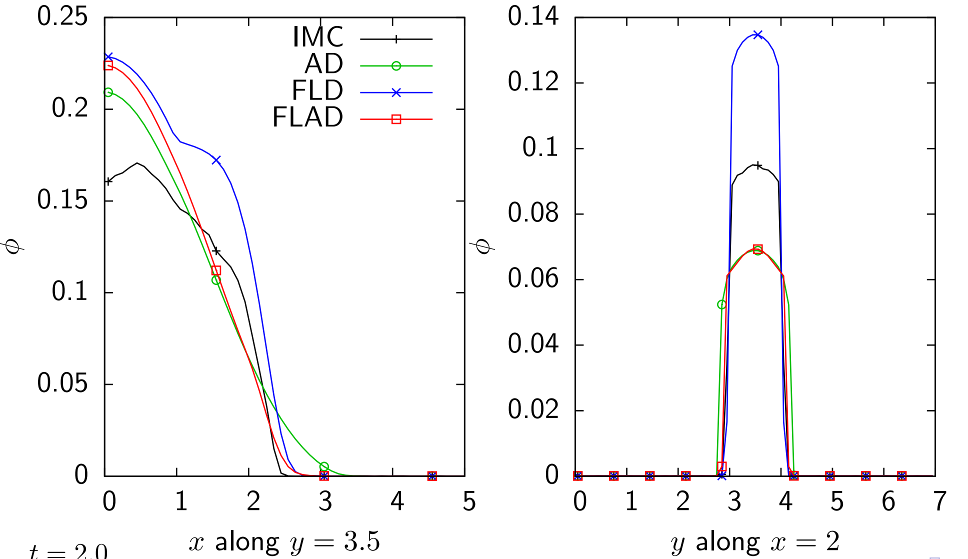
$t = 20$

Time evolution of radiation energy density



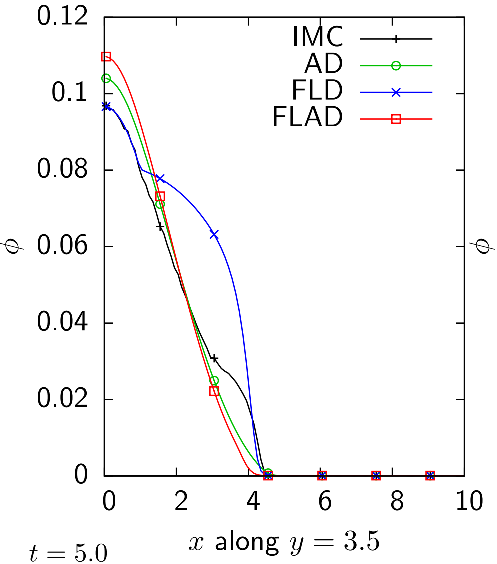
$t = 1.0$

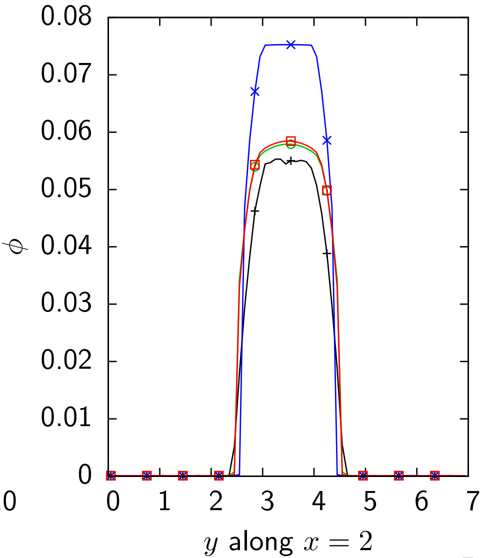
Time evolution of radiation energy density



$t = 2.0$

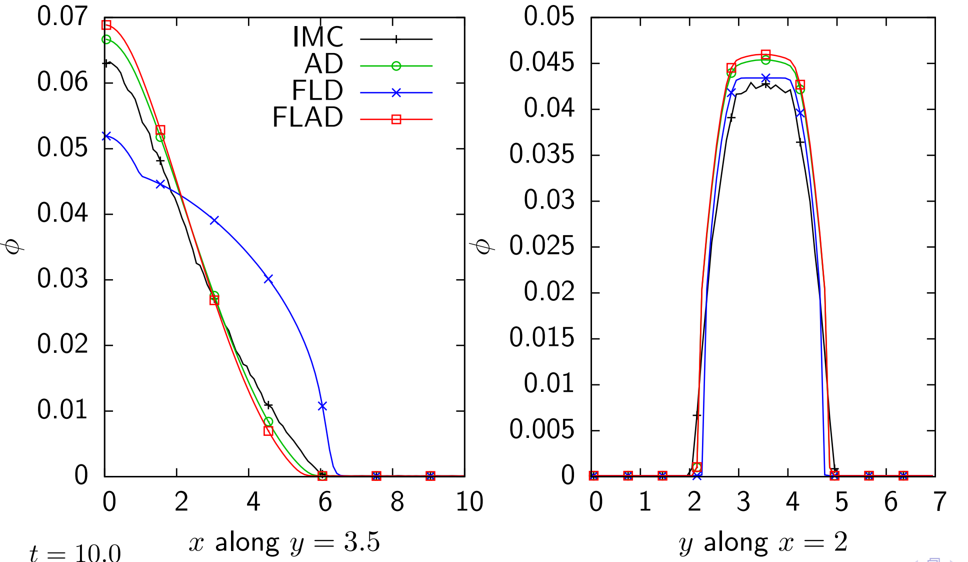
Time evolution of radiation energy density





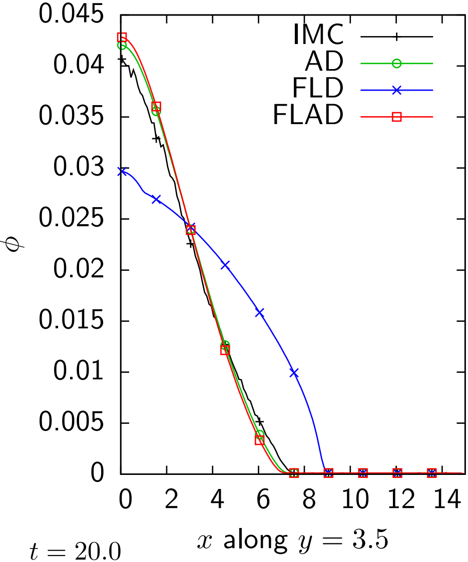
$t = 5.0$

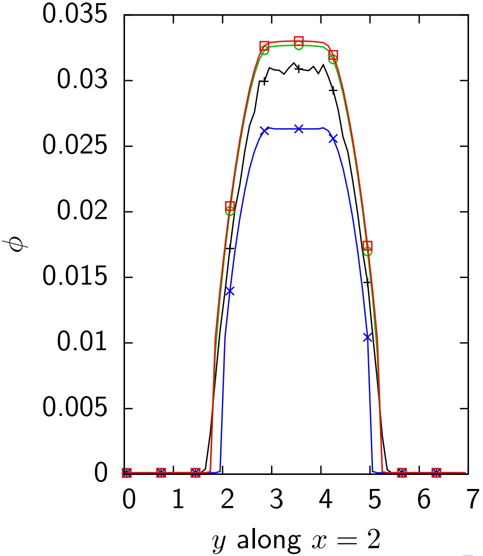
Time evolution of radiation energy density



$t = 10.0$

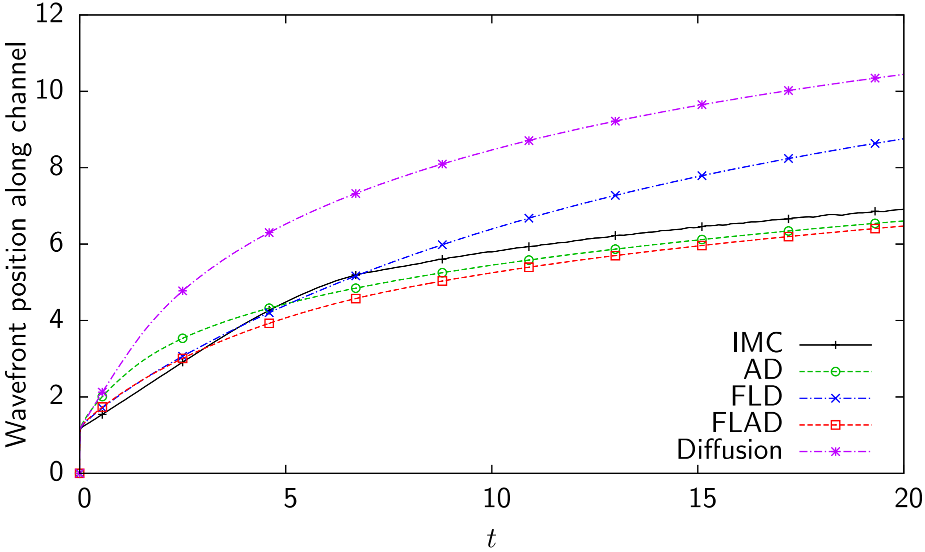
Time evolution of radiation energy density



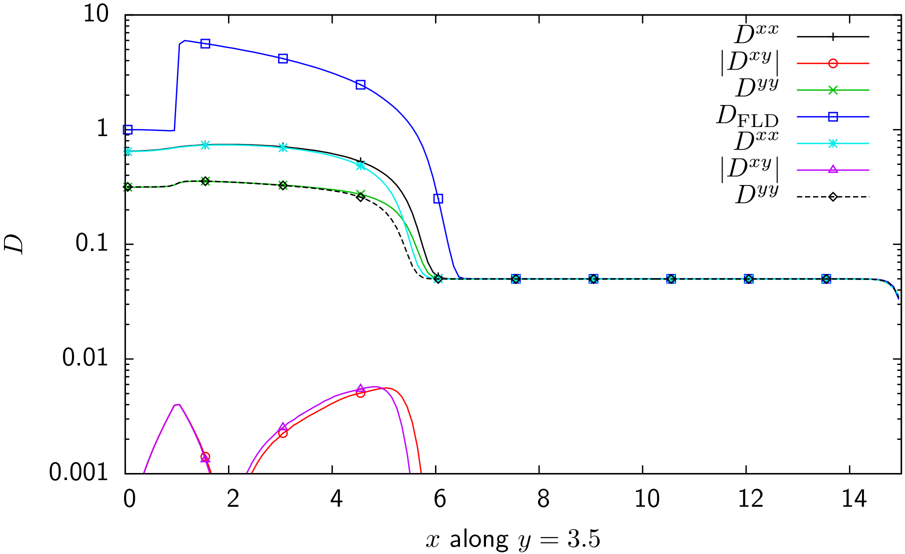


$t = 20.0$

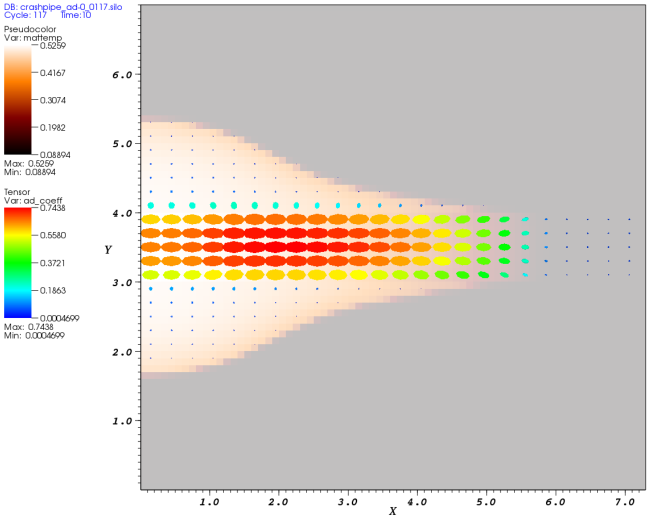
Time evolution of radiation temperature wavefront



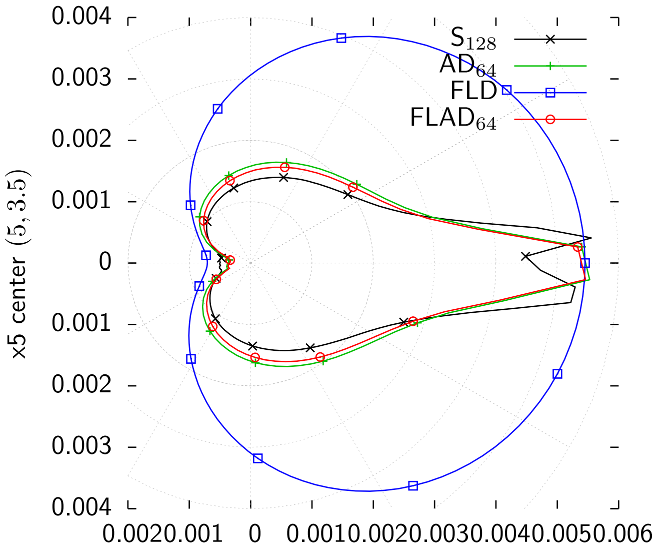
Diffusion coefficients ($t = 10$)



Anisotropic diffusion tensor visualization



Approximate representations of the angular flux



Timing results

Method	Wall time (s)
IMC	2730
FLD	21
D	20
AD_{64}	36
AD_{128}	59

Table 1: Approximate run times for pipe test problem with $\Delta_x = 0.1$.

Outline

Conclusions

Anisotropic diffusion:

- Accounts for some amount of arbitrary anisotropy in angular flux, unlike standard or current-limited diffusion, by preserving some transport physics
- Works best in problems with weaker derivatives, as suggested by theory and borne out by numerical experiments
- Accurately treats the nonlinear time-dependent flow of radiation through a tube like that found in CRASH experiments

Future work

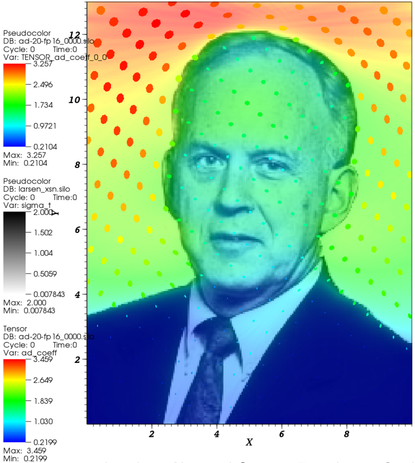
Me:

- Further analysis of boundary conditions
- Finish writing a dissertation
- Convince committee to let me graduate

Someone else:

- Implement and test "Anisotropic P_1" ($\frac{1}{c}\frac{\partial}{\partial t} = O(\epsilon)$ instead of $O(\epsilon^2)$)?
- Extend method to anisotropic internal sources
- Keep the $\boldsymbol{\nabla} \cdot \boldsymbol{J}$ term by ignoring assumption of $\int_{4\pi} \boldsymbol{\Omega}(\cdot)\,\mathrm{d}\Omega = O(\epsilon)$

Questions?



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