An anisotropic diffusion approximation to nonlinear radiation transport

Seth Johnson Ed Larsen

University of Michigan, Ann Arbor

May 24, 2011

MICHIGAN

Nuclear Energy University Programs
U.S. Department of Energy

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 ($\sigma \propto T^{-3}$)

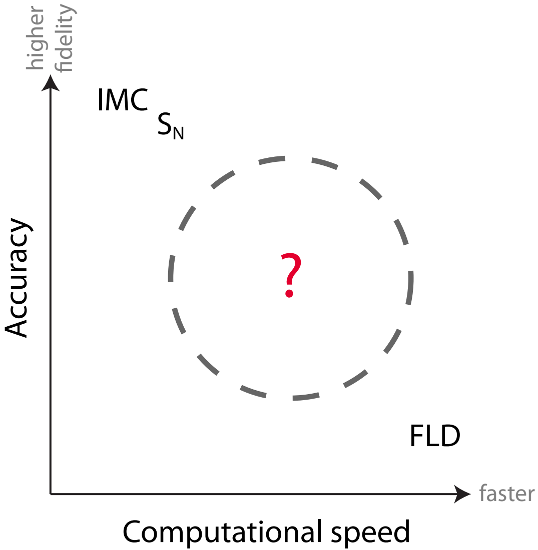
Difficulties in solving:

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

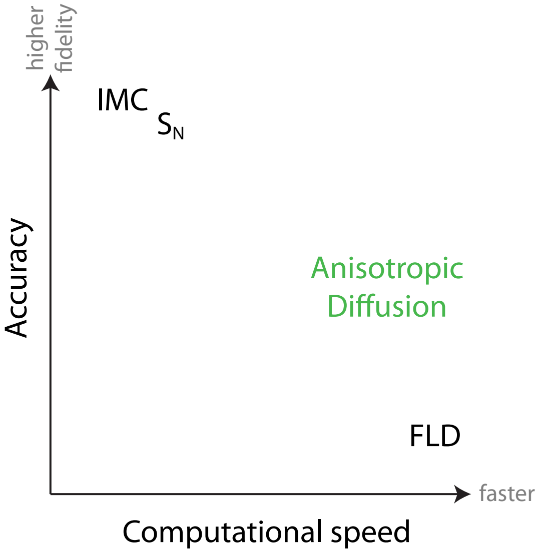
Particular application of this work: CRASH project

- 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
?
Accuracy
FLD
faster
Computational speed

Motivation


higher fidelity
IMC
S_N
Accuracy
Anisotropic Diffusion
FLD
faster
Computational speed

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, intensity $I(\boldsymbol{x}, \boldsymbol{\Omega}, t)$:

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

Material energy balance equation:

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

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 intensity as $\Psi = I - \frac{1}{4\pi}\phi$.
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 $I = O(1)$, $\frac{1}{c}\frac{\partial}{\partial t} = O(\epsilon^2)$, $\boldsymbol{\nabla} = O(\epsilon)$, $\int_{4\pi} \boldsymbol{\Omega}(\cdot)\, \mathrm{d}\Omega = O(\epsilon)$.
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 $\boldsymbol{F} = -\mathbf{D} \cdot \boldsymbol{\nabla}\phi$
6. Substitute $\boldsymbol{F}$ into the time-dependent particle conservation equation to get time-dependent anisotropic diffusion.

Transport equation (interior)

Inside a time step, with "frozen" opacities:

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

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

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

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

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

Anisotropic intensity equation

Define "anisotropic intensity":

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

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

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

Transport equation for Ψ:

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

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

Integral transport equation

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

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

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

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 intensity, very small time derivative:

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

Our first approximation: $\mathcal{I}_i[\cdot] = O(\epsilon^2)$ and $\boldsymbol{\nabla} \cdot \boldsymbol{F} = O(\epsilon^2)$:

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

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

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:

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

Thus,

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

An analogy to Fick's law

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

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

Substitute into radiation energy conservation equation:

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

Couple with the material energy balance equation:

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

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 intensity, 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, $\int_{4\pi} \boldsymbol{\Omega\Omega} f \, \mathrm{d}\Omega = \mathbf{I}/3\sigma$.

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:

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

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

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

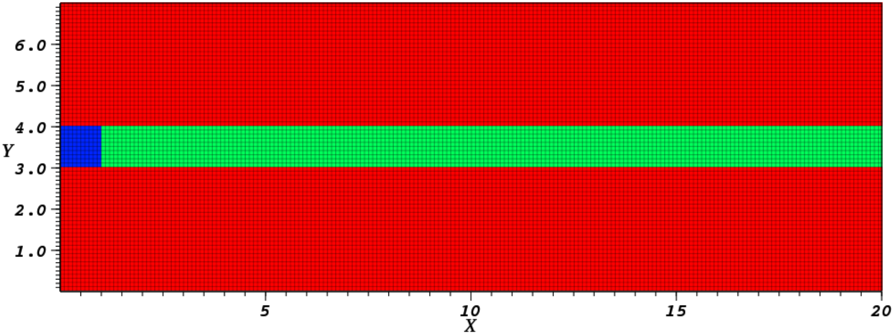
- Flux-limited anisotropic diffusion:

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

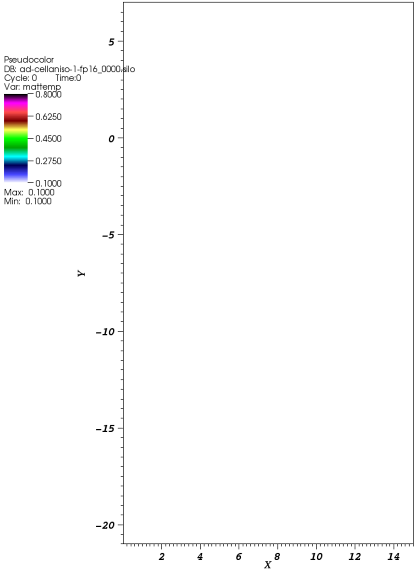
Problem description

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

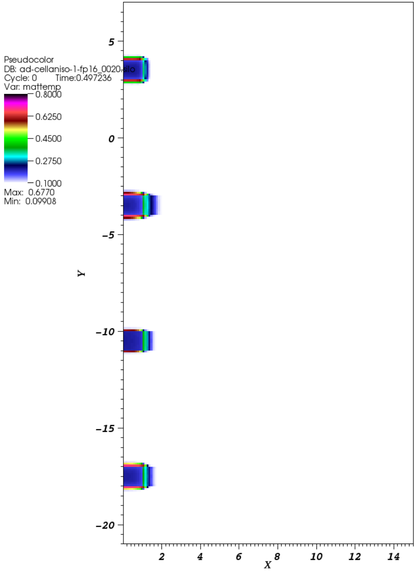
AD

FLD

FLAD

$t = 0$

Time evolution of material temperature



IMC

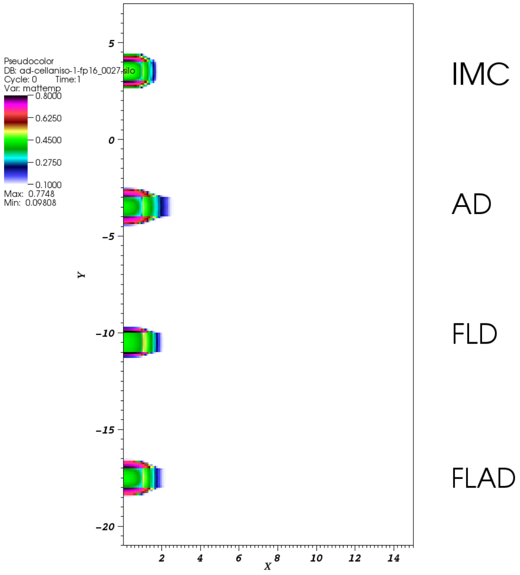
AD

FLD

FLAD

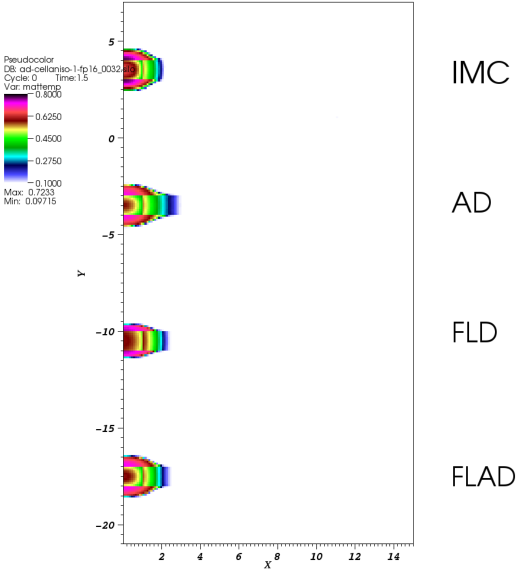
$t = 0.5$

Time evolution of material temperature



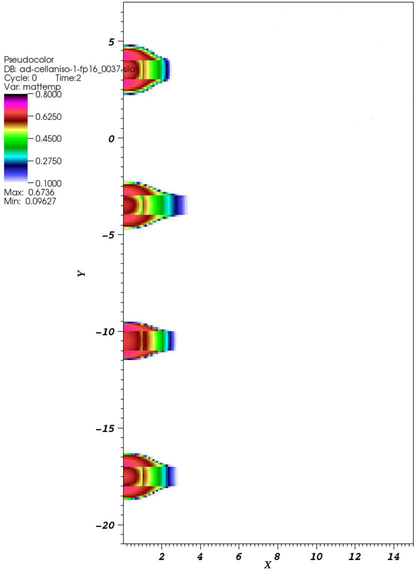
$t = 1.0$

Time evolution of material temperature



$t = 1.5$

Time evolution of material temperature



IMC

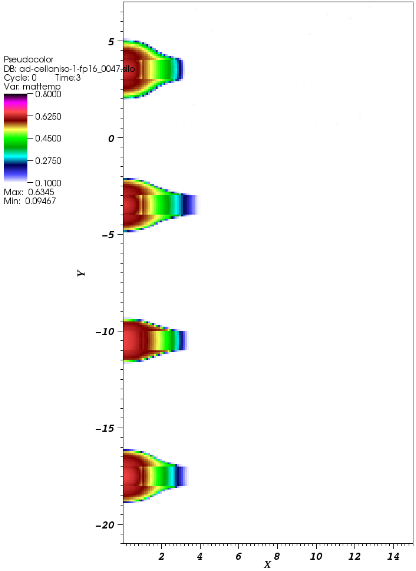
AD

FLD

FLAD

$t = 2$

Time evolution of material temperature



IMC

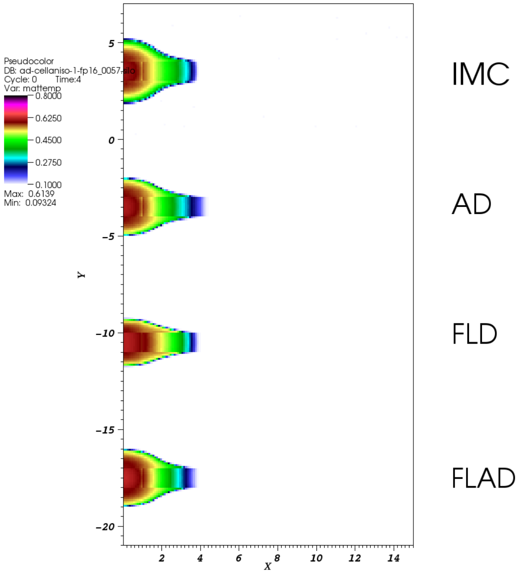
AD

FLD

FLAD

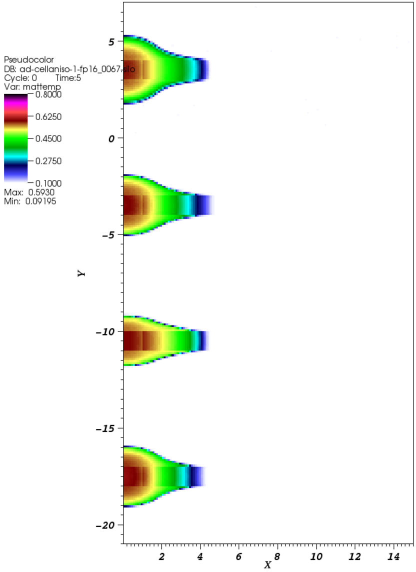
$t = 3$

Time evolution of material temperature



$t = 4$

Time evolution of material temperature



IMC

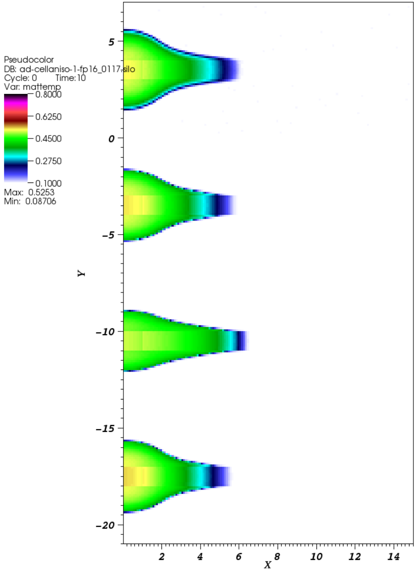
AD

FLD

FLAD

$t = 5$

Time evolution of material temperature



IMC

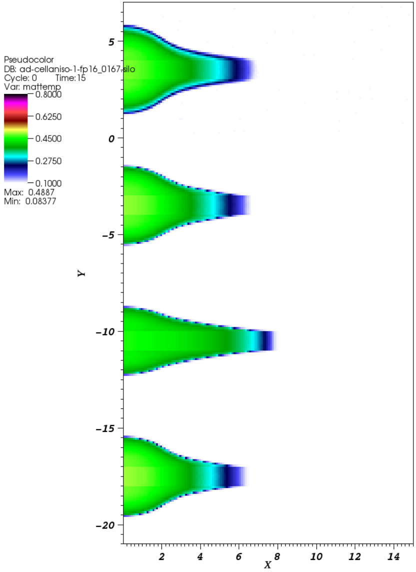
AD

FLD

FLAD

$t = 10$

Time evolution of material temperature



IMC

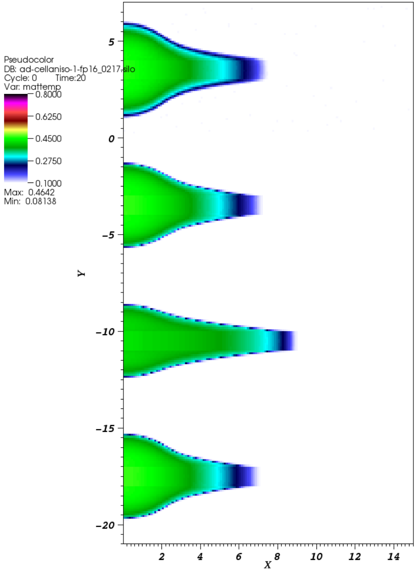
AD

FLD

FLAD

$t = 15$

Time evolution of material temperature



IMC

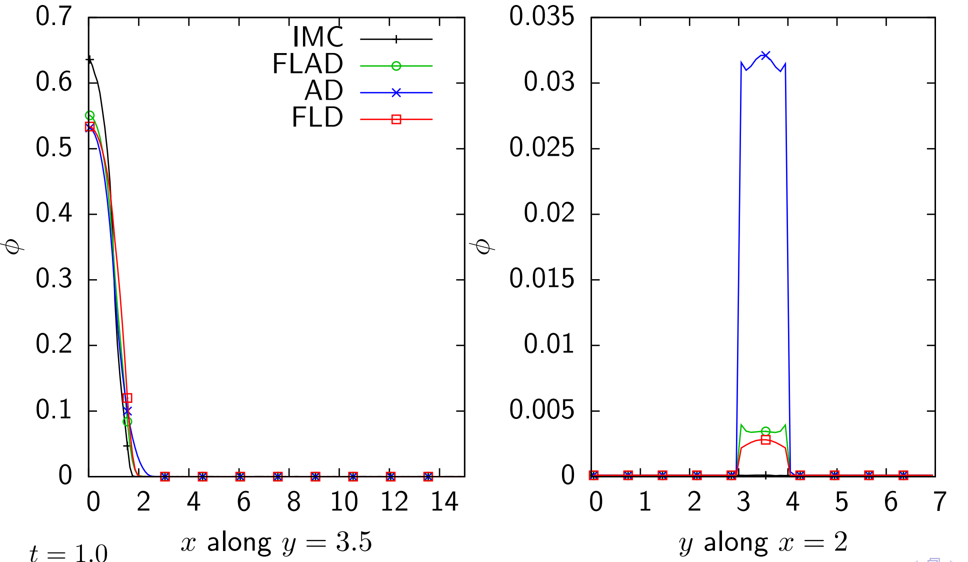
AD

FLD

FLAD

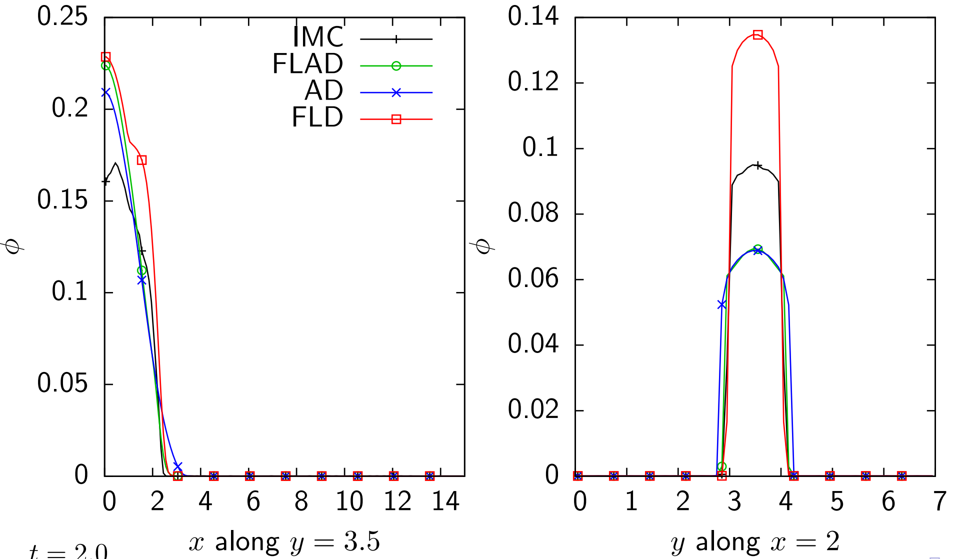
$t = 20$

Time evolution of radiation energy density



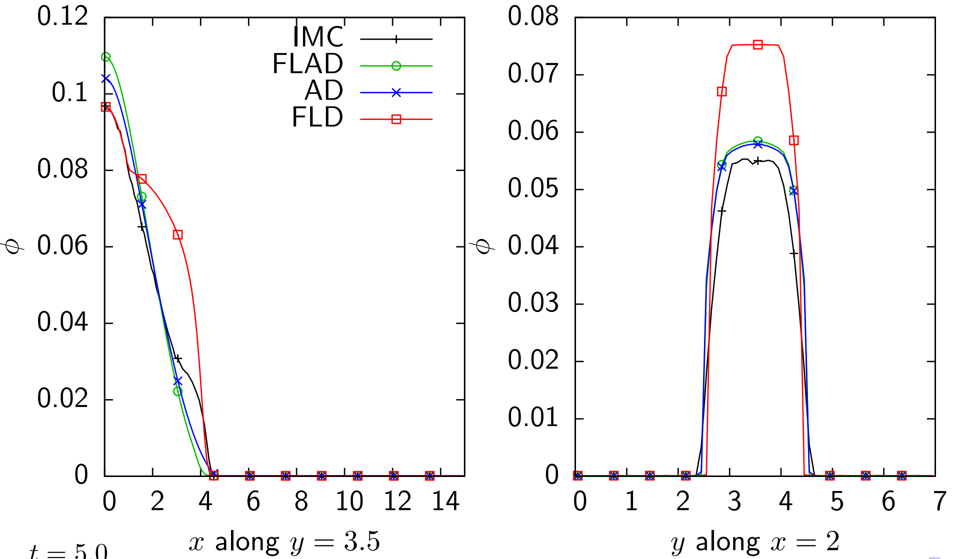
$t = 1.0$

Time evolution of radiation energy density



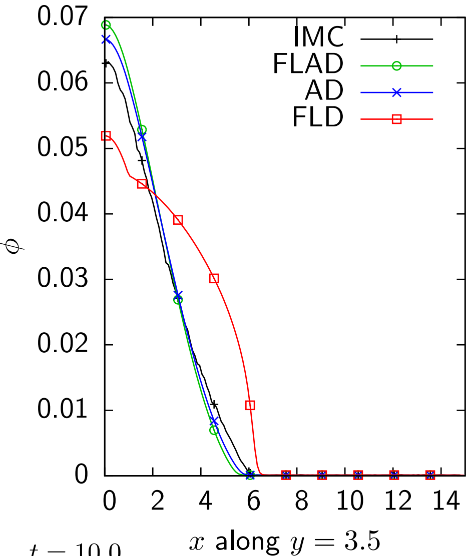
$t = 2.0$

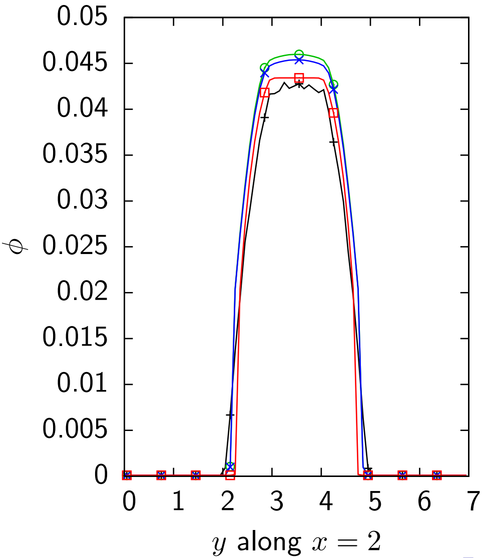
Time evolution of radiation energy density



$t = 5.0$

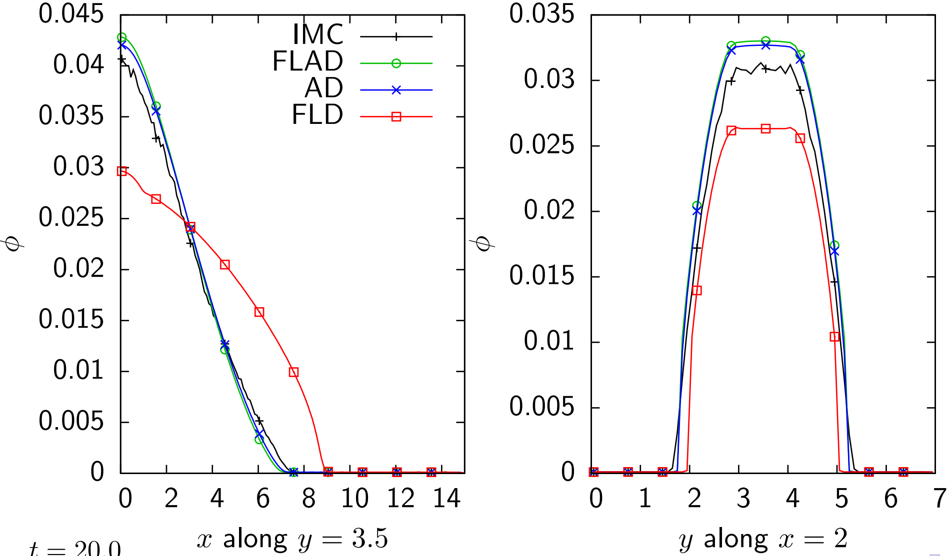
Time evolution of radiation energy density





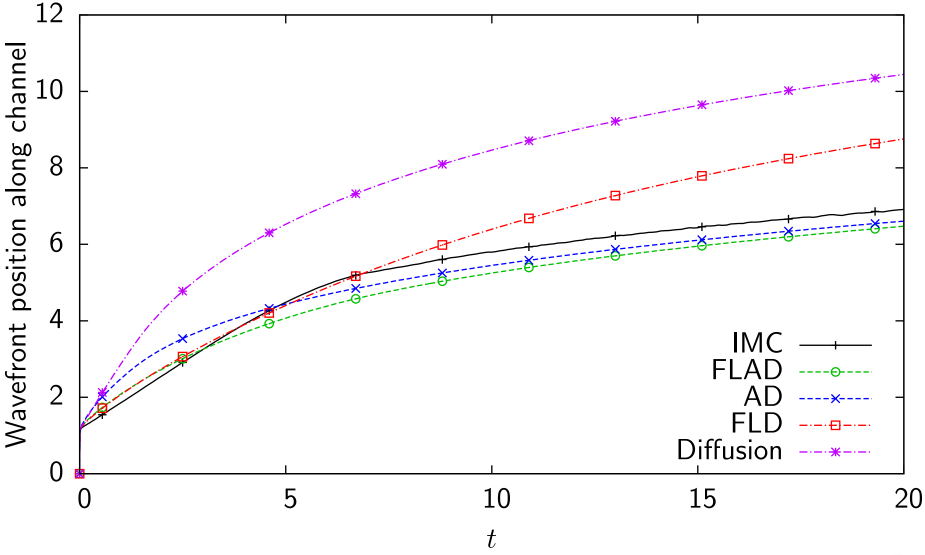
$t = 10.0$

Time evolution of radiation energy density

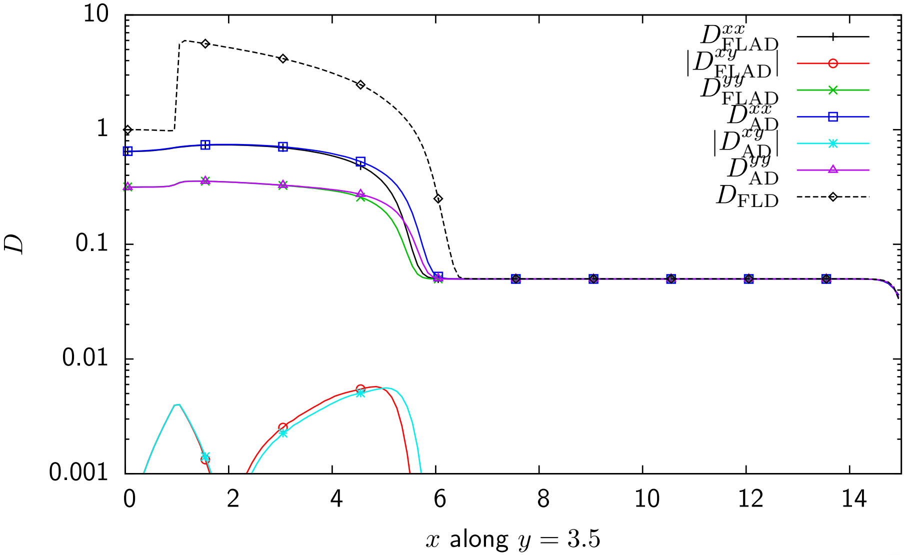


$t = 20.0$

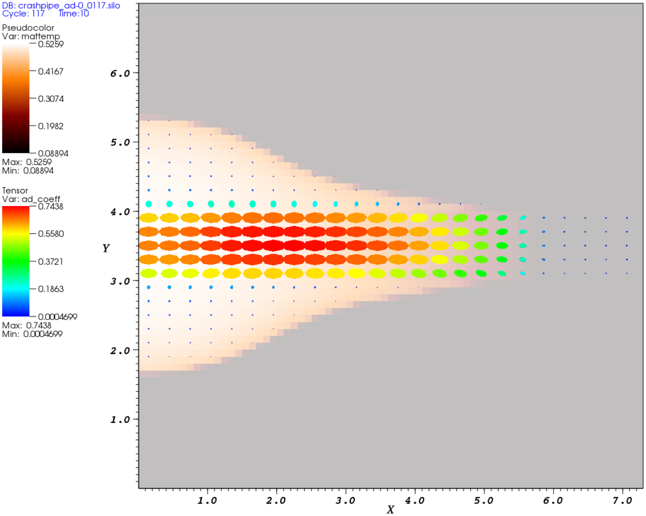
Time evolution of radiation temperature wavefront



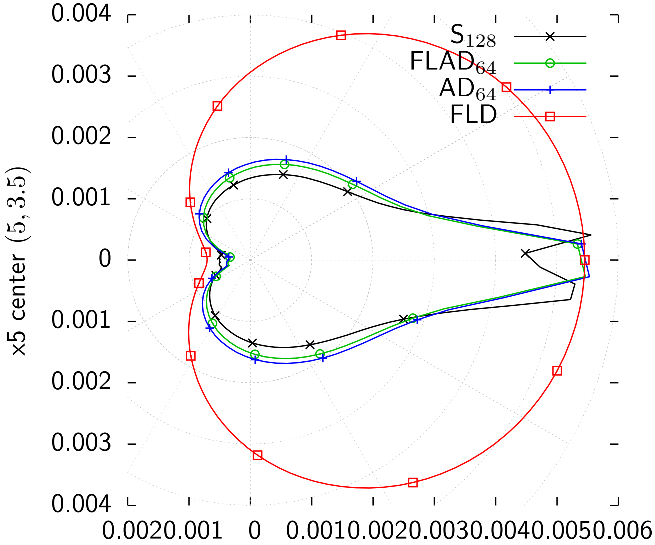
Diffusion coefficients ($t = 10$)



Anisotropic diffusion tensor visualization



Approximate representations of the intensity



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

1. Introduction
2. Theory
3. Results
4. Conclusions

Conclusions

Anisotropic diffusion:

- Accounts for some amount of arbitrary anisotropy in angular intensity, unlike standard or flux-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

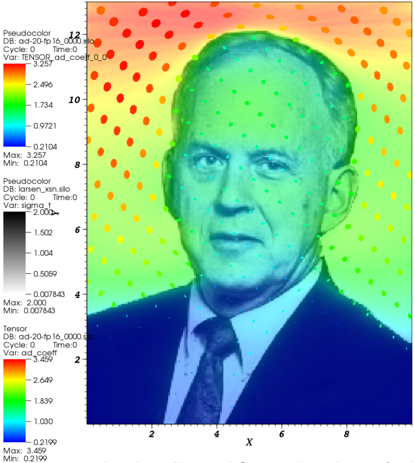
Me:

- 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 $\boldsymbol{\nabla} \cdot \boldsymbol{F}$ term by ignoring assumption of $\int_{4\pi} \boldsymbol{\Omega}(\cdot)\,\mathrm{d}\Omega = O(\epsilon)$

Questions?



This material is based upon work supported under a National Science Foundation Graduate Research Fellowship and a Department of Energy Nuclear Energy University Programs Graduate Fellowship. Any opinions, findings, conclusions or recommendations expressed in this publication are those of the author and do not necessarily reflect the views of the National Science Foundation or the Department of Energy Office of Nuclear Energy.

References

E. W. LARSEN and T. J. TRAHAN, "2-D Anisotropic Diffusion in Optically Thin Channels," in "Trans. Am. Nucl. Soc.", (2009), vol. 101, pp. 387–389.

J. E. MOREL, "A Non-Local Tensor Diffusion Theory," Tech. Rep. LA-UR-07-5257, Los Alamos National Laboratory (2007).

J. A. FLECK, JR. and J. D. CUMMINGS, "An Implicit Monte Carlo Scheme for Calculating Time and Frequency Dependent Nonlinear Radiation Transport," *Journal of Computational Physics*, **8**, 3, 313–342 (1971).

G. L. OLSON, L. H. AUER, and M. L. HALL, "Diffusion, P_1, and other approximate forms of radiation transport," *Journal of Quantitative Spectroscopy and Radiative Transfer*, **64**, 619–634 (2000).