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

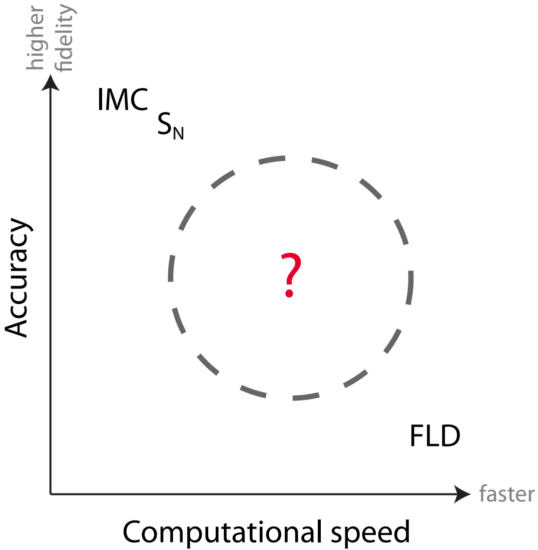
Difficulties in solving:

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

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:

- 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

Summary in advance (infinite medium)

1. Define the anisotropic intensity as $\Psi = I - \frac{1}{4\pi}\phi$. We will approximate Ψ rather than I.
2. From the radiation transport equation and conservation equation, we get a differential transport equation for Ψ. Transform this 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

Inside a time step, with "frozen" opacities:

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

and the initial condition

$$
I(\boldsymbol{x},\boldsymbol{\Omega},0) = I^i(\boldsymbol{x},\boldsymbol{\Omega},t)\,, \quad \boldsymbol{x} \in V,\ \boldsymbol{\Omega} \in 4\pi\,. \qquad \text{(2b)}
$$

For this presentation, only consider an infinite (non-homogeneous) medium.

Conservation equations

Operating on Eq. (2a) by $\int_{4\pi}(\cdot)\,\mathrm{d}\Omega$ gives

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

and on the initial condition, Eq. (2b),

$$\phi(\boldsymbol{x},0) = \int_{4\pi} I^i(\boldsymbol{x},\boldsymbol{\Omega})\,\mathrm{d}\Omega = \phi^i(\boldsymbol{x})\,. \tag{3b}$$

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

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

Anisotropic intensity equations

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. (2a); the isotropic source cancels:

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

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

Subtract Eq. (3b) from Eq. (2b):

$$\Psi(\boldsymbol{x}, \boldsymbol{\Omega}, 0) = I(\boldsymbol{x}, \boldsymbol{\Omega}, 0) - \frac{1}{4\pi}\phi(\boldsymbol{x}, 0) = I^i - \frac{\phi^i}{4\pi}$$

The exact solutions for I, ϕ, $\boldsymbol{F}$ satisfy these equations: still no approximations.

Integral transport equation

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

$$\begin{aligned}
\Psi(\boldsymbol{x}, \boldsymbol{\Omega}, t) &= \Psi^i(\boldsymbol{x} - ct\boldsymbol{\Omega}, \boldsymbol{\Omega})\, \mathrm{e}^{-\tau(\boldsymbol{x}, \boldsymbol{x} - ct\boldsymbol{\Omega})} \\
&\qquad + \int_0^\infty \left[\hat{Q}(\boldsymbol{x} - s\boldsymbol{\Omega}, \boldsymbol{\Omega}, t - s/c)\right] \mathrm{e}^{-\tau(\boldsymbol{x}, \boldsymbol{x} - s\boldsymbol{\Omega})}\, \mathrm{d}s\,. && \text{(6a)} \\
&\equiv \mathcal{L}_i^{-1}\left[\Psi^i\right] + \mathcal{L}_v^{-1}\left[\hat{Q}\right] && \text{(6b)} \\
&= \mathcal{L}_i^{-1}\left[\Psi^i\right] + \mathcal{L}_v^{-1}\left[\frac{1}{4\pi}\boldsymbol{\nabla} \cdot \boldsymbol{F}\right] - \mathcal{L}_v^{-1}\left[\frac{1}{4\pi}\boldsymbol{\Omega} \cdot \boldsymbol{\nabla}\phi\right]\,.
\end{aligned}$$

Here, 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: $\mathcal{L}_i^{-1}[\cdot] = O(\epsilon^2)$ and $\boldsymbol{\nabla} \cdot \boldsymbol{F} = O(\epsilon^2)$:

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

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

Taylor series expansion:

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

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

Internal approximation to Ψ

Applying the Taylor series expansion under the assumption of a smooth ϕ,

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

where $\mathcal{L}_v^{-1}\left[\frac{1}{4\pi}\right] \equiv f$ is the solution to a purely absorbing transport equation:

$$\boldsymbol{\Omega}\cdot\boldsymbol{\nabla} f(\boldsymbol{x},\boldsymbol{\Omega}) + \sigma^* f(\boldsymbol{x},\boldsymbol{\Omega}) = \frac{1}{4\pi}\,, \quad x\in V,\ \boldsymbol{\Omega}\in 4\pi\,, \tag{8a}$$

$$f(\boldsymbol{x},\boldsymbol{\Omega}) = 0\,, \quad \boldsymbol{x}\in\partial V,\ \boldsymbol{\Omega}\cdot\boldsymbol{n} < 0\,. \tag{8b}$$

An analogy to Fick's Law

To get an expression for the radiation flux (a.k.a. "current"), use the identity $\boldsymbol{F} = \int_{4\pi} \boldsymbol{\Omega}\Psi \,\mathrm{d}\Omega$,

$$\begin{aligned} \boldsymbol{F}(\boldsymbol{x},t) &= \int_{4\pi} \boldsymbol{\Omega} \left(-\mathcal{L}_v^{-1}\left[\frac{1}{4\pi}\right] \boldsymbol{\Omega}\cdot\boldsymbol{\nabla}\phi(\boldsymbol{x},t)\right) \mathrm{d}\Omega \\ &= -\left[\int_{4\pi} \boldsymbol{\Omega}\boldsymbol{\Omega} f \,\mathrm{d}\Omega\right]\cdot\boldsymbol{\nabla}\phi \\ &\equiv -\mathbf{D}\cdot\boldsymbol{\nabla}\phi\,. \end{aligned}$$

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 $\mathbf{D}$,

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

- Takes only one transport sweep to solve, since it is the description of a purely absorbing medium
- 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, $\int_{4\pi} \boldsymbol{\Omega} f \boldsymbol{\Omega} \, \mathrm{d}\Omega = \mathbf{I}/3\sigma$.
- For a finite medium, we must derive boundary conditions.

Properties of anisotropic diffusion

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

- Results from consistent approximations to the transport equation using physical coefficients
- Reduces to $\mathbf{I}/3\sigma$ for infinite homogeneous medium, which gives standard diffusion solution
- Has a greater "action" along the direction of a voided channel than across it (see later visualization)
- Does not "blow up" in void regions
- 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 [3] (implemented with variance reduction methods), 10^7 particles per time step
- Flux-limited diffusion with Larsen limiter [4], with semi-implicit treatment of diffusion coefficient and radiation:

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

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

$$\boldsymbol{F}^{n+1} = -D^n \boldsymbol{\nabla}\phi^{n+1} = -\frac{1}{3\sigma^n} \boldsymbol{\nabla}\phi^{n+1}$$

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

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

AD implementation

Approximations in the theory

- Assume weak gradients and angular moments for I (*don't* assume that I is a linear function of $\mathbf{\Omega}$!)
- Apply semi-implicit approximation for nonlinear material coupling and radiation

$\mathbb{D}$ transport equation

- S_N angular approximation
- DD spatial approximation

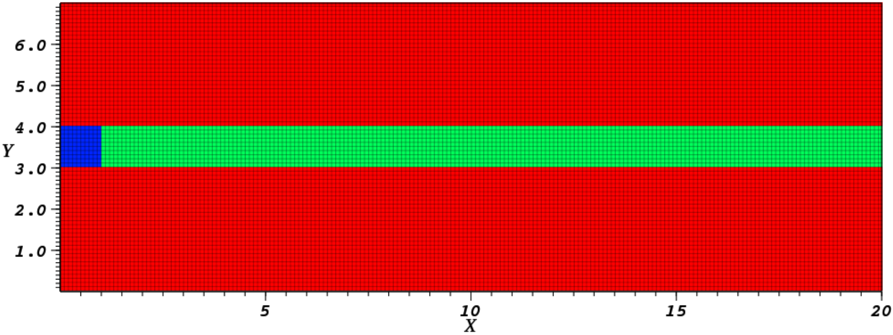
AD equation

- 9-point cell-centered finite difference spatial approximation

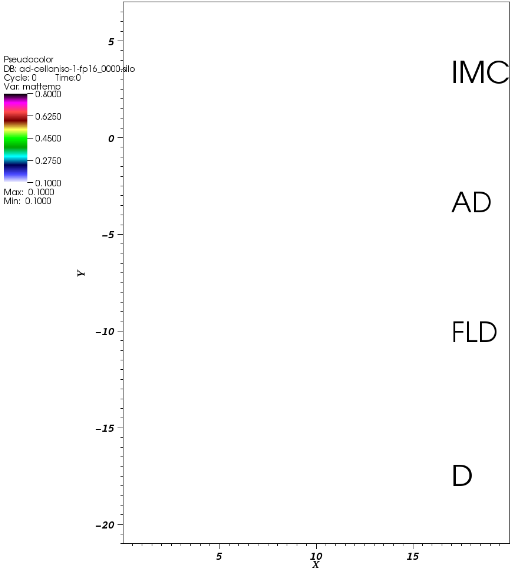
Problem description

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: $T = T_{\text{rad}} = 0.1$

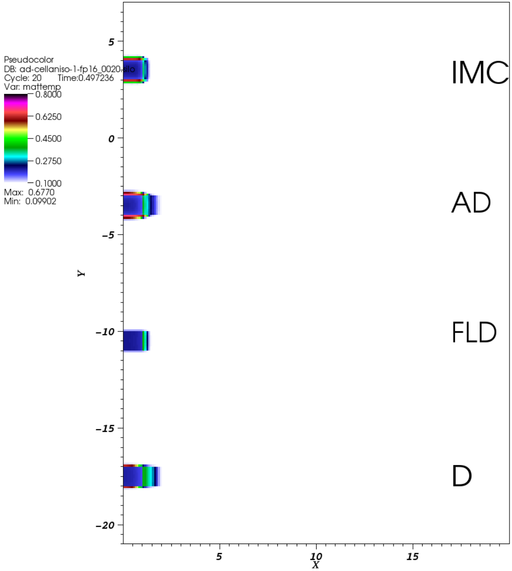


Time evolution of material temperature



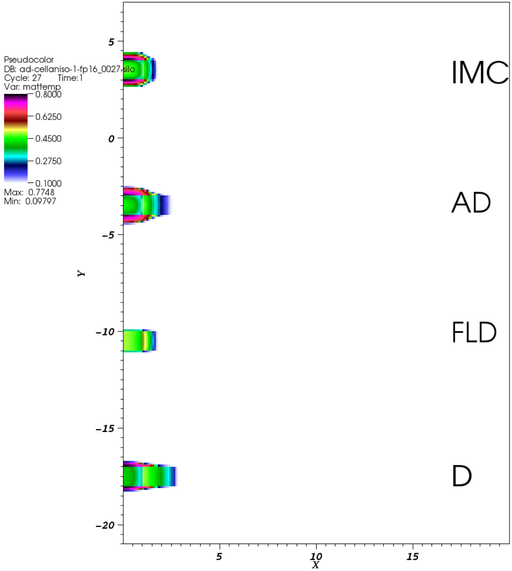
$t = 0$

Time evolution of material temperature



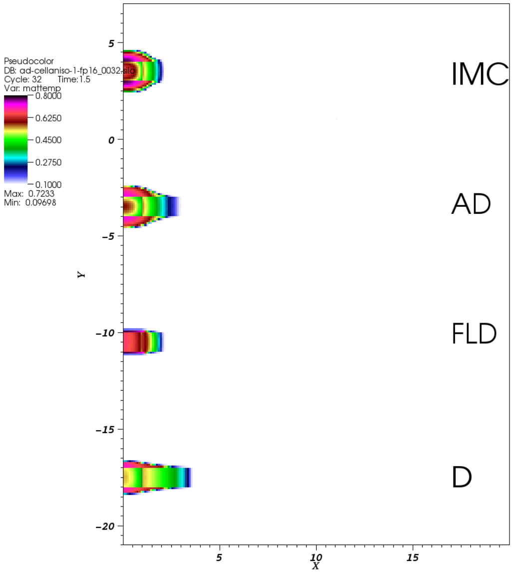
$t = 0.5$

Time evolution of material temperature



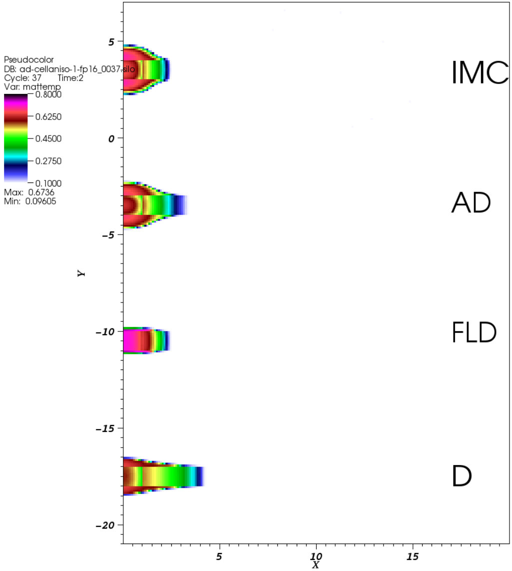
$t = 1.0$

Time evolution of material temperature



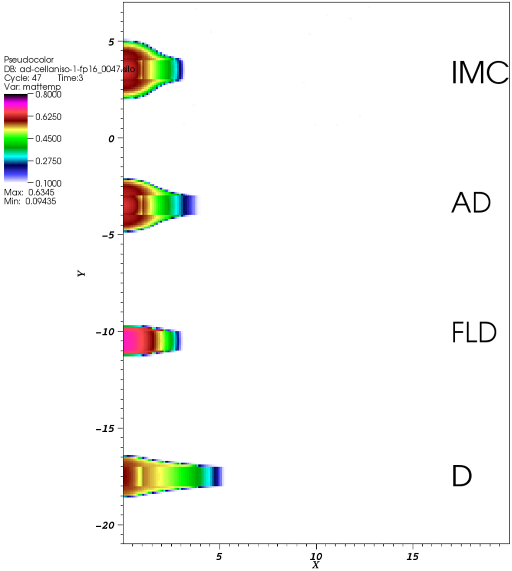
$t = 1.5$

Time evolution of material temperature



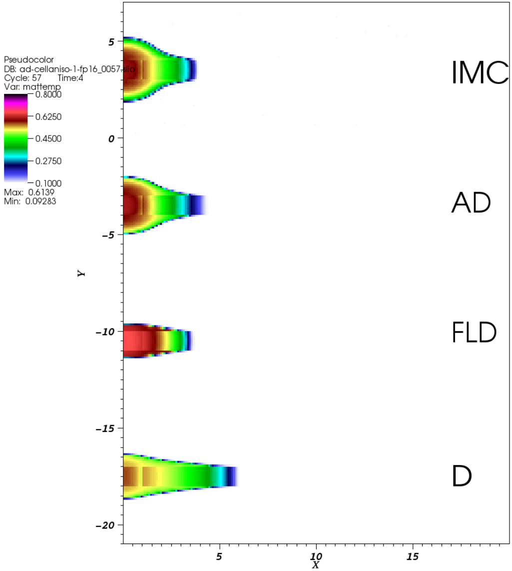
$t = 2$

Time evolution of material temperature



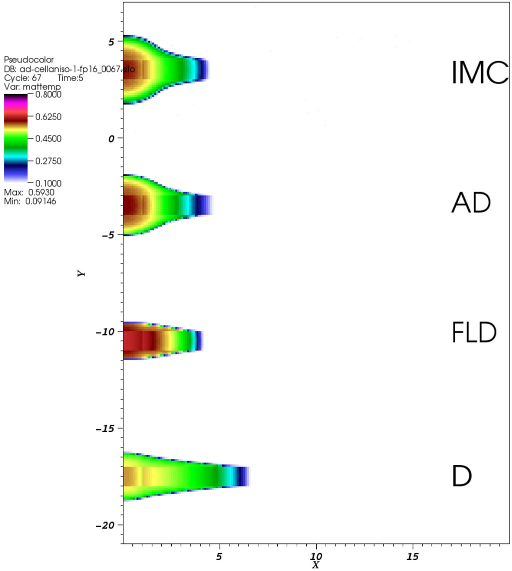
$t = 3$

Time evolution of material temperature



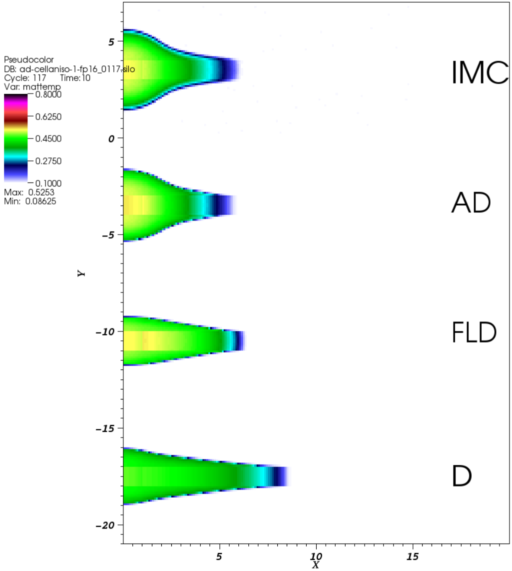
$t = 4$

Time evolution of material temperature



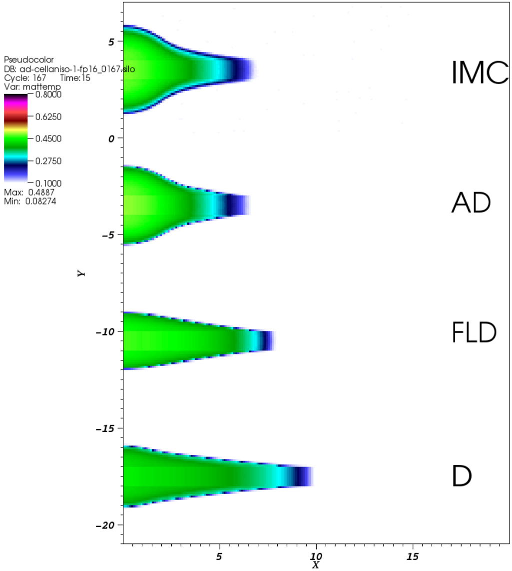
$t = 5$

Time evolution of material temperature



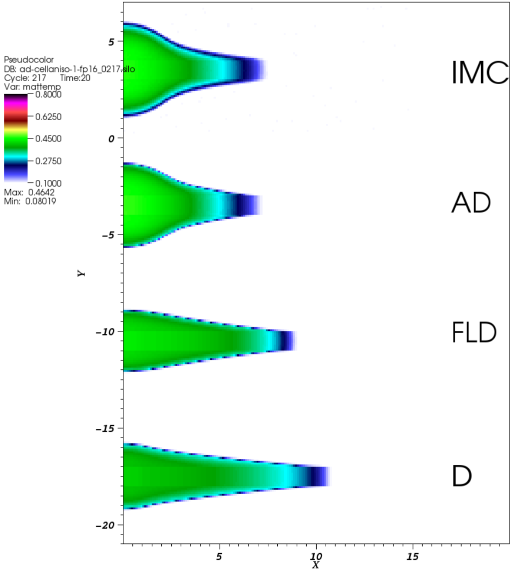
$t = 10$

Time evolution of material temperature



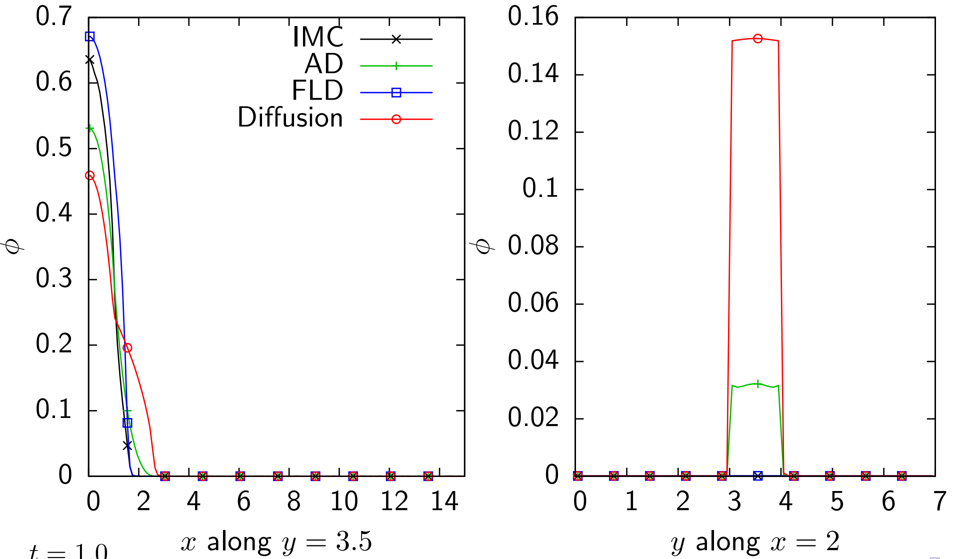
$t = 15$

Time evolution of material temperature



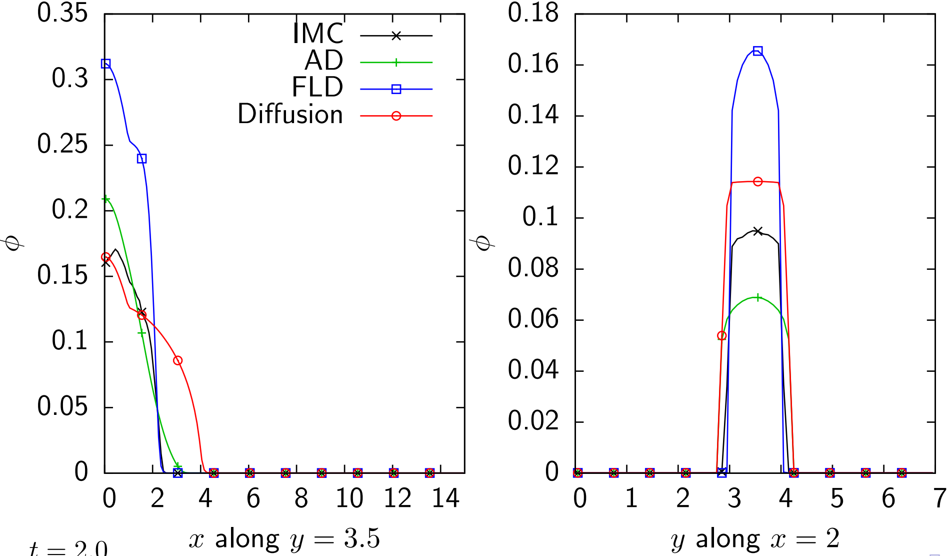
$t = 20$

Time evolution of radiation energy density



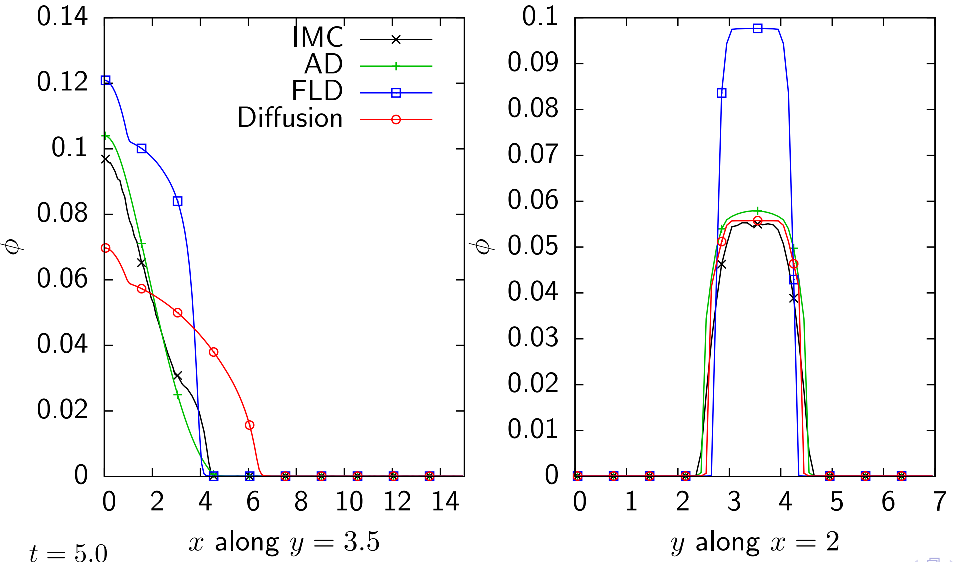
$t = 1.0$

Time evolution of radiation energy density



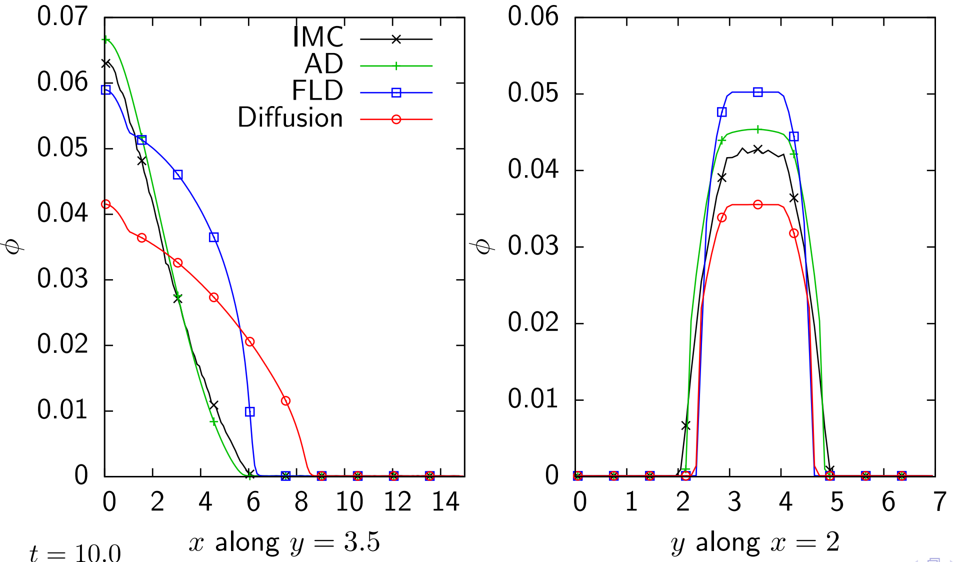
$t = 2.0$

Time evolution of radiation energy density



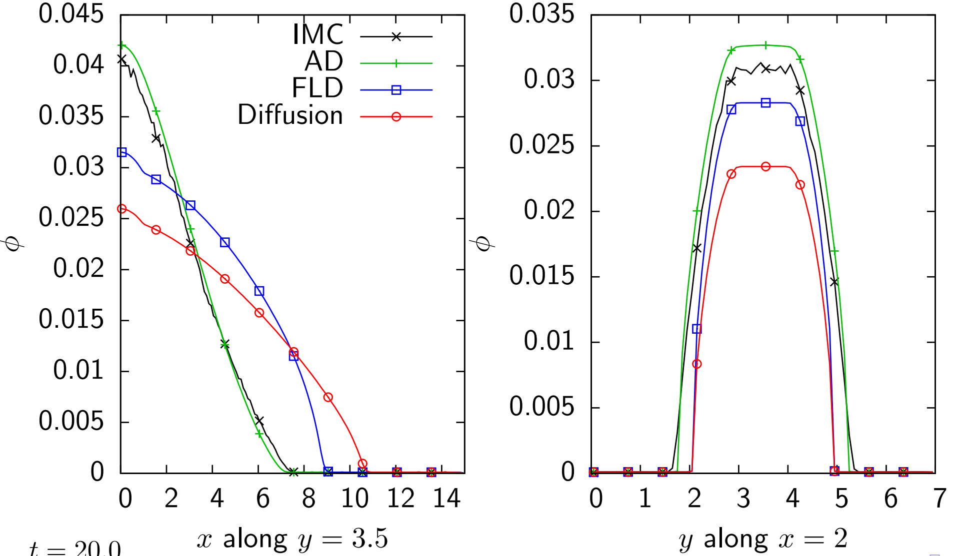
$t = 5.0$

Time evolution of radiation energy density



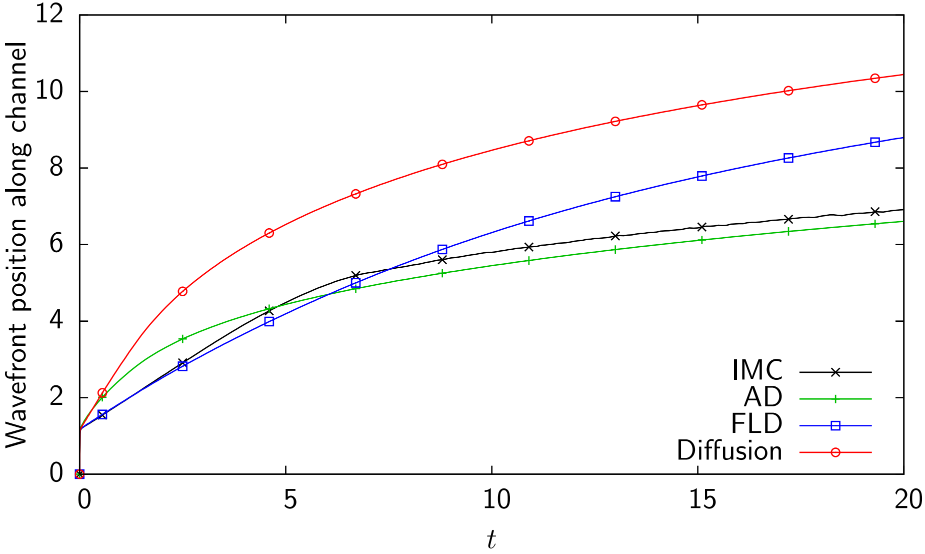
$t = 10.0$

Time evolution of radiation energy density

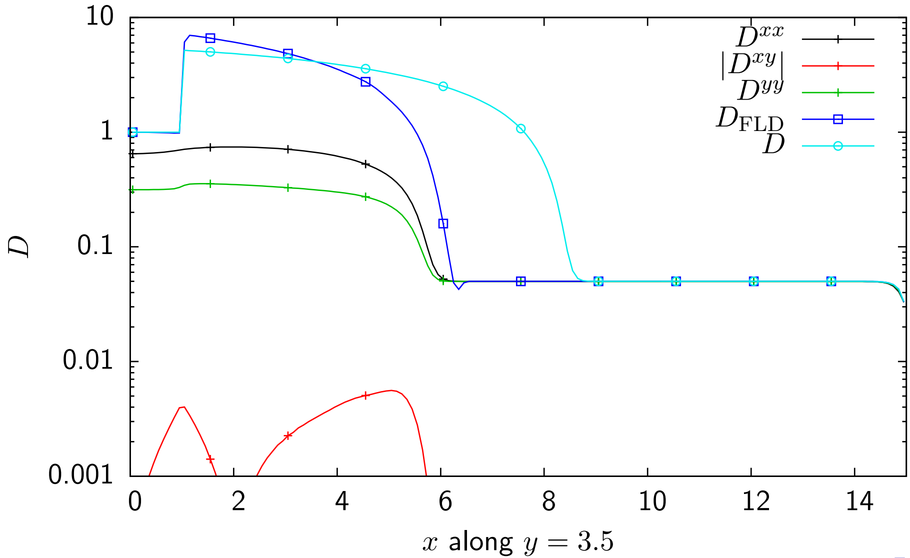


$t = 20.0$

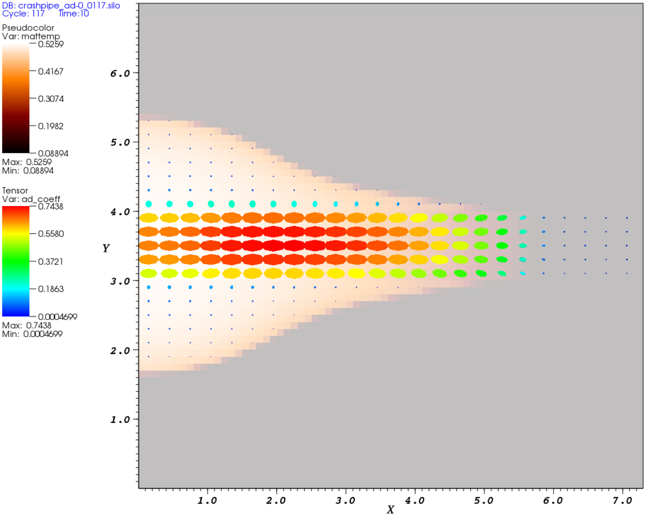
Time evolution of radiation temperature wavefront



Diffusion coefficients ($t = 10$)



Anisotropic diffusion tensor visualization ($t = 10$)



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

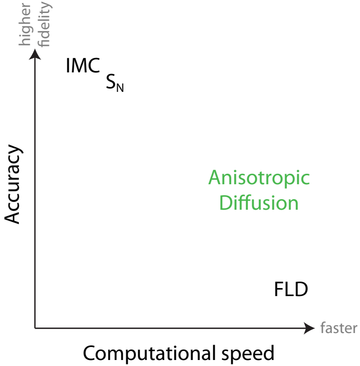
Anisotropic diffusion:

- Accounts for some amount of arbitrary anisotropy in angular 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

- Finalize derivation and analysis of transport-matched boundary conditions (not presented here).
- Implement and test "Anisotropic P_1" ($\frac{1}{c}\frac{\partial}{\partial t} = O(\epsilon)$ instead of $O(\epsilon^2)$).
- Extend the 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?



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