A Physics-Based Anisotropic Diffusion Method for Thermal Radiative Transfer

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Outline

Thermal radiative transfer

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

Applications in high energy density physics:

- Stellar astrophysics, strategic astrophysics
- Inertial confinement fusion
- CRASH (Center for RAdiative Shock Hydrodynamics) program: "Assessment of Predictive Capability"

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

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).

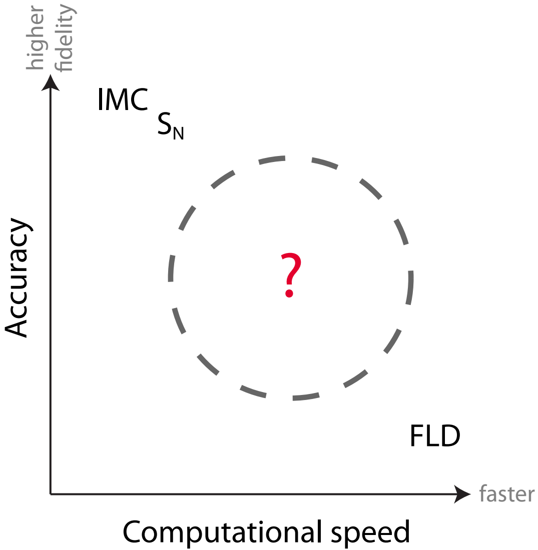
Radiation transfer equation, intensity $I(\boldsymbol{x}, \boldsymbol{\Omega}, t)$:

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

Material energy balance equation:

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

Motivation


higher fidelity
IMC
S_N
Accuracy
?
FLD
faster
Computational speed

Anisotropic diffusion work

Previous work:

- Steady-state VHTR-like problem with analytically calculated coefficients [2]
- Non-local tensor diffusion [3] for steady-state radiative transfer, no further development or analysis in literature

Current work:

- Time-dependent anisotropic diffusion for thermal radiative transfer!

Outline

Summary in advance

1. Make assumptions about weakness of derivatives and moments of intensity $I(\boldsymbol{x}, \boldsymbol{\Omega}, t)$.
2. Convert integrodifferential transport equation to integral transport equation along characteristic rays.
3. Substitute the left hand side of the particle conservation equation (zeroth moment of Boltzmann equation) into the integral equation
4. Apply Taylor series to non-local ϕ to get an approximate expression for $I(\boldsymbol{x}, \boldsymbol{\Omega}, t)$ as a function of $\phi(\boldsymbol{x}, t)$ and other problem-dependent quantities. Discard $O(\epsilon^2)$ and higher terms.
5. Take first moment of this approximate I to get $\boldsymbol{F}(\boldsymbol{x}, t)$.
6. Apply semi-implicit approximation to TRT equations.

Gray Boltzmann transport equation:

$$\frac{1}{c}\frac{\partial I}{\partial t}(\boldsymbol{x},\boldsymbol{\Omega},t) + \boldsymbol{\Omega}\cdot\boldsymbol{\nabla} I(\boldsymbol{x},\boldsymbol{\Omega},t) + \sigma(\boldsymbol{x},T)I(\boldsymbol{x},\boldsymbol{\Omega},t) = \frac{\sigma(\boldsymbol{x},T)ac[T(\boldsymbol{x},t)]^4}{4\pi} + \frac{cQ(\boldsymbol{x},t)}{4\pi} \qquad (2)$$

Radiation energy conservation by integrating over angles $\int_{4\pi}(\cdot)\,\mathrm{d}\Omega$:

$$\frac{1}{c}\frac{\partial \phi}{\partial t}(\boldsymbol{x},t) + \boldsymbol{\nabla}\cdot\boldsymbol{F}(\boldsymbol{x},t) + \sigma(\boldsymbol{x},T)\phi(\boldsymbol{x},t) = \sigma(\boldsymbol{x},T)ac[T(\boldsymbol{x},t)]^4 + cQ(\boldsymbol{x},t) \qquad (3)$$

Asymptotic importance ansatz

$$I = O(1), \qquad \sigma = O(1),$$

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

Integral time-dependent transport equation [5], neglecting boundary and initial conditions:

$$I(\boldsymbol{x}, \boldsymbol{\Omega}, t) = \int_0^\infty \mathrm{e}^{-\tau(\boldsymbol{x}, \boldsymbol{x}-s\boldsymbol{\Omega}, \boldsymbol{\Omega}, t)} \left[\frac{\sigma a c T^4}{4\pi} + \frac{cQ}{4\pi} \right]_{(\boldsymbol{x}-s\boldsymbol{\Omega}, t-s/c)} \mathrm{d}s \tag{4}$$

where the optical thickness from $(\boldsymbol{x}, t)$ to the boundary along $\boldsymbol{\Omega}$ is

$$\tau(\boldsymbol{x}, \boldsymbol{x}', \boldsymbol{\Omega}, t) = \int_0^{\|\boldsymbol{x}-\boldsymbol{x}'\|} \sigma(\boldsymbol{x} - s'\boldsymbol{\Omega}, t - s'/c)\, \mathrm{d}s' \,. \tag{5}$$

Substituting left hand side of conservation equation (3):

$$\begin{aligned} I(\boldsymbol{x}, \boldsymbol{\Omega}, t) &= \frac{1}{4\pi} \int_0^\infty \mathrm{e}^{-\tau(\boldsymbol{x}, \boldsymbol{x}-s\boldsymbol{\Omega}, \boldsymbol{\Omega}, t)} \left[\sigma a c T^4 + cQ \right]_{(\boldsymbol{x}-s\boldsymbol{\Omega}, t-s/c)} \mathrm{d}s \\ &= \frac{1}{4\pi} \int_0^\infty \mathrm{e}^{-\tau(\boldsymbol{x}, \boldsymbol{x}-s\boldsymbol{\Omega}, \boldsymbol{\Omega}, t)} \Bigg[\underbrace{\sigma\phi}_{O(1)} + \underbrace{\frac{1}{c}\frac{\partial \phi}{\partial t}}_{O(\epsilon)} + \underbrace{\boldsymbol{\nabla} \cdot \boldsymbol{F}}_{O(\epsilon^2)} \Bigg]_{(\boldsymbol{x}-s\boldsymbol{\Omega}, t-s/c)} \mathrm{d}s \end{aligned} \tag{6}$$

Consider the integral's three components separately.

First term in Eq. (6):

$$\frac{1}{4\pi}\int_0^\infty \mathrm{e}^{-\int_0^s \sigma(\boldsymbol{x}-s'\boldsymbol{\Omega},t-s'/c)\,\mathrm{d}s'}\sigma(\boldsymbol{x}-s\boldsymbol{\Omega},t-s/c)\phi(\boldsymbol{x}-s\boldsymbol{\Omega},t-s/c)\,\mathrm{d}s$$

Fundamental theorem of calculus:

$$=\frac{1}{4\pi}\int_0^\infty\left(-\frac{\mathrm{d}}{\mathrm{d}s}\,\mathrm{e}^{-\int_0^s \sigma(\boldsymbol{x}-s'\boldsymbol{\Omega},t-s'/c)\,\mathrm{d}s'}\right)\phi(\boldsymbol{x}-s\boldsymbol{\Omega},t-s/c)\,\mathrm{d}s$$

Integration by parts with $u=\phi(\boldsymbol{x}-s\boldsymbol{\Omega},t-s/c)$ and $\mathrm{d}v=\frac{\mathrm{d}}{\mathrm{d}s}\,\mathrm{e}^{-\tau}\,\mathrm{d}s$:

$$\begin{aligned}
&=-\frac{1}{4\pi}\left[\mathrm{e}^{-\int_0^s \sigma(\boldsymbol{x}-s'\boldsymbol{\Omega},t-s'/c)\,\mathrm{d}s'}\phi(\boldsymbol{x}-s\boldsymbol{\Omega},t-s/c)\Big|_0^\infty\right.\\
&\qquad\left.-\int_0^\infty \mathrm{e}^{-\int_0^s \sigma(\boldsymbol{x}-s'\boldsymbol{\Omega},t-s'/c)\,\mathrm{d}s'}\frac{\mathrm{d}}{\mathrm{d}s}\phi(\boldsymbol{x}-s\boldsymbol{\Omega},t-s/c)\,\mathrm{d}s\right]\\
&=-\frac{1}{4\pi}\left[0-\mathrm{e}^0\phi(\boldsymbol{x},t)-\int_0^\infty \mathrm{e}^{-\tau(\boldsymbol{x},\boldsymbol{x}-s\boldsymbol{\Omega},\boldsymbol{\Omega},t)}\frac{\mathrm{d}}{\mathrm{d}s}\phi(\boldsymbol{x}-s\boldsymbol{\Omega},t-s/c)\,\mathrm{d}s\right]\\
&=\frac{1}{4\pi}\phi(\boldsymbol{x},t)+\frac{1}{4\pi}\int_0^\infty \mathrm{e}^{-\tau}\left[-\boldsymbol{\Omega}\cdot\boldsymbol{\nabla}-\frac{1}{c}\frac{\partial}{\partial t}\right]\phi(\boldsymbol{x}-s\boldsymbol{\Omega},t-s/c)\,\mathrm{d}s
\end{aligned}$$

Approximate using Taylor series

Taylor series expansion of nonlocal unknown ϕ in space and time:

$$\begin{aligned}\phi(\boldsymbol{x} - s\boldsymbol{\Omega}, t - s/c) &\sim \phi(\boldsymbol{x}, t) - s\boldsymbol{\Omega} \cdot \boldsymbol{\nabla}\phi(\boldsymbol{x}, t) - s\frac{1}{c}\frac{\partial \phi}{\partial t}(\boldsymbol{x}, t) + \cdots \\ &= \phi(\boldsymbol{x}, t) - s\left[\boldsymbol{\Omega} \cdot \boldsymbol{\nabla} + \frac{1}{c}\frac{\partial}{\partial t}\right]\phi(\boldsymbol{x}, t) + \cdots \\ &= O(1) + O(\epsilon) + \cdots\end{aligned}$$

Taylor series in time for σ embedded in optical thickness τ:

$$\begin{aligned}\sigma(\boldsymbol{x} - s\boldsymbol{\Omega}, t - s/c) &\sim \sigma(\boldsymbol{x} - s\boldsymbol{\Omega}, t) - s\frac{1}{c}\frac{\partial \sigma}{\partial t}(\boldsymbol{x} - s\boldsymbol{\Omega}, t) + \cdots \\ &= O(1) + O(\epsilon^{(?)}) + \cdots\end{aligned}$$

Keep only the leading order terms.

The expansion in ϕ allows it to be moved outside the integral, and the expansion in σ obviates the storage of all prior σ:

$$\int_0^\infty \mathrm{e}^{-\int_0^s \sigma(\boldsymbol{x}-s'\boldsymbol{\Omega},t-s'/c)\,\mathrm{d}s'} \left[-\boldsymbol{\Omega}\cdot\boldsymbol{\nabla} - \frac{1}{c}\frac{\partial}{\partial t}\right] \phi(\boldsymbol{x}-s\boldsymbol{\Omega}, t-s/c)\,\mathrm{d}s$$

$$\sim \int_0^\infty \mathrm{e}^{-\int_0^s \sigma(\boldsymbol{x}-s'\boldsymbol{\Omega},t)\,\mathrm{d}s'}\,\mathrm{d}s \left[-\boldsymbol{\Omega}\cdot\boldsymbol{\nabla} - \frac{1}{c}\frac{\partial}{\partial t}\right] \phi(\boldsymbol{x},t)$$

Therefore the $\sigma\phi$ component of I is approximated as

$$\frac{1}{4\pi}\int_0^\infty \mathrm{e}^{-\tau(\boldsymbol{x},\boldsymbol{x}-s\boldsymbol{\Omega},\boldsymbol{\Omega},t)}\sigma(\boldsymbol{x}-s\boldsymbol{\Omega},t-s/c)\phi(\boldsymbol{x}-s\boldsymbol{\Omega},t-s/c)\,\mathrm{d}s$$

$$\sim \frac{1}{4\pi}\underbrace{\phi(\boldsymbol{x},t)}_{O(1)} + \frac{1}{4\pi}\int_0^\infty \mathrm{e}^{-\int_0^s \sigma(\boldsymbol{x}-s'\boldsymbol{\Omega},t)\,\mathrm{d}s'}\,\mathrm{d}s\,\underbrace{\left[-\boldsymbol{\Omega}\cdot\boldsymbol{\nabla} - \frac{1}{c}\frac{\partial}{\partial t}\right]}_{O(\epsilon)}\phi(\boldsymbol{x},t)\,.$$

Next term in Eq. (6): apply the same Taylor series to σ and ϕ, discarding $O(\epsilon^2)$ and higher terms:

$$\frac{1}{4\pi}\int_0^\infty \mathrm{e}^{-\tau(\boldsymbol{x},\boldsymbol{x}-s\boldsymbol{\Omega},\boldsymbol{\Omega},t)}\frac{1}{c}\frac{\partial}{\partial t}\phi(\boldsymbol{x}-s\boldsymbol{\Omega},t-s/c)\,\mathrm{d}s \sim \frac{1}{4\pi}\int_0^\infty \mathrm{e}^{-\int_0^s \sigma(\boldsymbol{x}-s'\boldsymbol{\Omega},t)\,\mathrm{d}s'}\,\mathrm{d}s\,\underbrace{\frac{1}{c}\frac{\partial}{\partial t}}_{O(\epsilon)}\phi(\boldsymbol{x},t)\,.$$

This cancels the time derivative term from the $\sigma\phi$ component!
Third term in Eq. (6),

$$\frac{1}{4\pi}\int_0^\infty \mathrm{e}^{-\tau(\boldsymbol{x},\boldsymbol{x}-s\boldsymbol{\Omega},\boldsymbol{\Omega},t)}\boldsymbol{\nabla}\cdot\boldsymbol{F}(\boldsymbol{x}-s\boldsymbol{\Omega},t-s/c)\,\mathrm{d}s\,,$$

is $O(\epsilon^2)$, so neglect it.
Result:

$$I(\boldsymbol{x},\boldsymbol{\Omega},t) \approx \frac{1}{4\pi}\phi(\boldsymbol{x},t) - \left[\int_0^\infty \frac{1}{4\pi}\,\mathrm{e}^{-\int_0^s \sigma(\boldsymbol{x}-s'\boldsymbol{\Omega},t)\,\mathrm{d}s'}\,\mathrm{d}s\right]\boldsymbol{\Omega}\cdot\boldsymbol{\nabla}\phi(\boldsymbol{x},t) \quad (7)$$

Analogy to Fick's law

Take the first angular moment of Eq. (7) to find the radiation flux ("current" in the neutron world):

$$\begin{aligned}
\boldsymbol{F}(\boldsymbol{x},t) &= \int_{4\pi} \boldsymbol{\Omega} I(\boldsymbol{x},\boldsymbol{\Omega},t)\,\mathrm{d}\Omega \\
&= \frac{1}{4\pi}\phi(\boldsymbol{x},t)\int_{4\pi} \boldsymbol{\Omega}\,\mathrm{d}\Omega \\
&\qquad - \int_{4\pi} \boldsymbol{\Omega}\left[\int_0^\infty \frac{1}{4\pi}\,\mathrm{e}^{-\int_0^s \sigma(\boldsymbol{x}-s'\boldsymbol{\Omega},t)\,\mathrm{d}s'}\,\mathrm{d}s\right]\boldsymbol{\Omega}\,\mathrm{d}\Omega \cdot \boldsymbol{\nabla}\phi(\boldsymbol{x},t) \\
&= -\left[\int_{4\pi} \boldsymbol{\Omega} f(\boldsymbol{x},\boldsymbol{\Omega},t)\boldsymbol{\Omega}\,\mathrm{d}\Omega\right]\cdot \boldsymbol{\nabla}\phi(\boldsymbol{x},t) \\
&= -\mathbf{D}(\boldsymbol{x},t)\cdot\boldsymbol{\nabla}\phi(\boldsymbol{x},t)
\end{aligned}$$

where f satisfies the "steady-state" transport equation

$$\boldsymbol{\Omega}\cdot\boldsymbol{\nabla} f(\boldsymbol{x},\boldsymbol{\Omega},t) + \sigma(\boldsymbol{x},t) f(\boldsymbol{x},\boldsymbol{\Omega},t) = \frac{1}{4\pi}\,. \tag{8}$$

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 smaller magnitude across a channel than along it
- Does not "blow up" in void regions
- Is continuous in $\boldsymbol{x}$, so the anisotropic solution ϕ has continuous first derivatives

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

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

- Takes only one transport sweep to solve, since it is the description of a purely absorbing medium
- Only needs to be calculated once if σ is constant in time
- 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, $\int_{4\pi} \mathbf{\Omega} f \mathbf{\Omega} \, \mathrm{d}\Omega = \mathbf{I}/3\sigma$.

Zeroth moment of radiative transfer equation:

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

Radiation flux equation from anisotropic diffusion calculation:

$$\boldsymbol{F}(\boldsymbol{x}, t) \cong -\mathbf{D}(\boldsymbol{x}, \sigma) \cdot \boldsymbol{\nabla}\phi(\boldsymbol{x}, t)$$

Material energy balance equation:

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

Semi-implicit discretization freezes c_v/T^3 and σ at the initial time value t^n explicitly and treats ϕ implicitly. Some manipulation gives a linear transport equation (with "effective scattering" that emulates photon absorption and reëmission) over the time step, and an equation to update the new material temperature.

Outline

Compared methods

- Implicit Monte Carlo [1] (implemented with variance reduction methods), 10^6 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:

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

Summary of AD approximations

Thermal radiative transfer equations

- Assume weak gradients and angular moments for I (*don't* assume that I is a linear function of $\mathbf{\Omega}$!)
- Neglect boundary and initial conditions
- Semi-implicit approximation for the nonlinearities

AD equation

- Cell-centered finite difference spatial approximation
- Discard D^{xy} and D^{yx} terms*

$\mathbb{D}$ transport equation

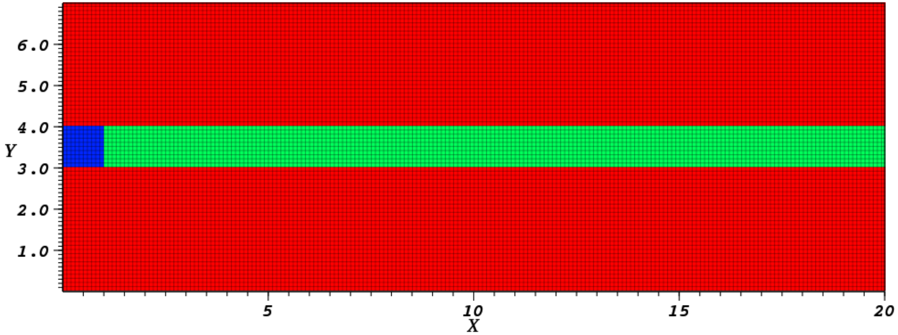
- Discrete ordinates angular approximation
- Diamond difference* spatial approximation (16* azimuthal ordinates per quadrant)

*Numerical experiments support using these approximations

Problem description

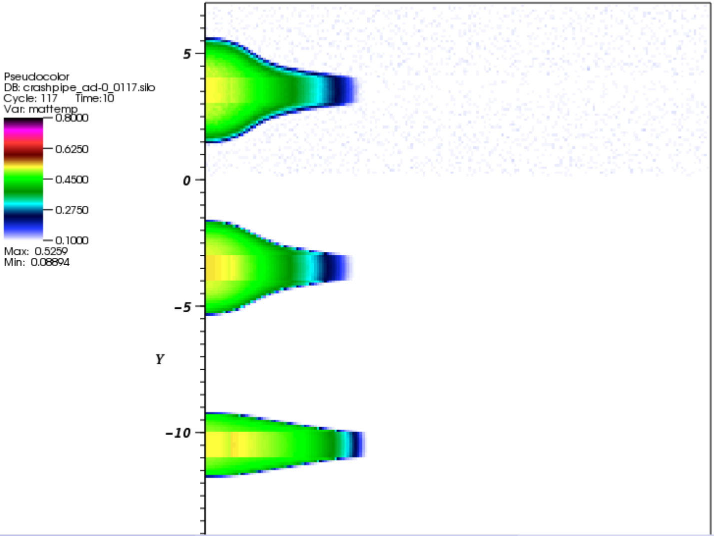
Flatland geometry!
Uniform spatial grid: $\Delta_x = 0.1$
Piecewise linear time grid:
$\Delta_t = 0.1$ for $t \geq 1$
Reflecting bndy on left, others vacuum

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

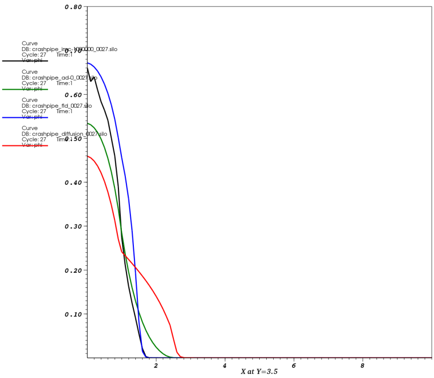


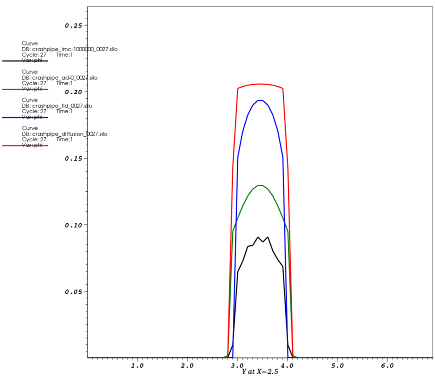
Time evolution of material temperature

(Replaced with movie)



Time evolution of radiation energy density

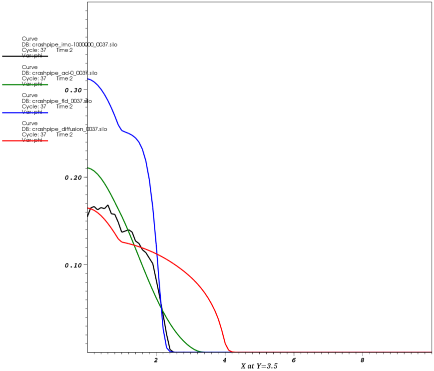


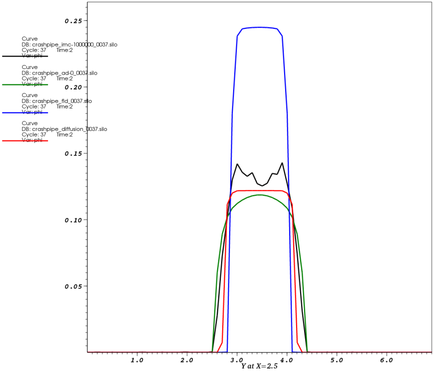


along $y = 3.5$ $\quad t = 1.0 \quad$ along $x = 2.5$

IMC **AD** **FLD** **Diffusion**

Time evolution of radiation energy density

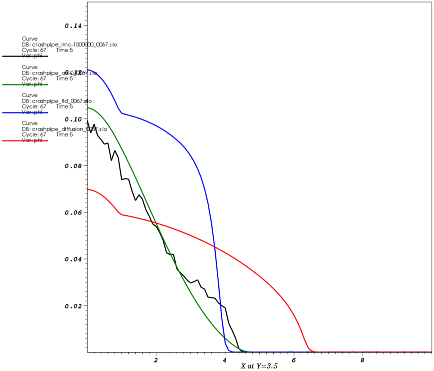


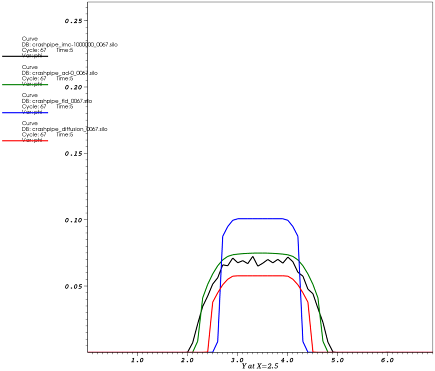


along $y = 3.5$ $\quad t = 2.0 \quad$ along $x = 2.5$

IMC **AD** **FLD** **Diffusion**

Time evolution of radiation energy density

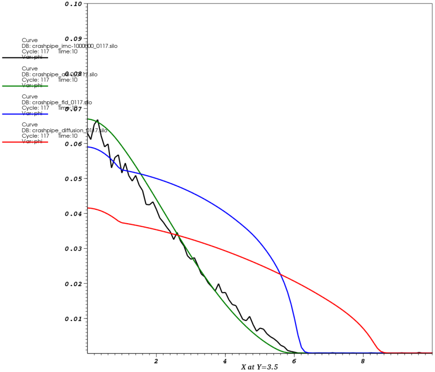


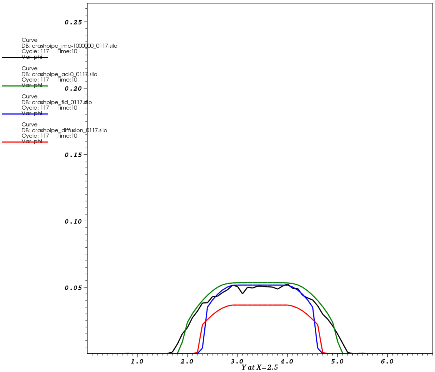


along $y = 3.5$ $t = 5.0$ along $x = 2.5$

IMC AD FLD Diffusion

Time evolution of radiation energy density

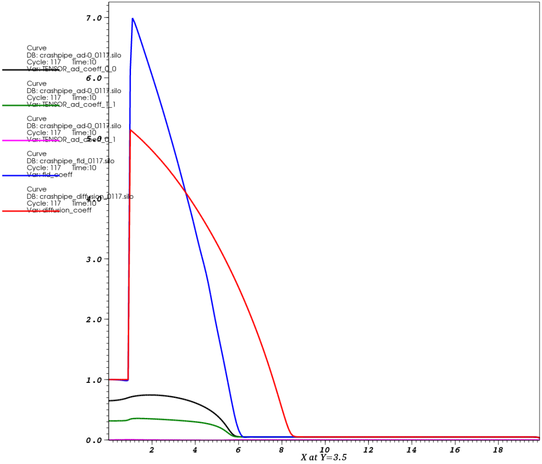




along $y = 3.5$ $\qquad t = 10.0 \qquad$ along $x = 2.5$

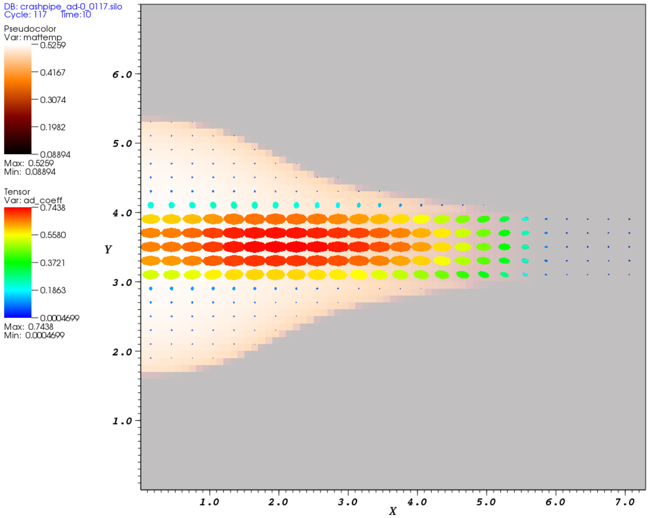
IMC **AD** **FLD** **Diffusion**

Diffusion coefficients



D^{xx} D^{xy} D^{yy} D_{FLD} D

Anisotropic diffusion tensor visualization



Timing results

Method	Time (s)
IMC	477
FLD	8
D	8
AD_{64}	13
AD_{128}	22

Table 1: Run times for pipe test problem, 14000 cells. Average of three runs.

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

- Improved time-dependent behavior, with wavefront propagation speed of c
- Boundary conditions for both anisotropic diffusion problem and purely absorbing transport problem (solution of f)
- Improve performance by reducing time spent in transport sweeps
  - Evaluate $\mathbf{D}$ on coarser spatial grid, since it is smooth
  - Update $\mathbf{D}$ less frequently
  - Advanced quadrature set for *a priori* problem geometry
- Quantify the penalty of omitting the D^{xy} terms for various problems, or find an effective discretization scheme to include them

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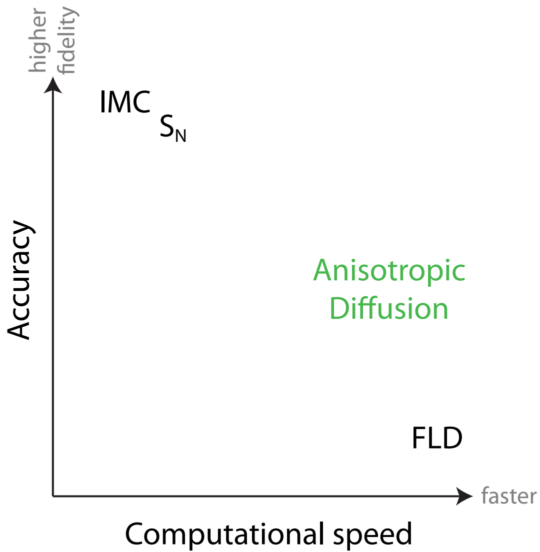
Questions?


higher fidelity
IMC
S_N
Accuracy
Anisotropic Diffusion
FLD
faster
Computational speed

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