

# A Physics-Based Anisotropic Diffusion Method for Thermal Radiative Transfer

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# Outline

1 Introduction

2 Theory

3 Results

4 Conclusions

# 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 ( $\mathbf{x}, \mathbf{\Omega}, h\nu, t$ )
- Highly nonlinear coupled partial differential equations for radiation field  $I(\mathbf{x}, \mathbf{\Omega}, h\nu, t)$  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).

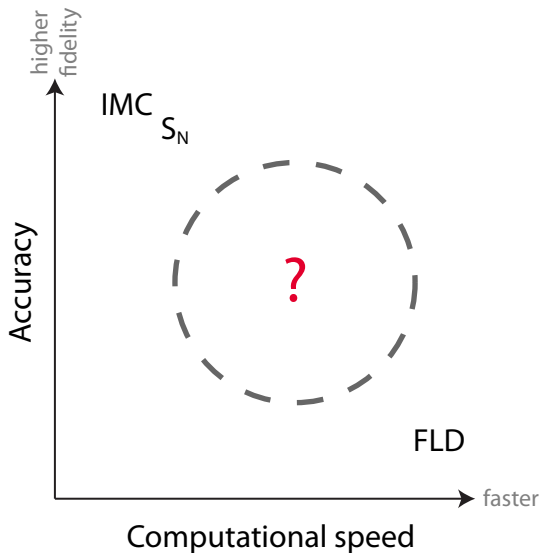
Radiation transfer equation, intensity  $I(\mathbf{x}, \boldsymbol{\Omega}, t)$ :

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

Material energy balance equation:

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

# Motivation



# 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!

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# Summary in advance

- 1 Make assumptions about weakness of derivatives and moments of intensity  $I(\mathbf{x}, \boldsymbol{\Omega}, t)$ .
- 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  $\phi$  to get an approximate expression for  $I(\mathbf{x}, \boldsymbol{\Omega}, t)$  as a function of  $\phi(\mathbf{x}, t)$  and other problem-dependent quantities. Discard  $O(\epsilon^2)$  and higher terms.
- 5 Take first moment of this approximate  $I$  to get  $\mathbf{F}(\mathbf{x}, t)$ .
- 6 Apply semi-implicit approximation to TRT equations.



Gray Boltzmann transport equation:

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

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

$$\frac{1}{c} \frac{\partial \phi}{\partial t}(\mathbf{x}, t) + \nabla \cdot \mathbf{F}(\mathbf{x}, t) + \sigma(\mathbf{x}, t) \phi(\mathbf{x}, t) = \sigma(\mathbf{x}, t) a c [T(\mathbf{x}, t)]^4 + c Q(\mathbf{x}, t) \quad (3)$$

Asymptotic importance ansatz

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

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

$$I(\mathbf{x}, \mathbf{\Omega}, t) = \int_0^\infty e^{-\tau(\mathbf{x}, \mathbf{x}-s\mathbf{\Omega}, \mathbf{\Omega}, t)} \left[ \frac{\sigma ac T^4}{4\pi} + \frac{cQ}{4\pi} \right]_{(\mathbf{x}-s\mathbf{\Omega}, t-s/c)} ds \quad (4)$$

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

$$\tau(\mathbf{x}, \mathbf{x}', \mathbf{\Omega}, t) = \int_0^{\|\mathbf{x}-\mathbf{x}'\|} \sigma(\mathbf{x} - s'\mathbf{\Omega}, t - s'/c) ds'. \quad (5)$$

Substituting left hand side of conservation equation (3):

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

Consider the integral's three components separately.

First term in Eq. (6):

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

Fundamental theorem of calculus:

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

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

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

# Approximate using Taylor series

Taylor series expansion of nonlocal unknown  $\phi$  in space and time:

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

Taylor series in time for  $\sigma$  embedded in optical thickness  $\tau$ :

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

Keep only the leading order terms.

The expansion in  $\phi$  allows it to be moved outside the integral, and the expansion in  $\sigma$  obviates the storage of all prior  $\sigma$ :

$$\begin{aligned} \int_0^\infty e^{-\int_0^s \sigma(\mathbf{x}-s'\mathbf{\Omega}, t-s'/c) ds'} \left[ -\mathbf{\Omega} \cdot \mathbf{\nabla} - \frac{1}{c} \frac{\partial}{\partial t} \right] \phi(\mathbf{x} - s\mathbf{\Omega}, t - s/c) ds \\ \sim \int_0^\infty e^{-\int_0^s \sigma(\mathbf{x}-s'\mathbf{\Omega}, t) ds'} ds \left[ -\mathbf{\Omega} \cdot \mathbf{\nabla} - \frac{1}{c} \frac{\partial}{\partial t} \right] \phi(\mathbf{x}, t) \end{aligned}$$

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

$$\begin{aligned} \frac{1}{4\pi} \int_0^\infty e^{-\tau(\mathbf{x}, \mathbf{x}-s\mathbf{\Omega}, \mathbf{\Omega}, t)} \sigma(\mathbf{x} - s\mathbf{\Omega}, t - s/c) \phi(\mathbf{x} - s\mathbf{\Omega}, t - s/c) ds \\ \sim \frac{1}{4\pi} \underbrace{\phi(\mathbf{x}, t)}_{O(1)} + \frac{1}{4\pi} \int_0^\infty e^{-\int_0^s \sigma(\mathbf{x}-s'\mathbf{\Omega}, t) ds'} ds \underbrace{\left[ -\mathbf{\Omega} \cdot \mathbf{\nabla} - \frac{1}{c} \frac{\partial}{\partial t} \right] \phi(\mathbf{x}, t)}_{O(\epsilon)}. \end{aligned}$$

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

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

This cancels the time derivative term from the  $\sigma\phi$  component!

Third term in Eq. (6),

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

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

Result:

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

# Analogy to Fick's law

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

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

where  $f$  satisfies the “steady-state” transport equation

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

# Properties of anisotropic diffusion

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

- 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  $\mathbf{x}$ , so the anisotropic solution  $\phi$  has continuous first derivatives



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

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

- Takes only one transport sweep to solve, since it is the description of a purely absorbing medium
- Only needs to be calculated once if  $\sigma$  is constant in time
- Requires no storage of the angular flux, just accumulation of second moment,  $D_{ij} = \int_{4\pi} \Omega_i \Omega_j f \, d\Omega$
- Has the solution  $f = 1/4\pi\sigma$  if  $\sigma$  is a constant. Then,  $\int_{4\pi} \boldsymbol{\Omega} f \boldsymbol{\Omega} \, d\Omega = \mathbf{I}/3\sigma$ .

Zeroth moment of radiative transfer equation:

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

Radiation flux equation from anisotropic diffusion calculation:

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

Material energy balance equation:

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

Semi-implicit discretization freezes  $c_v/T^3$  and  $\sigma$  at the initial time value  $t^n$  explicitly and treats  $\phi$  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.

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# 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:

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

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

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

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

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

# 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  $\Omega$ !)
- 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\*

## 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  $t \geq 1$

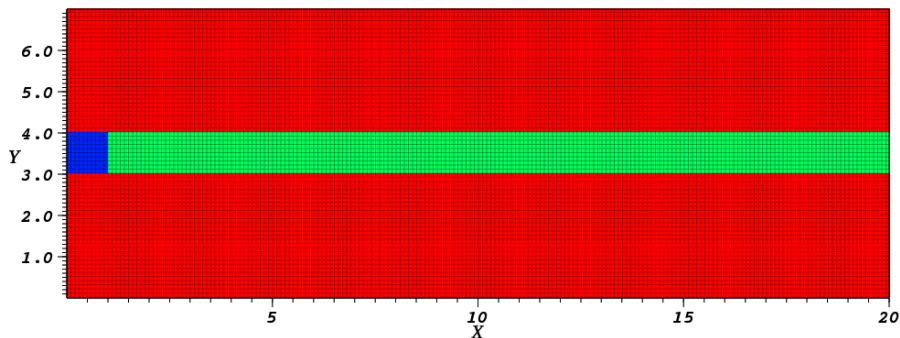
Reflecting bndy on left, others  
vacuum

**Source:**  $c_v = 0.5$ ,  $\sigma = 0.5$ ;  $Q = 1$   
for  $0 \leq t \leq 1$ ,  $Q = 0$  for  $t > 1$ .

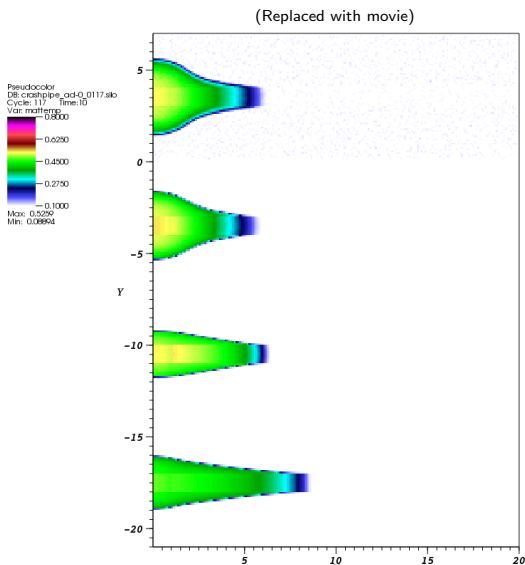
**Diffusive:**  $c_v = 0.1$ ,  $\sigma = T^{-3}$

**Channel:**  $c_v = 0.1$ ,  $\sigma = 0.01T^{-3}$

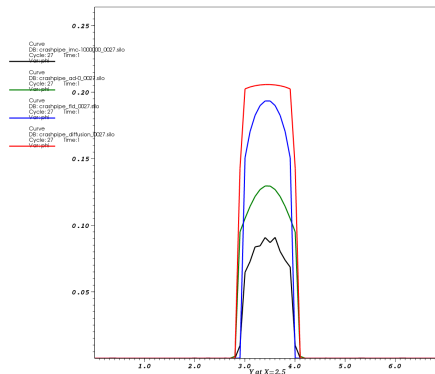
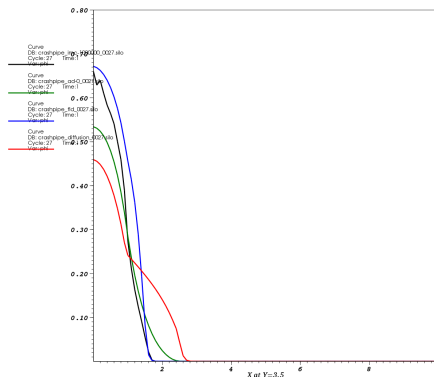
Initial condition:  $T = T_{\text{rad}} = 0.1$



# Time evolution of material temperature



# Time evolution of radiation energy density



along  $y = 3.5$

$t = 1.0$

along  $x = 2.5$

**IMC**

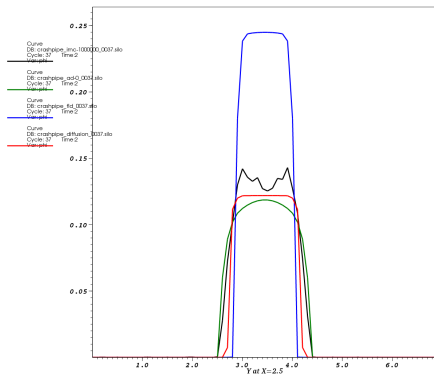
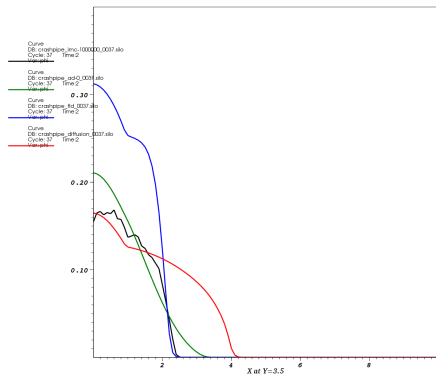
**AD**

**FLD**

**Diffusion**



# Time evolution of radiation energy density



along  $y = 3.5$

$t = 2.0$

along  $x = 2.5$

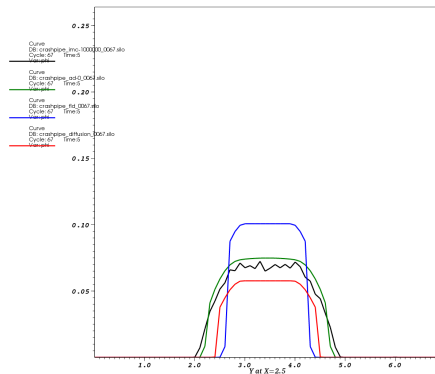
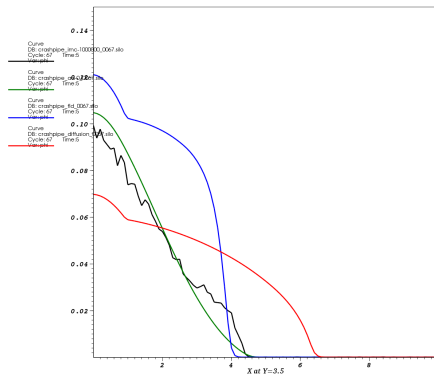
**IMC**

**AD**

**FLD**

**Diffusion**

# Time evolution of radiation energy density



along  $y = 3.5$

$t = 5.0$

along  $x = 2.5$

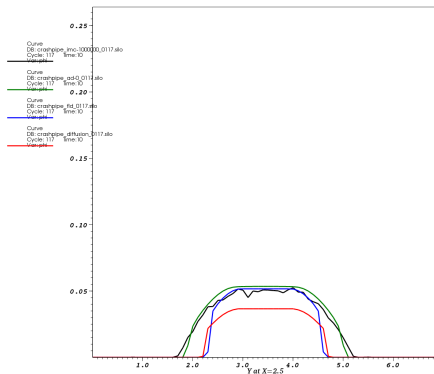
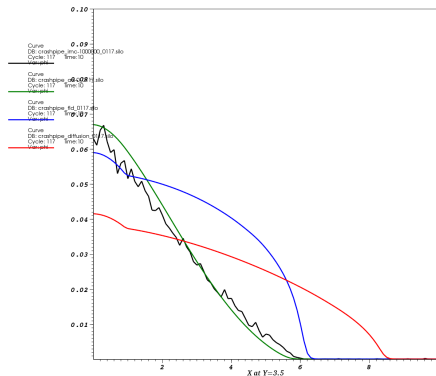
**IMC**

**AD**

**FLD**

**Diffusion**

# Time evolution of radiation energy density



along  $y = 3.5$

$t = 10.0$

along  $x = 2.5$

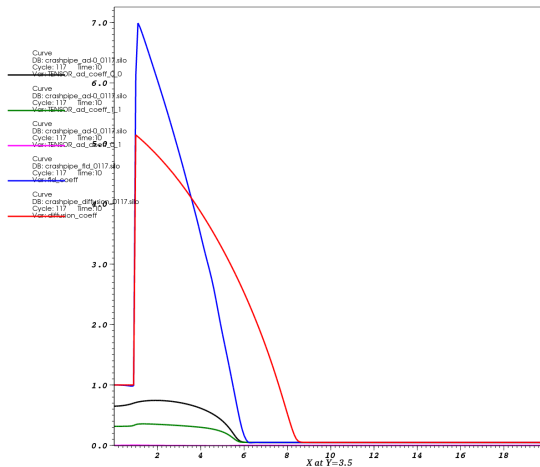
**IMC**

**AD**

**FLD**

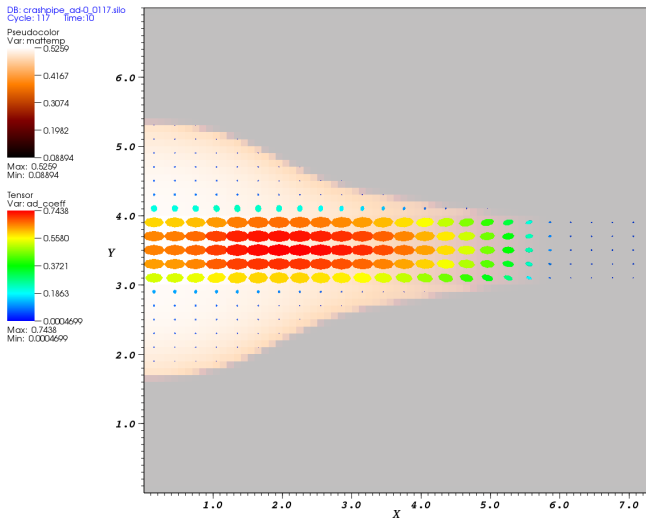
**Diffusion**

# 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 <sub>64</sub>	13
AD <sub>128</sub>	22

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

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# Conclusions

## Anisotropic diffusion:

- Accounts for some amount of arbitrary anisotropy in angular flux, 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



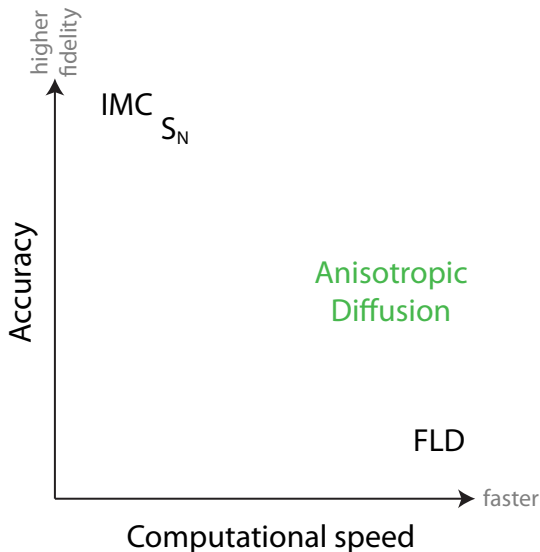
# Future work

- 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?



# References

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