An anisotropic diffusion approximation to nonlinear radiation transport

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Outline

- Introduction
- 2 Theory
- Results
- 4 Conclusions



Thermal radiative transfer

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

Difficulties in solving:

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

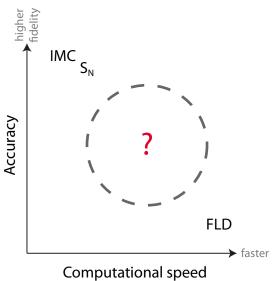
Particular application of this work: CRASH project

- 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

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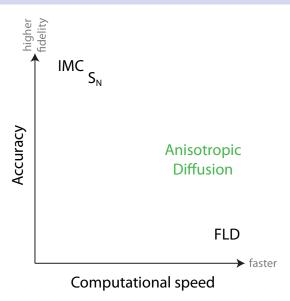
Motivation





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Motivation





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

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

Material energy balance equation:

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

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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

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- **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 .
- Use Taylor series to approximate nonlocal unknowns with local unknowns, discarding small terms. This yields

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

- **3** Take the first angular moment of Ψ to get $oldsymbol{J} = \mathbf{D} \cdot oldsymbol{
 abla} \phi$
- $footnote{\bullet}$ Substitute J into the time-dependent particle conservation equation to get time-dependent anisotropic diffusion.

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Transport equation (interior)

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

with a boundary condition and initial condition.

Operating on Eq. (2) by $\int_{4\pi} (\cdot) d\Omega$ gives the conservation equation:

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

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

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

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Anisotropic angular flux equation

Define "anisotropic angular flux":

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

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

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

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 , J satisfy this equation: no approximations.

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Integral transport equation

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

$$\Psi(\boldsymbol{x}, \boldsymbol{\Omega}, t) = \Psi^{i}(\boldsymbol{x} - ct\boldsymbol{\Omega}, \boldsymbol{\Omega}) e^{-\tau(\boldsymbol{x}, \boldsymbol{x} - ct\boldsymbol{\Omega})}
+ \int_{0}^{\infty} \left[\hat{Q}(\boldsymbol{x} - s\boldsymbol{\Omega}, \boldsymbol{\Omega}, t - s/c) \right] e^{-\tau(\boldsymbol{x}, \boldsymbol{x} - s\boldsymbol{\Omega})} ds .$$

$$\equiv \mathcal{I}_{i} \left[\Psi^{i} \right] + \mathcal{I}_{v} \left[\hat{Q} \right]$$
(6b)

where we have defined the optical thickness is

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

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

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Time for some approximations

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

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

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

$$\begin{split} \Psi &= \mathcal{I}_i \big[\Psi^i \big] + \mathcal{I}_v \bigg[\frac{1}{4\pi} \boldsymbol{\nabla} \cdot \boldsymbol{J} \bigg] - \mathcal{I}_v \bigg[\frac{1}{4\pi} \boldsymbol{\Omega} \cdot \boldsymbol{\nabla} \phi \bigg] \\ \Psi &\approx - \mathcal{I}_v \bigg[\frac{1}{4\pi} \boldsymbol{\Omega} \cdot \boldsymbol{\nabla} \phi \bigg] + O(\epsilon^2) \end{split}$$

Taylor series expansion:

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

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

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Taylor series applied

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

$$-\mathcal{I}_{v}\left[\frac{1}{4\pi}\mathbf{\Omega}\cdot\mathbf{\nabla}\phi\right] = -\int_{0}^{\infty} \left[\frac{1}{4\pi}\mathbf{\Omega}\cdot\mathbf{\nabla}\phi\right]_{(\boldsymbol{x}-s\mathbf{\Omega},t-s/c)} e^{-\tau(\boldsymbol{x},\boldsymbol{x}-s\mathbf{\Omega})} ds$$

$$\sim -\int_{0}^{\infty} \left[\frac{1}{4\pi}\right] e^{-\tau(\boldsymbol{x},\boldsymbol{x}-s\mathbf{\Omega})} ds \mathbf{\Omega}\cdot\mathbf{\nabla}\phi(\boldsymbol{x},t) + O(\epsilon^{2})$$

$$= -\mathcal{I}_{v}\left[\frac{1}{4\pi}\right] \mathbf{\Omega}\cdot\mathbf{\nabla}\phi(\boldsymbol{x},t). \tag{8}$$

Thus,

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

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An analogy to Fick's law

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

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

Substitute into radiation energy conservation equation:

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

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.



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The transport problem used to calculate ${f D}$ is

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

with boundary condition

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

- 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, $D_{ij}=\int_{4\pi}\Omega_i\Omega_jf\,\mathrm{d}\Omega$
- Has the solution $f=1/4\pi\sigma$ if σ is a constant. Then, $\int_{4\pi} {\bf \Omega} {\bf \Omega} f \, {\rm d}\Omega = {\bf I}/3\sigma.$



Properties of anisotropic diffusion

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

- Does not "blow up" in void regions
- Has a greater "action" along the direction of a voided channel than across it
- Reduces to $I/3\sigma$ 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 x, so the approximate AD-calculated ϕ has continuous first derivatives (i.e., ϕ is smooth like our ansatz requires)



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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:

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

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Problem description

Flatland geometry!

Uniform spatial grid: $\Delta_r = 0.1$

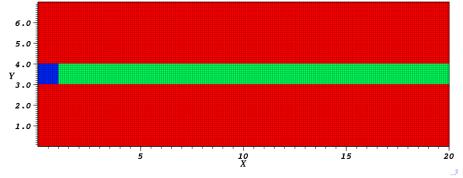
Piecewise linear time grid: $\Delta_t = 0.1$

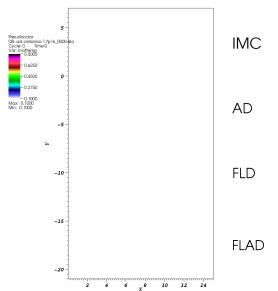
for t > 1

Reflecting bndy on left, others

vacuum

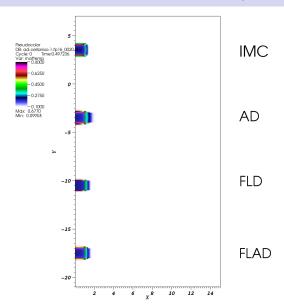
Source: $c_v = 0.5$, $\sigma = 0.5$; Q = 1for $0 \le t \le 1$, Q = 0 for t > 1. **Diffusive**: $c_v = 0.1$, $\sigma = T^{-3}$ **Channel**: $c_v = 0.1$, $\sigma = 0.01T^{-3}$ Initial condition: $T = T_{rad} = 0.1$



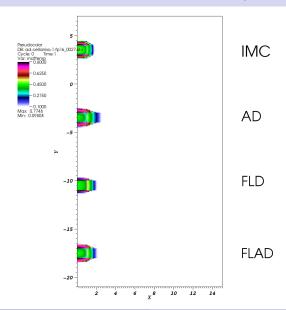


t = 0

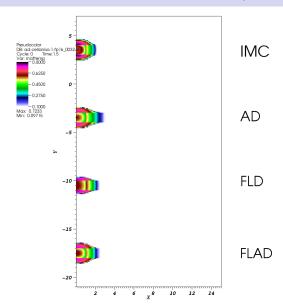
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t = 0.5

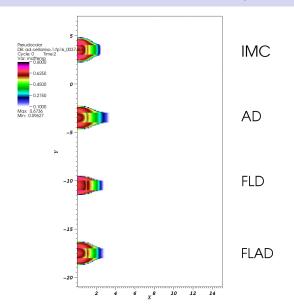


t = 1.0



t = 1.5

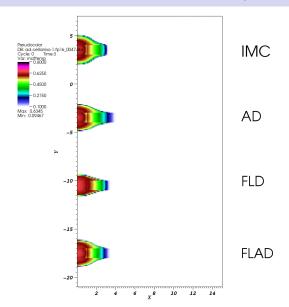
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t=2

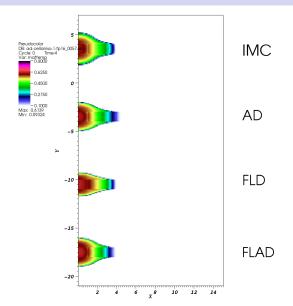
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t = 3

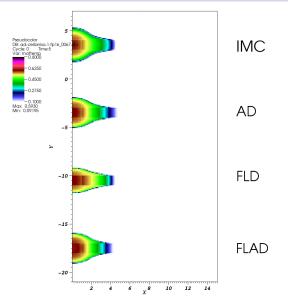
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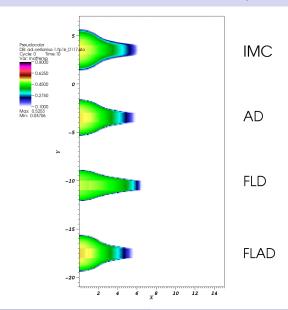
t = 4

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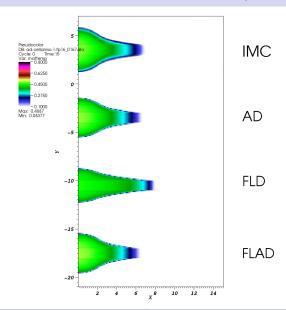
t=5



t = 10

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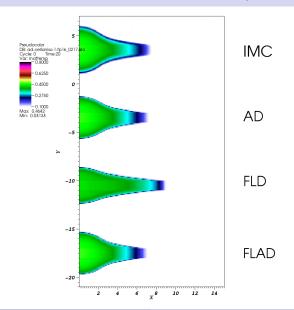
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t = 15

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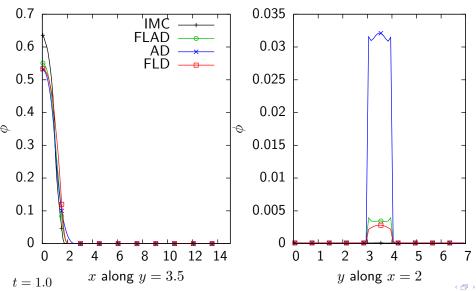
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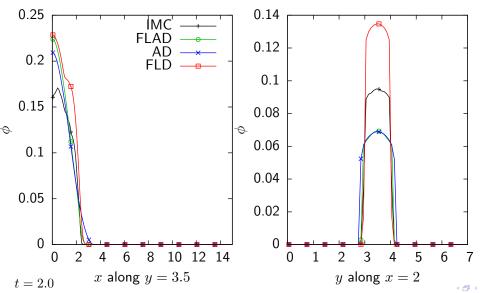
t = 20

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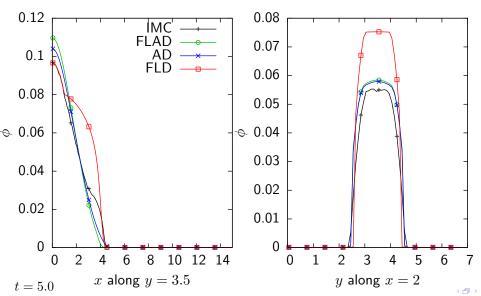
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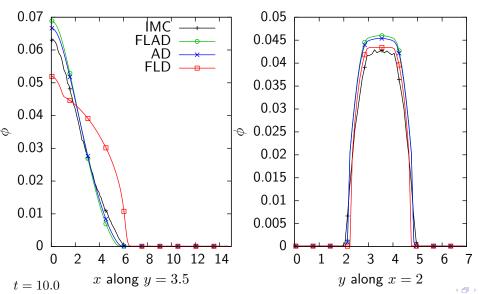


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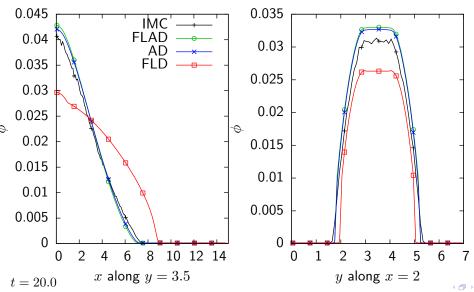


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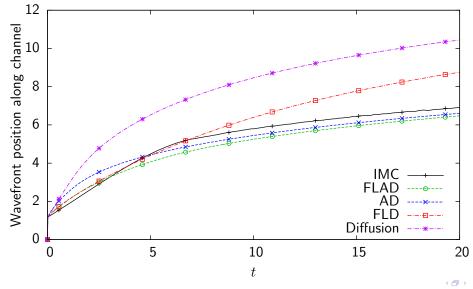
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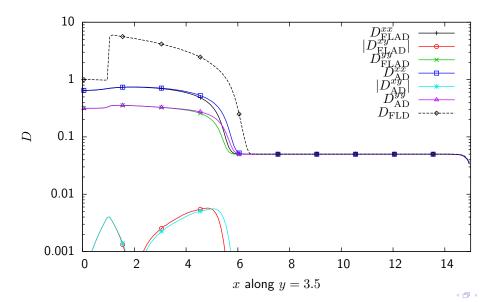
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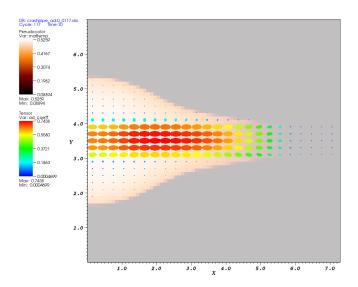
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Diffusion coefficients (t = 10)



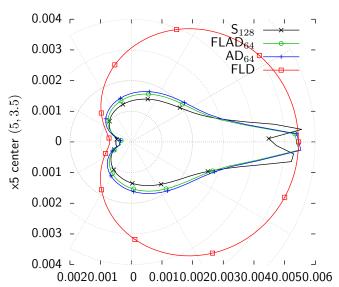
Anisotropic diffusion tensor visualization





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Approximate representations of the angular flux



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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 $\Delta_x = 0.1$.

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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:

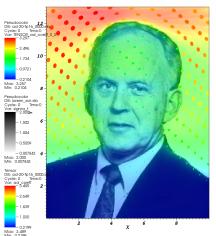
- Further analysis of boundary conditions
- Finish writing a dissertation
- Convince committee to let me graduate

Someone else:

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



Questions?



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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).

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