A fast algorithm for radiative transfer

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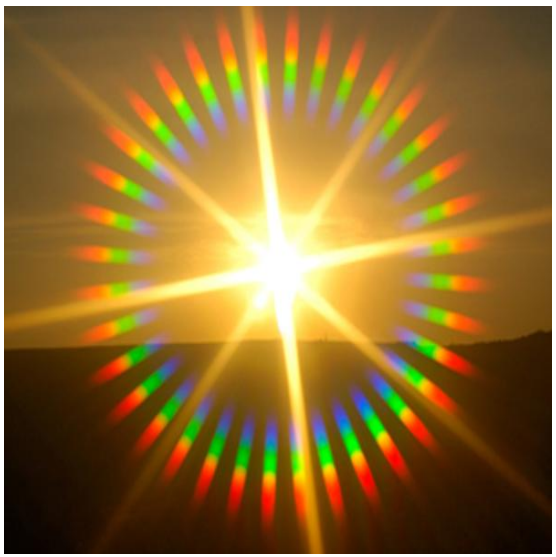
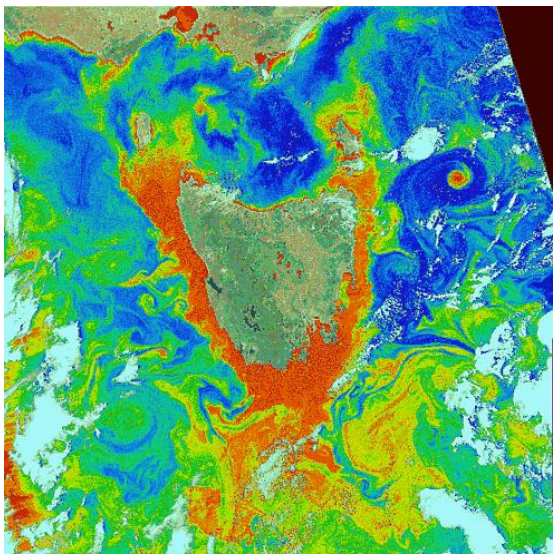
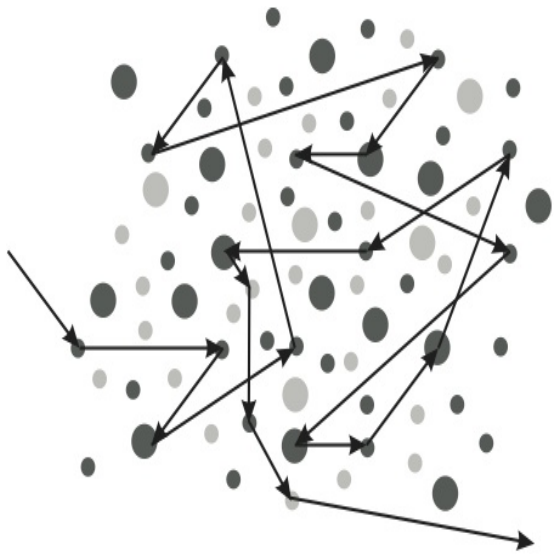
Introduction of radiative transfer

Radiative transport describes the propagation of **particles** through a medium which is affected by *absorption*, *emission*, *scattering*. It has a wide variety of applications in optics, astrophysics, remote sensing, nuclear engineering, biomedical imaging.







Steady-state radiative transfer

Here we consider following steady-state equation of radiative transport in medium $D \subset \mathbb{R}^d$, $u(\mathbf{x}, \mathbf{v})$ is the density of particles at $\mathbf{x} \in D$ along unit direction $\mathbf{v} \in \mathbb{S}^{d-1}$,

$$\mathbf{v} \cdot \nabla u(\mathbf{x}, \mathbf{v}) + (\sigma_s(\mathbf{x}) + \sigma_a(\mathbf{x}))u = \sigma_s(\mathbf{x}) \int_{\mathbb{S}^{d-1}} K(\mathbf{v}, \mathbf{v}')u(\mathbf{x}, \mathbf{v}')d\mathbf{v}' + q(\mathbf{x})$$

σ_a is absorption coefficient, σ_s is scattering coefficient. $K(\mathbf{v}, \mathbf{v}')$ is scattering phase function, describes the probability of each particle altering direction from $\mathbf{v}'$ to $\mathbf{v}$. Here $q(\mathbf{x})$ is an isotropic source for simplicity purpose. Let $\sigma_t = \sigma_s + \sigma_a$ be extinction coefficient and assume there is *vacant incoming boundary conditions*.

Numerical difficulties for radiative transfer

Numerical solutions to radiative transfer in general need enormous of computing efforts, due to *high dimensionality* of the solution space $D \times \mathbb{S}^{d-1}$. In recent decades, some numerical methods are developed for solution of radiative transfer.

1. Spherical Harmonics Method (P_n, SP_n) : accurate for scattering dominated medium.
2. Discrete Ordinates Method : high dimensionality, false scattering, ray effect.
3. Stochastic-based Method (Monte-Carlo) : computational cost.

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Isotropic scattering

Under *isotropic* setting, $K(\mathbf{v}, \mathbf{v}') \equiv \frac{1}{\mathrm{Vol}(\mathbb{S}^{d-1})}$. Let

$$\Phi(\mathbf{x}) = \frac{1}{\mathrm{Vol}(\mathbb{S}^{d-1})} \int_{\mathbb{S}^{d-1}} u(\mathbf{x}, \mathbf{v}) d\mathbf{v},$$

then equation is equivalent to a linear transport with unknown source R

$$(\mathbf{v} \cdot \nabla + \sigma_t) u = \sigma_s \Phi(\mathbf{x}) + q(\mathbf{x}) = \underline{R(\mathbf{x})}$$

Isotropic scattering

Along **v**, above equation is one-dimensional ODE, the solution for this linear transport is known (with vacant incoming boundary condition)

$$u(\mathbf{x},\mathbf{v}) = \int_0^{\tau^-(\mathbf{x},\mathbf{v})} \exp\Big(-\int_0^{\rho} \sigma_t(\mathbf{x}-\rho'\mathbf{v})d\rho'\Big) R(\mathbf{x}-\rho\mathbf{v})d\rho$$

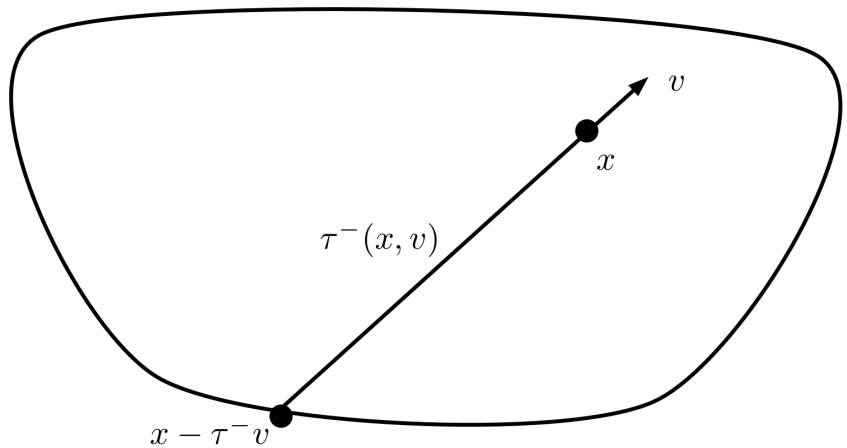

Figure: Illustration for 1D transport along **v**

Integral formulation for isotropic scattering

Integrate $u(\mathbf{x}, \mathbf{v})$ over $\mathbb{S}^{d-1}$ and take average (Φ)

$$\Phi(\mathbf{x}) = \frac{1}{\mathrm{Vol}(\mathbb{S}^{d-1})} \int_{\mathbb{S}^{d-1}} \int_0^{\tau^-(\mathbf{x},\mathbf{v})} \exp\left(- \int_0^{\rho} \sigma_t(\mathbf{x} - \rho' \mathbf{v}) d\rho' \right) R(\mathbf{x} - \rho \mathbf{v}) d\rho d\mathbf{v}$$

If we take $\mathbf{y} = \mathbf{x} - \rho \mathbf{v}$, and let

$$E(\mathbf{x}, \mathbf{y}) = \exp(- \int_0^{\rho} \sigma_t(\mathbf{x} - \rho' \mathbf{v}) d\rho'),$$

where E is equivalent to a line integral for σ_t from $\mathbf{x}$ to $\mathbf{y}$.

Integral formulation for isotropic scattering

Simplify the equation with $E(\mathbf{x}, \mathbf{y})$, we obtain

$$\Phi(\mathbf{x}) = \frac{1}{\mathrm{Vol}(\mathbb{S}^{d-1})} \int_{\mathbb{S}^{d-1}} \int_0^{\tau^-(\mathbf{x},\mathbf{v})} E(\mathbf{x}, \mathbf{y}) R(\mathbf{y}) \underline{d\rho d\mathbf{v}},$$

where the $d\rho d\mathbf{v}$ fits into polar coordinate.

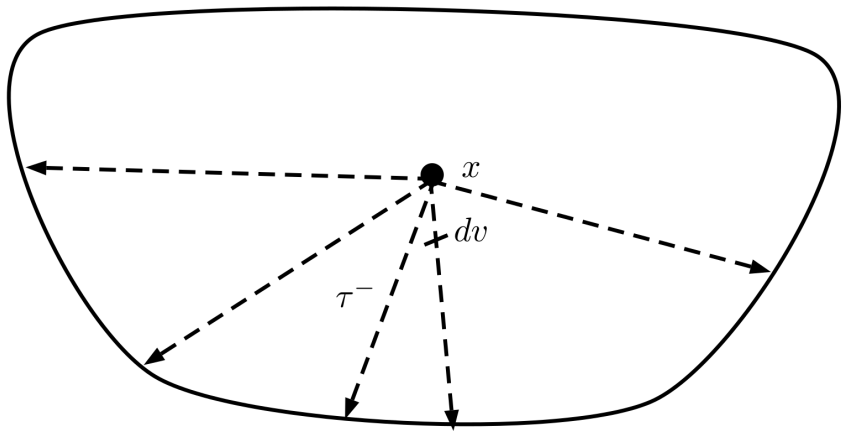

Figure: Illustration of polar coordinate

Integral formulation for isotropic scattering

We transform from polar coordinate back to Cartesian coordinate

$$d\mathbf{y} = \rho^{d-1} d\rho d\mathbf{v},$$

and replace source R with $\sigma_s \Phi + q$, observing $\rho = |\mathbf{x} - \mathbf{y}|$,

$$\Phi(\mathbf{x}) = \frac{1}{\mathrm{Vol}(\mathbb{S}^{d-1})} \int_D \frac{E(\mathbf{x}, \mathbf{y})}{|\mathbf{x} - \mathbf{y}|^{d-1}} \left(\sigma_s(\mathbf{y})\Phi(\mathbf{y}) + q(\mathbf{y})\right) d\mathbf{y}$$

we obtain an second kind integral equation about Φ depending $\mathbf{x}$ only.

Integral formulation for isotropic scattering

In terms of operator, we can write as

$$(\mathcal{I} - \mathcal{K}\sigma_s)\Phi = \mathcal{K}q, \tag{1}$$

where linear integral operator

$$\mathcal{K}f = \frac{1}{\mathrm{Vol}(\mathbb{S}^{d-1})} \int_D \frac{E(\mathbf{x}, \mathbf{y})}{|\mathbf{x} - \mathbf{y}|^{d-1}} f(\mathbf{y}) d\mathbf{y}. \tag{2}$$

Some observations

1. $E(\mathbf{x}, \mathbf{y})$ exponentially decays as $|\mathbf{x} - \mathbf{y}|$ increases.
2. If σ_t is constant number, then

$$E(\mathbf{x}, \mathbf{y}) = \exp(-\sigma_t |\mathbf{x} - \mathbf{y}|), \tag{3}$$

   then operator $\mathcal{K}$ is convolution product.
3. If σ_t is analytically known, then $E(\mathbf{x}, \mathbf{y})$ might be calculated explicitly.
4. If σ_t is not analytical (e.g. piecewise defined), it will require some fast algorithm for evaluation of line integrals.

Discretization

For simplicity, We discretize the integral equation as

$$(I - K\Sigma_s)\Psi = KQ,$$

where

$$K_{ij} = \frac{1}{\mathrm{Vol}(\mathbb{S}^{d-1})} \frac{E(\mathbf{x}_i, \mathbf{x}_j)}{|\mathbf{x}_i - \mathbf{x}_j|^{d-1}}, \quad i \neq j$$

for $i = j$, we analytically integrate the kernel locally.

$$\Sigma_s = \mathrm{diag}(\sigma_s(\mathbf{x}_1), \dots),$$

$$Q = (q(\mathbf{x}_1), \dots)^T.$$

we can show that first order error can be achieved by above *bruteforce* discretization.

Iterative method for integral equation

We solve the linear system by iterative scheme `GMRES(m)`.

But the iteration number approximated is proportional to σ_s. We need a preconditioner.

For practical use, we assume σ_t and σ_s are piecewisely defined, so time complexity of *naively* evaluating $E(\mathbf{x}, \mathbf{y})$ is proportional to $|\mathbf{x} - \mathbf{y}|$.

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Fast multipole method: a brief idea

The idea of FMM is to accelerate matrix-vector multiplication $\mathbf{y}_{n\times 1} = A_{n\times n}\mathbf{x}_{n\times 1}$, by seeking for low rank approximation of A:

If A has good property that given ε, we can find $m \ll n$ that

$$\|A_{n\times n} - U_{n\times m}S_{m\times m}V^*_{m\times n}\| \leqslant \varepsilon \tag{4}$$

then cost of applying A can be approximated be $O(2mn + m^2)$.

There are many kinds of variants of FMM nowadays: KIFMM, BBFMM, PVFMM, randomized methods,etc.

Fast multipole method

For matrix-vector multiplication with matrix K, we implemented BBFMM – interpolative FMM with Chebyshev polynomial, which was first introduced by Darve and Fong.

Some good things:

1. very easy to implement (about 1k lines C/C++).
2. time complexity still remains $O(N)$ as original FMM taking evaluation time of E into account.

Therefore applying low rank approximation of $(I - K\Sigma_s)$ is $O(N)$.

A not-too-slow preconditioner ?

It is frustrating that the iteration number be large if σ_s is large.

We need to find an operator $\hat{K} \sim K$ which makes $I - \hat{K}\Sigma_s$ also easy to invert.

When σ_s and σ_t are constant, $I - K\Sigma_s$ is convolution product after periodical extension. But exact inversion is not available !

But when σ_s is large, so is σ_t, which means decay is fast, then we can use zero extension to get approximated inversion.

Numerical experiments in 2D

We perform numerical experiments on unit square $D = (0,1)^2$ and discretized by uniform squares of length 2^{-M} ($M = 5, 6, 7, 8, 9$) and place sampling points at centers of these squares with first order scheme.

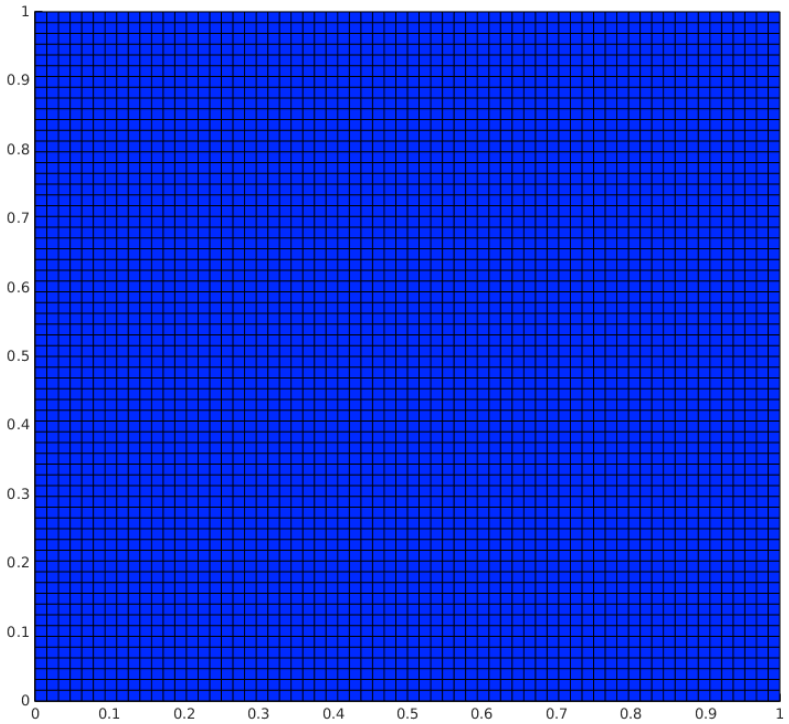
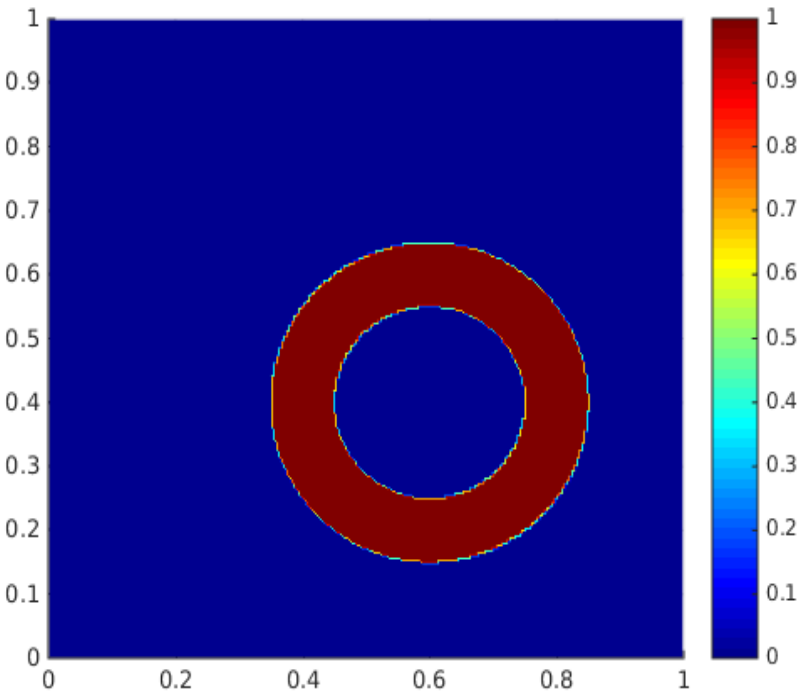
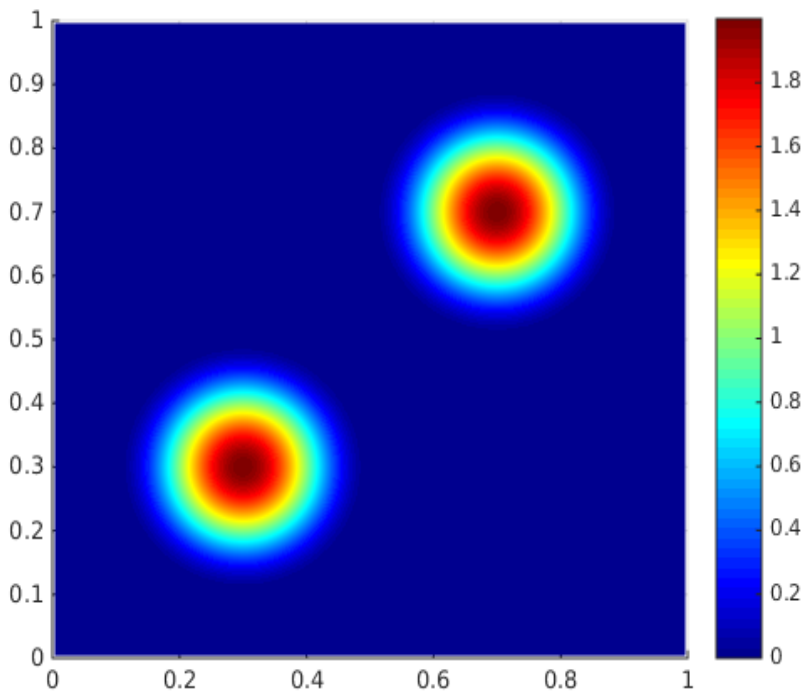


Figure: discretization with 64×64.

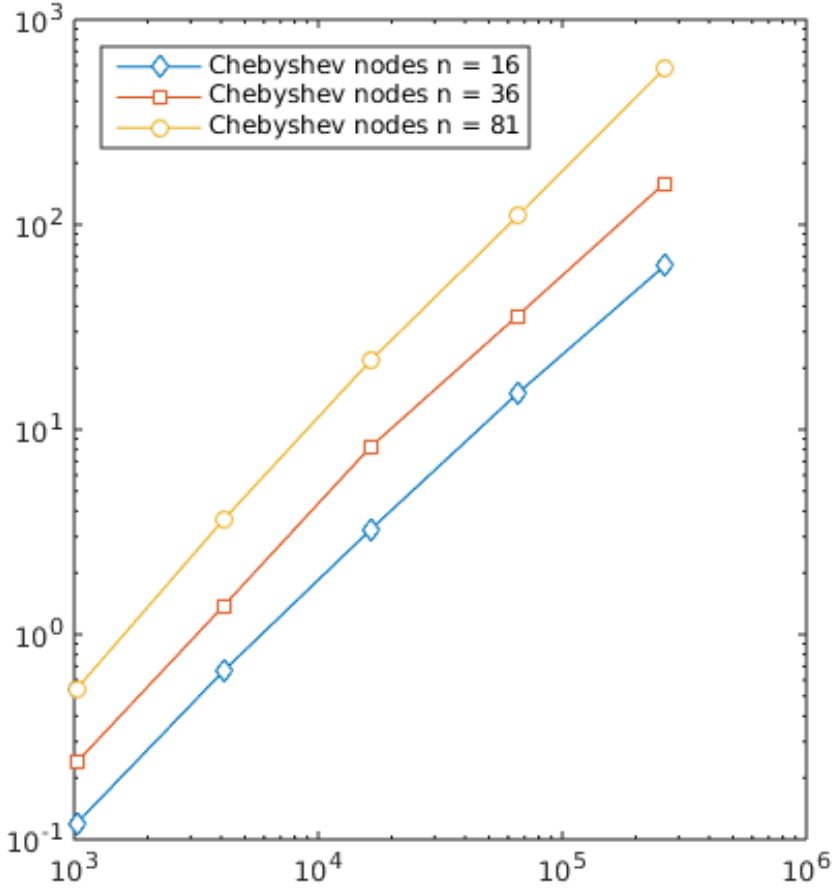
Numerical experiments in 2D

We select two source functions as examples below. In following experiments, $\sigma_a \equiv 0.2$ and $\sigma_s = 2.0, 5.0, 10.0$ respectively.





Strong scaling for FMM solution



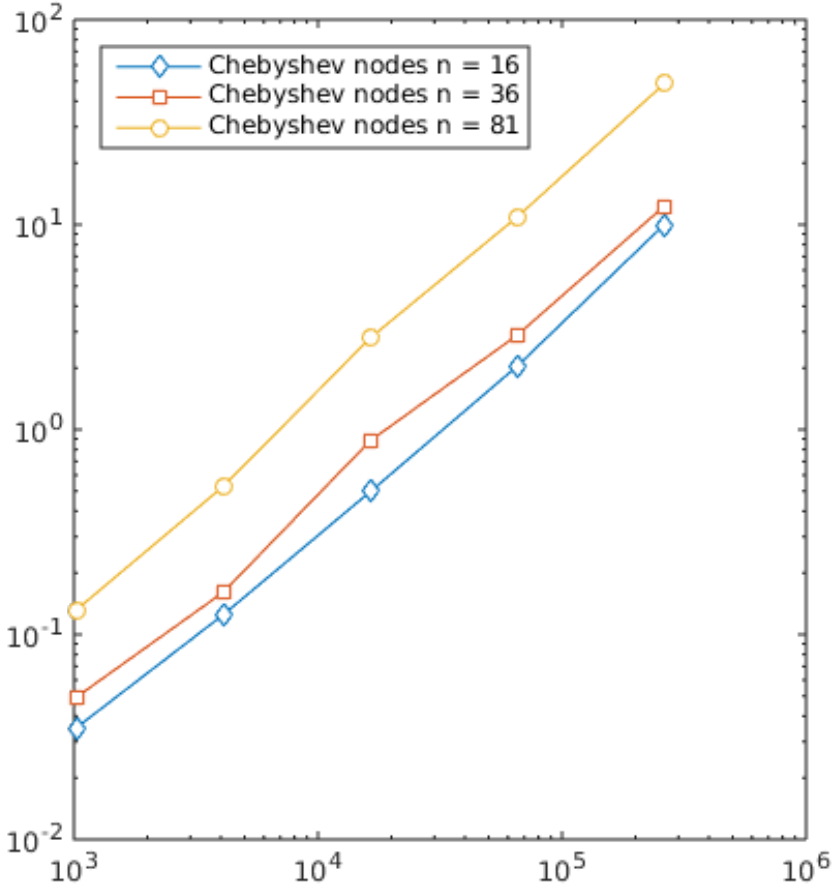
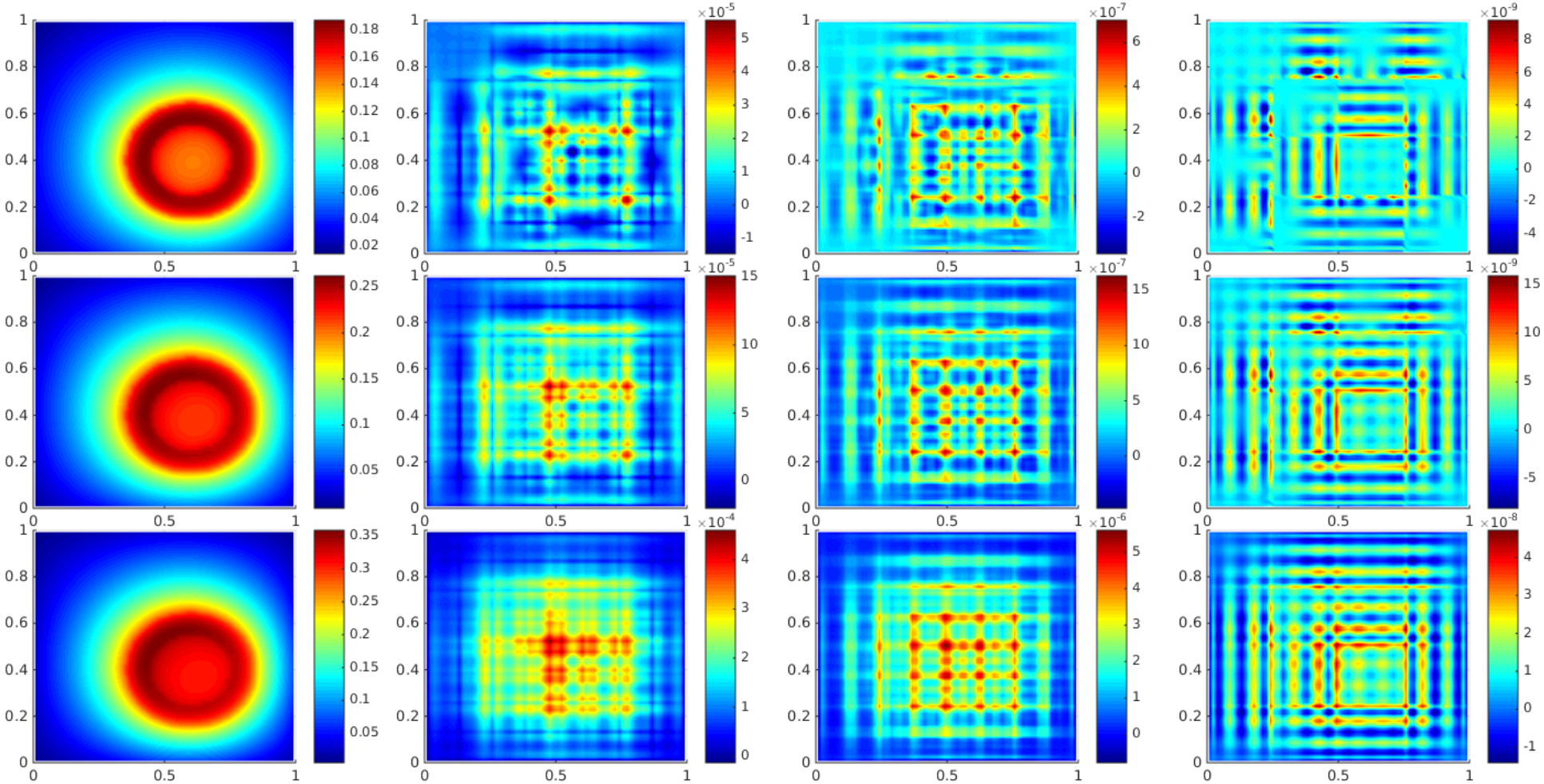
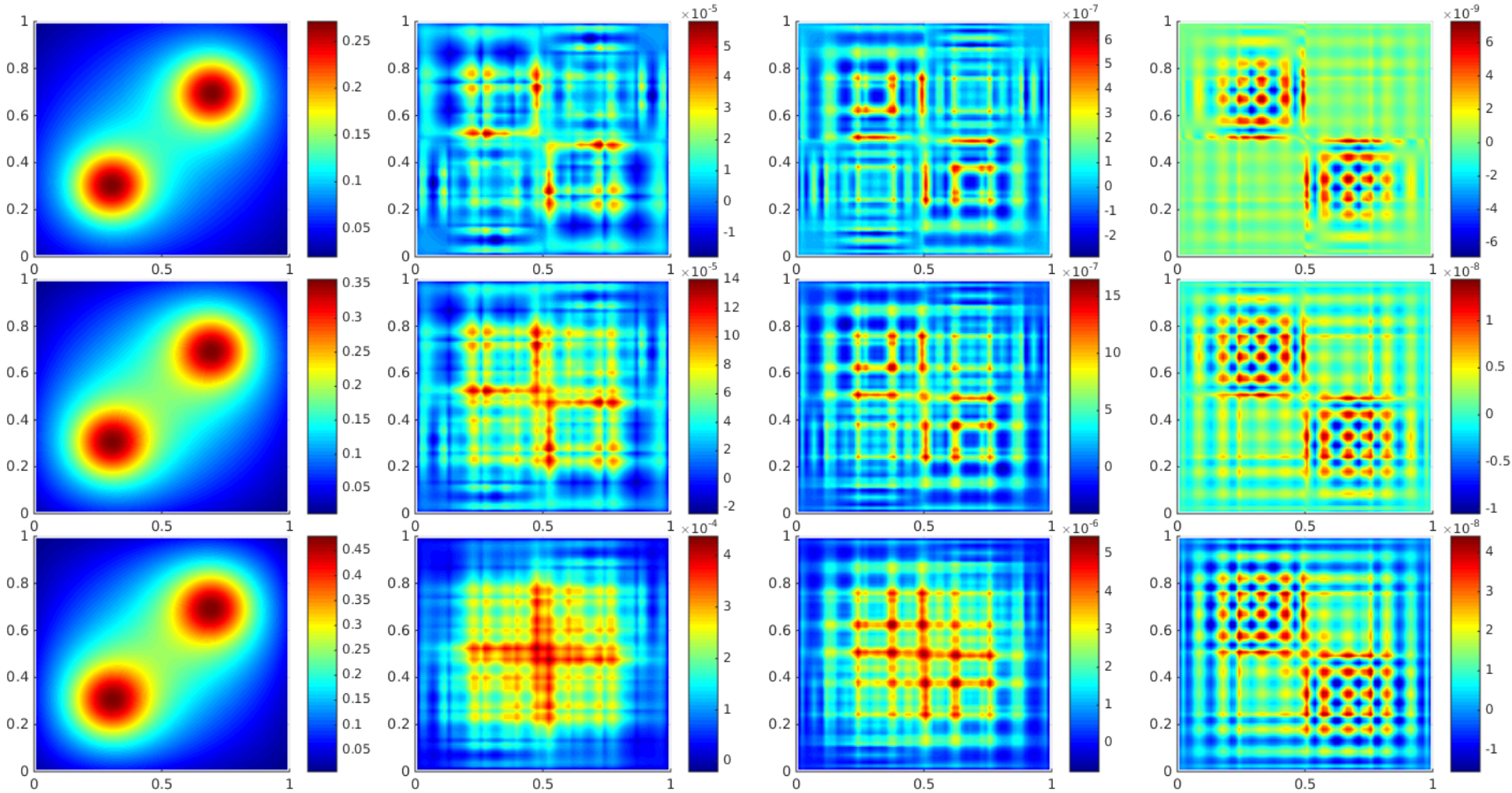


Figure: Left: Time (s) for preparation. Right: Time(s) for GMRES iterations

Error from FMM (first source)



Error from FMM (second source)



Error against Monte Carlo solution

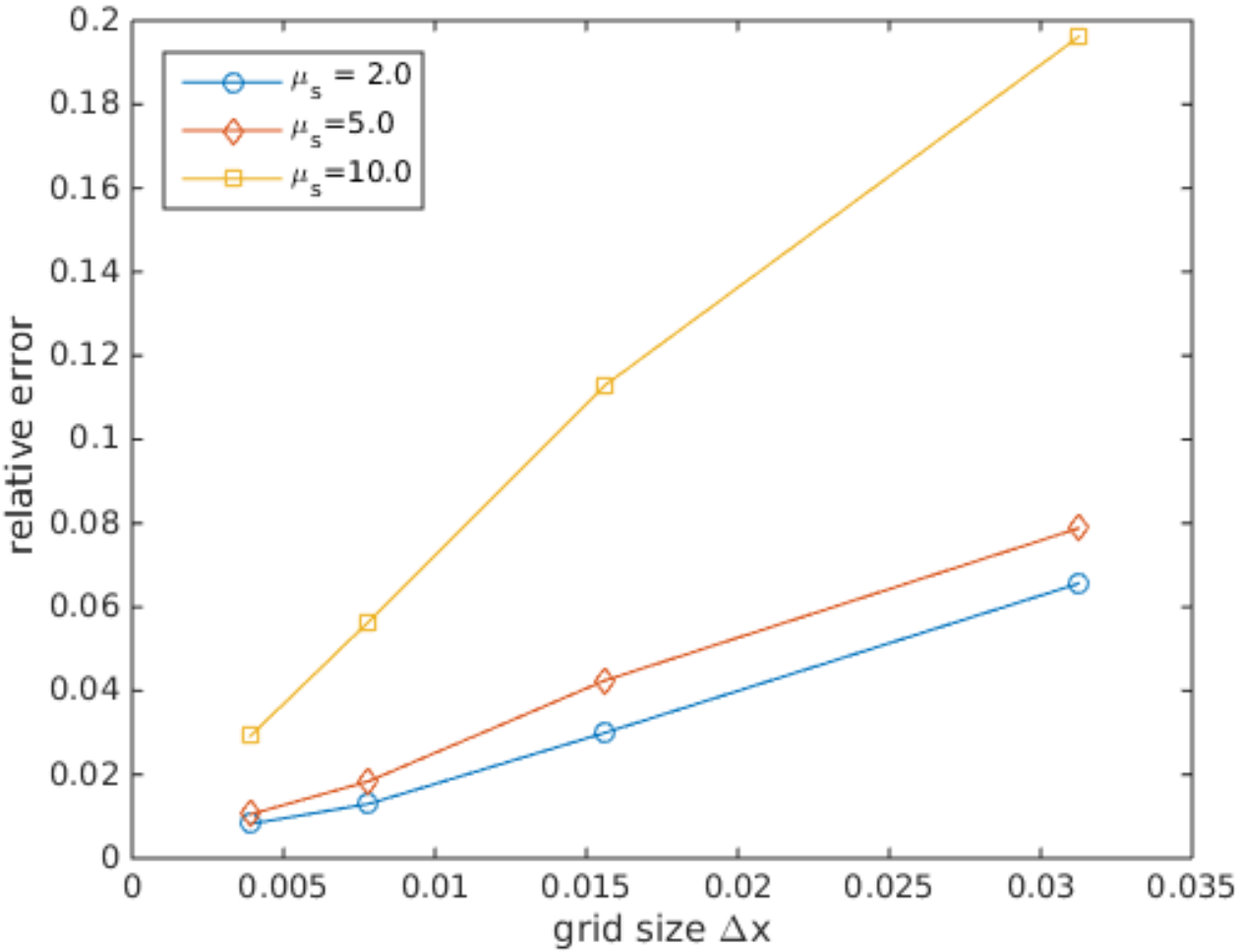


Figure: First order error for FMM solver

An intuitive approach to anisotropy

Since our formulation highly depends on integral formulation of the solution, thus anisotropic scattering might not be the most efficient. We consider Henyey-Greenstein phase function $p_{HG}(\mathbf{v}\cdot\mathbf{v}')$, that

$$\mathbf{v}\cdot\nabla u(\mathbf{x},\mathbf{v})+(\sigma_s(\mathbf{x})+\sigma_a(\mathbf{x}))u=\sigma_s(\mathbf{x})\int_{\mathbb{S}^{d-1}}p_{HG}(\mathbf{v}\cdot\mathbf{v}')u(\mathbf{x},\mathbf{v}')d\mathbf{v}'+q(\mathbf{x})$$

where

$$p_{HG}=\frac{1}{4\pi}\sum_{k=0}^{\infty}(2k+1)g^kP_k(\mathbf{v}\cdot\mathbf{v}')$$

and if we expand the formula further

$$p_{HG}(\mu,\theta,\mu',\theta')=\sum_{m=0}^{\infty}\sum_{l=m}^{\infty}\chi_l^mP_l^m(\mu)P_l^m(\mu')\cos m(\theta-\theta')$$

An intuitive approach to anisotropy

Because $\cos m(\theta - \theta') = \cos m\theta \cos m\theta' + \sin m\theta \sin m\theta'$, we can see the decoupling of $\mathbf{v}$ and $\mathbf{v}'$ is completed here. Let

$$\Phi_l^m(\mu, \theta) = P_l^m(\mu) \cos m\theta, \quad \Psi_l^m(\mu, \theta) = P_l^m(\mu) \sin m\theta$$

and let

$$C_l^m(\mathbf{y}) = \int_{\mathbb{S}^2} u(\mathbf{y}, \mu, \theta) \Phi_l^m(\mu, \theta) d\mu d\theta$$
$$S_l^m(\mathbf{y}) = \int_{\mathbb{S}^2} u(\mathbf{y}, \mu, \theta) \Psi_l^m(\mu, \theta) d\mu d\theta$$

then multiply the integral formulation by Φ_r^n and Ψ_r^n on both sides, we can obtain an integral equation system on C_r^n and S_r^n.

An intuitive approach to anisotropy

The system about (C_r^n, S_r^n) is written as,

$$C_r^n(\mathbf{x}) = \int_D \frac{E(\mathbf{x},\mathbf{y})}{|\mathbf{x}-\mathbf{y}|^{d-1}} \left(\sigma_s(\mathbf{y}) \sum_{l,m} \chi_l^m \Phi_r^n (\Phi_l^m C_l^m(\mathbf{y}) + \Psi_l^m S_l^m(\mathbf{y})) + \Phi_r^n q(\mathbf{y}) \right)$$

$$S_r^n(\mathbf{x}) = \int_D \frac{E(\mathbf{x},\mathbf{y})}{|\mathbf{x}-\mathbf{y}|^{d-1}} \left(\sigma_s(\mathbf{y}) \sum_{l,m} \chi_l^m \Psi_r^n (\Phi_l^m C_l^m(\mathbf{y}) + \Psi_l^m S_l^m(\mathbf{y})) + \Psi_r^n q(\mathbf{y}) \right)$$

where all θ, μ can be transformed into Cartesian coordinate with simple algebra.

Numerical experiments in 2D on δ-Eddington approximation

δ-Eddington approximation uses first order expansion. We adopt one of our previous source function to run simulation under setting $\mu_a \equiv 0.2$ and $\mu_s \equiv 5.0$, and $g' = g/(1+g) \leqslant 0.5$, we take

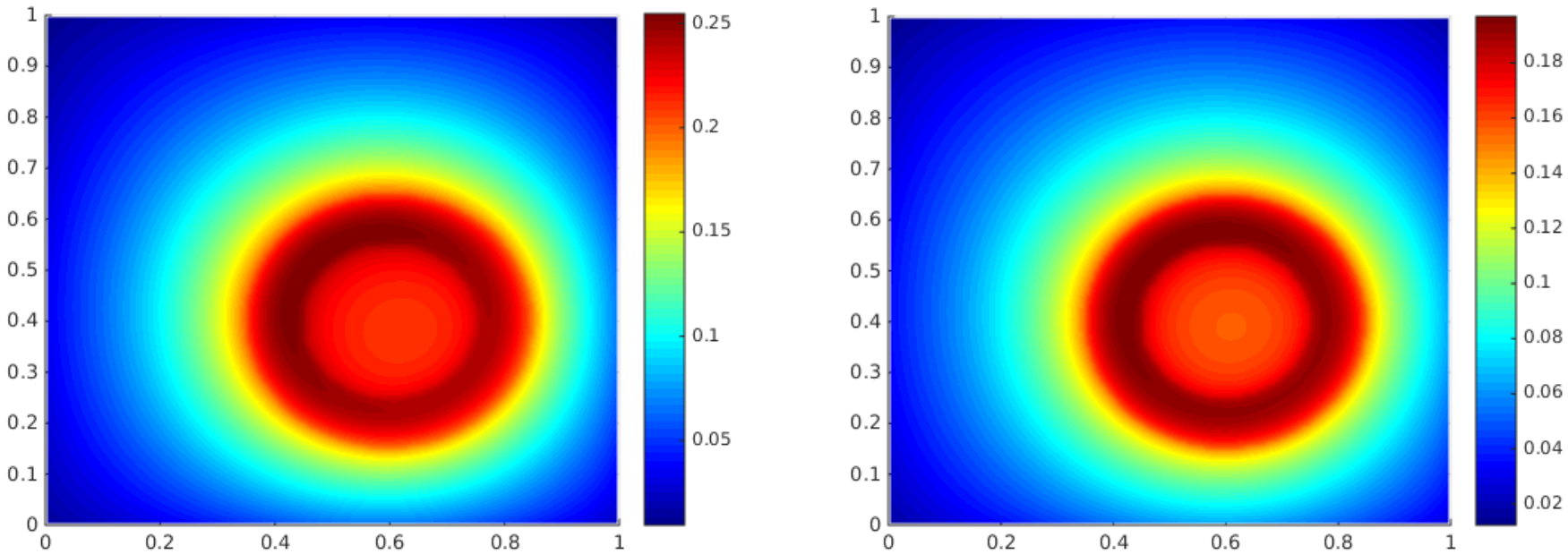


Figure: Fluence, from left to right, $g' = 0.05, 0.25$.

Numerical Experiments in 2D on δ-Eddington Approximation

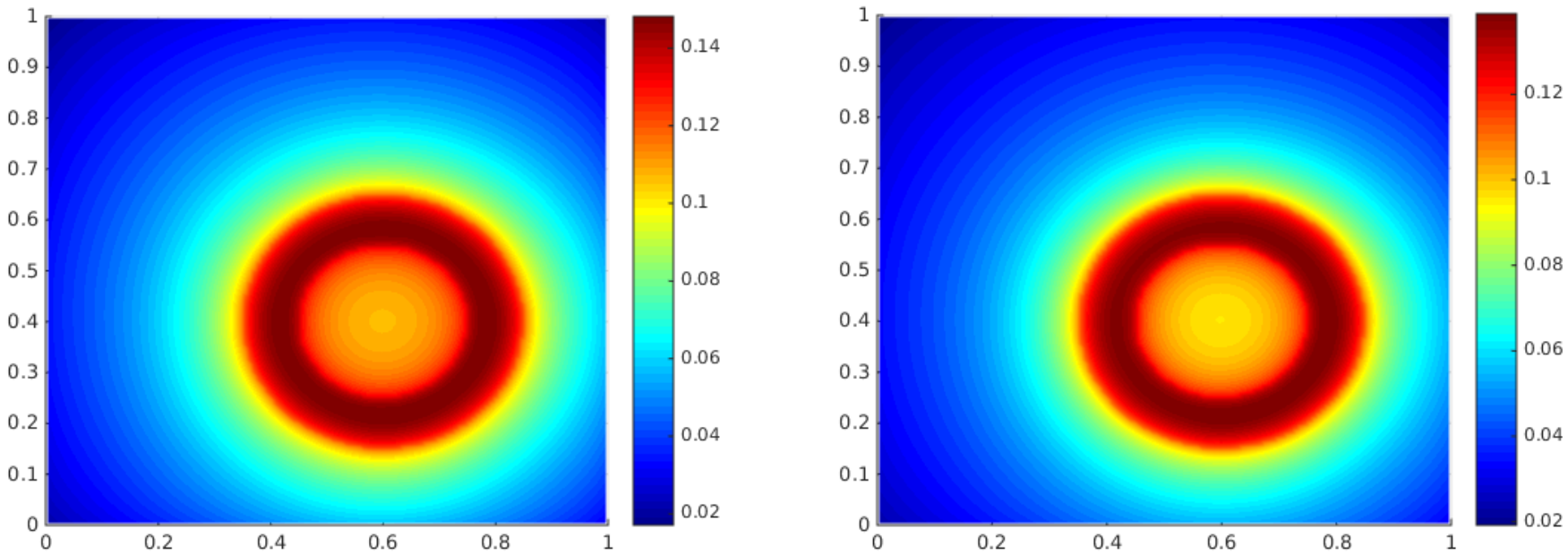


Figure: Fluence, from left to right, $g' = 0.40, 0.45$.

Summary and More

1. This method reduced the dimensionality of problem.
2. For isotropic scattering media, we propose a fast algorithm for radiative transfer equation, which can be used as a good preconditioner to the actual solution, the time complexity is $O(N)$.
3. And this method can extend to anisotropic scattering media with extra cost but solves in linear time and can be highly parallelized.
4. 3D isotropic parallel solver is implemented.
5. Future work might be on high order quadrature scheme, optimization of algorithm, time dependent problems and non-intuitive method under anisotropic scattering, inverse problem solver, etc.