FMM Preconditioner for Radiative Transport

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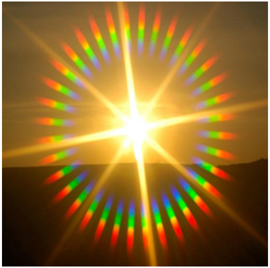
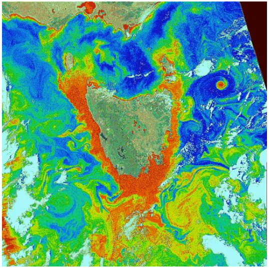
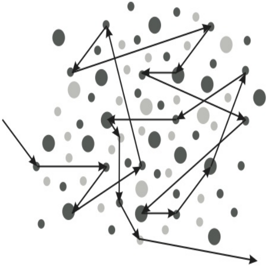
Introduction of Radiative Transport

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.







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 $\mathbf{x}$ along unit direction $\mathbf{v}$,

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

where $\mathbf{v} \in \mathbb{S}^{d-1}$, $\mathbf{x} \in D$, 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 $\mathbf{v}$. $q(\mathbf{x})$ is certain isotropic source. For simplicity, we call $\sigma_t = \sigma_s + \sigma_a$ be extinction coefficient and assume there is vanishing incoming boundary conditions.

Numerical methods for Radiative Transport

Solutions to radiative transport in general needs enormous of computing efforts, which is due to high dimensionality of the solution space. In recent decades, some numerical methods are developed for solution of radiative transport.

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

Integral Representation for Isotropic case

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 equation

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

Integral Representation for Isotropic case

Along $\mathbf{v}$, it is 1D transport (ODE), the solution for this equation is known

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

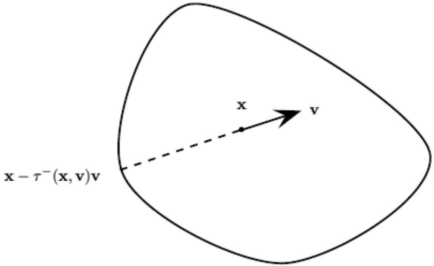


Figure: Illustration for 1D transport along $\mathbf{v}$

Integral Representation for Isotropic case

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

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

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 Representation for Isotropic case

Put E back into the equation, 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 $d\rho d\mathbf{v}$ actually fits polar coordinate.

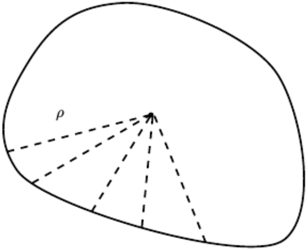


Figure: Illustration of polar coordinate

Integral Representation for Isotropic case

We transform from polar coordinate back to Cartesian $d\mathbf{y} = \rho^{d-1} d\rho d\mathbf{v}$, and replace R with $\sigma_s \Phi + q$, observing $\rho = |\mathbf{x} - \mathbf{y}|$,

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

we obtain an integral equation about Φ.

Observation 1: This equation does not contain angular variable $\mathbf{v}$.
Observation 2: This work does not require q to be isotropic.

Integral Representation for Isotropic case

In terms of operator, we can write as

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

where integral operator

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

Remark: $\mathcal{K}$ is compact, thus $\mathcal{I} - \mathcal{K}\Sigma_s$ is Fredholm. Since when $q = 0$, this equation only admits zero solution, by Fredholm alternative, $\mathcal{I} - \mathcal{K}\Sigma_s$ is invertible.

Algorithm for Integral Equation

Discretize the integral equation, take $\Psi = (\Phi(\mathbf{x}_1), \Phi(\mathbf{x}_2), \dots, \Phi(\mathbf{x}_n))^t$, then

$$\Psi = \mathcal{K}(\Sigma_s \Psi + Q)$$

where $\Sigma_s = \mathrm{diag}(\sigma_s(\mathbf{x}_1), \dots, \sigma_s(\mathbf{x}_n))$, and $Q = (q(\mathbf{x}_1), \dots, q(\mathbf{x}_n))^t$. Finally we obtain

$$\underline{(\mathcal{I} - \mathcal{K}\Sigma_s)\Psi = (\mathcal{K}Q)}$$

where matrix $\mathcal{K}$ is

$$\mathcal{K}_{ij} = \frac{1}{\mathrm{Vol}(\mathbb{S}^{d-1})} \frac{E(\mathbf{x}_i, \mathbf{x}_j)}{|\mathbf{x}_i - \mathbf{x}_j|^{d-1}} w_{ij}$$

where w_{ij} are weights to control the order of accuracy. For singularity part, we handle that separately.

Algorithm for Integral Equation

For linear system $(\mathcal{I} - \mathcal{K}\Sigma_s)\Psi = (\mathcal{K}Q)$,

1. Observe that when $|\mathbf{x}_i - \mathbf{x}_j|$ increases, $\mathcal{K}_{ij}$ decreases dramatically, which means (far) off-diagonal parts of $\mathcal{K}$ could be small (low rank), thus Krylov subspace method (e.g. GMRES) might work well for such linear system.
2. During each iteration of GMRES, we have to apply operator $\mathcal{I} - \mathcal{K}\Sigma_s$ multiple times, in general, if all entries are known, the matrix-vector multiplication is $O(N^2)$ complexity, which could be very expensive (running serially) when N is large.
3. To calculate the entries, we need to mention the computational cost of calculating $E(\mathbf{x}_i, \mathbf{x}_j)$.

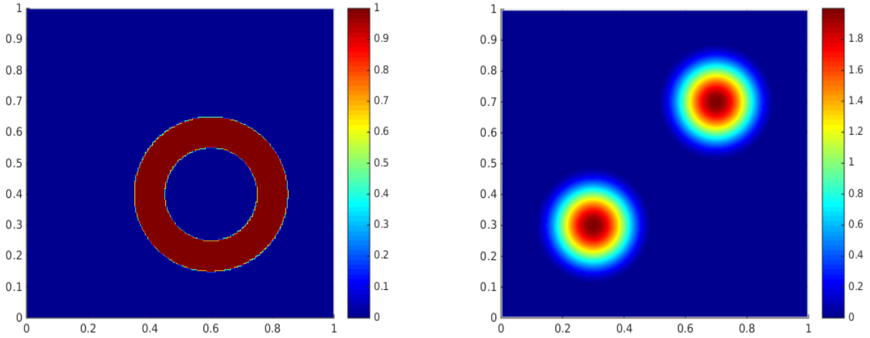
Algorithm for Integral Equation

1. Due to the low rank property of $\mathcal{K}$, we can adopt interpolative fast multipole method (FMM), such as Chebyshev polynomial, to accelerate the application of operator $(\mathcal{I} - \mathcal{K}\Sigma_s)$.
2. $O(N)$ time complexity of FMM for calculation of $(\mathcal{I} - \mathcal{K}\Sigma_s)\Psi$.

Observation 3: For piecewise defined σ_a and σ_s, the calculation of $E(\mathbf{x}_i, \mathbf{x}_j)$ does not change the time complexity due to FMM's hierarchical structure.
Observation 4: The total time cost is $O(M^2 N)$, M is iteration number.
Observation 5: Since GMRES will re-use the same operator, thus caching all expensive information will be beneficial.
Observation 6: It is symmetric operator, can reduce storage in half.

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

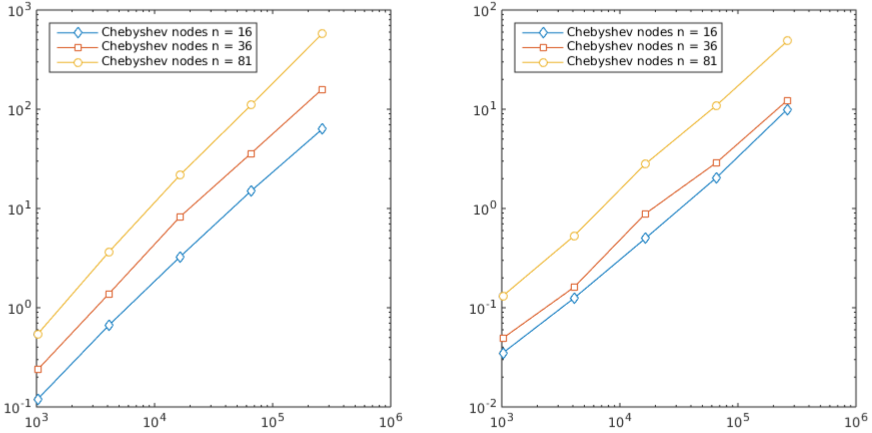
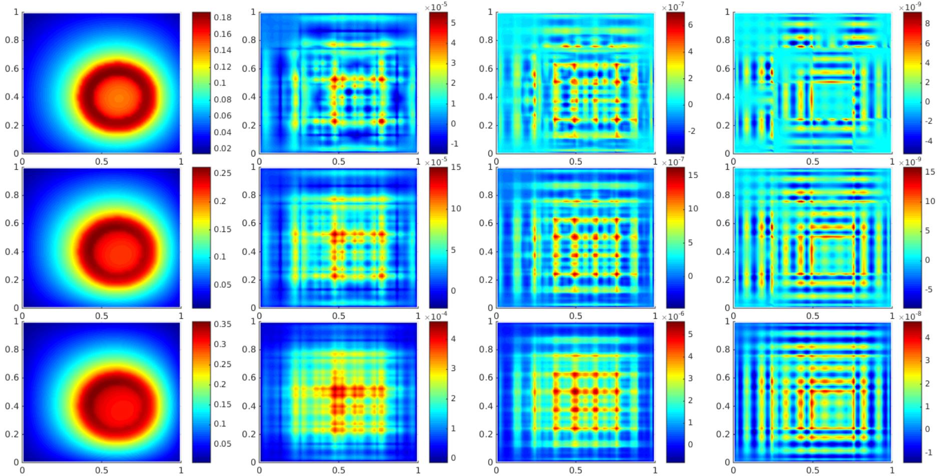
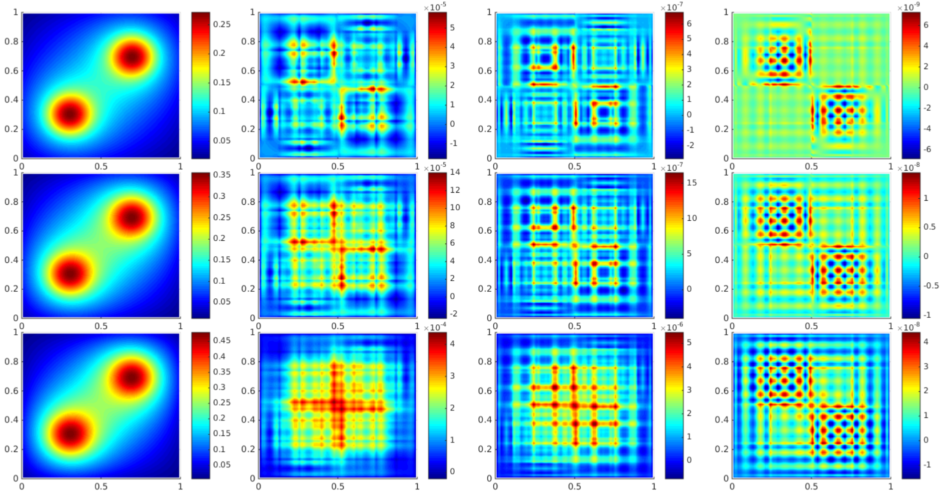


Figure: Left: Time (s) for preparation. Right: Time(s) for GMRES iterations

Error from FMM (first source)



Error from FMM (second source)



Anisotropic Case: An Intuitive Approach

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

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

and if we expand the formula further

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

Anisotropic Case: An Intuitive Approach

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

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

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.

Anisotropic Case: An Intuitive Approach

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

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

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

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

Observation 7: This system is truncated at $m = L$ for some small L.

Observation 8: This system is symmetric.

Observation 9: The time cost is $O(M^2 L^2 N)$, where M is iteration number.

Numerical Experiments in 2D on δ-Eddington Approximation

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

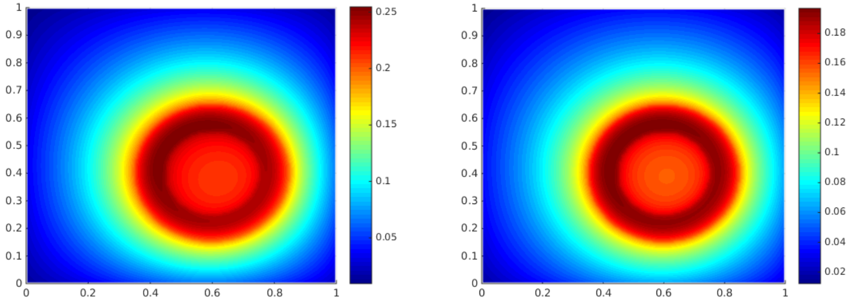
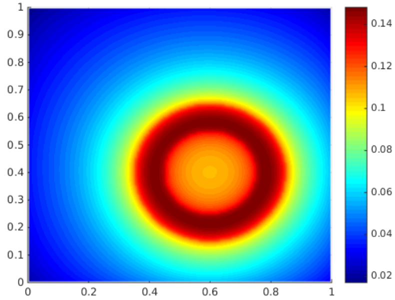


Figure: averaged solution, from left to right, $g' = 0.05, 0.25$.

Numerical Experiments in 2D on δ-Eddington Approximation

The integral operator system is 3 by 3, but only 5 entries have to be calculated.



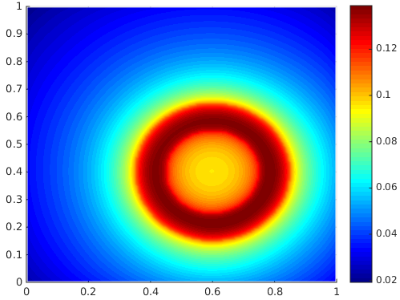


Figure: averaged solution, from left to right, $g' = 0.40, 0.45$.

Summary and More

1. This method reduced the dimensionality of the problem.
2. For isotropic scattering media, we propose a fast algorithm for radiative transport equation, which can be used as a good preconditioner or approximation to the actual solution, the time complexity is $O(N)$.
3. This method does not require specific geometry or mesh.
4. And this method can extend to anisotropic scattering media with extra cost but solves in linear time and can be highly parallelized.
5. 3D isotropic parallel solver is implemented.
6. Future work might be on optimization of algorithm, time dependent problems and non-intuitive method under anisotropic scattering, etc.