A low-rank method for two-dimensional time-dependent radiation transport calculations

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Abstract

The low-rank approximation is a complexity reduction technique to approximate a tensor or a matrix with a reduced rank, which has been applied to the simulation of high dimensional problems to reduce the memory required and computational cost. In this work, a dynamical low-rank approximation method is developed for the time-dependent radiation transport equation in 1-D and 2-D Cartesian geometries. Using a finite volume discretization in space and a spherical harmonics basis in angle, we construct a system that evolves on a low-rank manifold via an operator splitting approach. Numerical results on four test problems demonstrate that the low-rank solution requires less memory than solving the full rank equations with the same accuracy. It was furthermore shown that the low-rank algorithm can obtain much better results at a moderate extra cost by refining the discretization while keeping the rank fixed.

Keywords: Low-rank approximation, Radiation transport

1. Introduction

The numerical simulation of the radiation transport process is fundamental in a wide range of applications from supernovas to medical imaging, where accurate numerical solutions of a linear Boltzmann equation, also known as the
radiative transfer equation (RTE), are required. In this equation, we are solving for the specific intensity, which is a seven-dimensional function that describes the movement of the flow of particles in terms of time, position, direction, and energy. Despite the rapid development of high-performance computing, the numerical solution of the RTE remains challenging due to the high computational costs and the large memory requirements caused by such a high-dimensional phase space. In this paper, we focus on reducing the memory required to solve the RTE to enable better performance on exascale-class computers [1].

Due to the rich phase space, computational methods for radiation transport require discretizations in energy and direction, in addition to spatial and temporal discretizations. For the energy variable, the multigroup method is commonly used [2]. The direction, or angular variables, can be treated by solving the equations along particular directions via the discrete ordinates or $S_N$ method [3]. An alternative technique employs a basis expansion using the natural basis for the sphere: spherical harmonics. The spherical harmonics or $P_N$ method uses a truncated expansion to approximate the angular dependence [4–6]. Low-order approximations are also used such as flux-limited diffusion [7, 8], simplified $P_N$ [9–11] along with hybrid methods such as quasi-diffusion [12]. Finally, stochastic methods based on the implicit Monte Carlo method [13–16] are an alternative approach, though often requiring significant computational cost.

Although the aforementioned methods require many degrees of freedom to describe the phase-space dependence of the solution, it is known that many transport problems require only a subspace of the full phase space (called a manifold in mathematical parlance) to describe the transport of particles. An example of this phenomenon is problems in the diffusion limit: these problems require only a linear dependence on angular variables. One can also formulate problems where this manifold over which the solution depends evolves over time: a beam entering a scattering medium would be described by a delta-function in

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1The terminology direction and angle are typically used interchangeably to describe the angular component of the phase space.
space and angle at time zero, but eventually, relax to much smoother distribution that we could characterize using a simple basis expansion.

We desire to generalize this idea, and possibly automatically discover the manifold that describes the system evolution. We accomplish this task by expressing the solution to a transport problem as a basis expansion in space and angle and using techniques to determine what subspace of those bases are needed to describe the solution and how that subspace evolves. We use the dynamical low-rank approximation (DLRA) of Koch and Lubich to evolve time-dependent matrices by tangent-space projection \[17\]. DLRA has been extended to tensors \[18\], and further results can be found in \[19\]. DLRA has been used to reduce the computational complexity of quantum propagation \[20\] by restricting the evolution to lower-rank amongst other work \[21–23\]. The asymptotic analysis of the DLRA in a one-dimensional radiative transport equation with the backward Euler and Crank-Nicolson scheme was made in \[24\]. In this work, we apply DLRA to neutral particle transport.

Here we give a brief mathematical introduction to the robust and accurate projector-splitting method developed by Lubich \[25\] to perform the DLRA for matrix differential equations of the form

\[
\frac{\partial}{\partial t} A(t) = \dot{A}(t) = F(A(t)),
\]

for \( A(t) \in \mathbb{R}^{m \times n} \). DLRA seeks to find an approximating matrix \( Y(t) = U(t)S(t)V^T(t) \), where \( U(t) \in \mathbb{R}^{m \times r}, V(t) \in \mathbb{R}^{n \times r} \) are orthonormal matrices and \( S(t) \in \mathbb{R}^{r \times r} \) so that \( Y(t) \) has rank \( r \). Note that rank \( r \) matrices are a manifold, \( \mathcal{M}_r \), in the space \( \mathbb{R}^{m \times n} \). We evolve the solution on \( \mathcal{M}_r \) directly by inserting the ansatz for \( Y(t) \) into the equation and projecting the right-hand side onto the tangent space of \( \mathcal{M}_r \).

In this work, we develop a reduced system of the radiative transfer equation with this low-rank method, where the intensity only involves in its low-rank orthogonal bases rather the full phase space. We design a numerical scheme for the 2-D RTE with a finite volume discretization in space and a spherical harmonic (P\(_N\)) expansion in angle. We further demonstrate the memory saving
features by comparing the low-rank results with full-rank solutions and benchmark results.

2. Derivation of Method

We consider a energy-independent radiation transport equation
\[
\frac{1}{c} \frac{\partial \psi(r, \hat{\Omega}, t)}{\partial t} + \hat{\Omega} \cdot \nabla \psi(r, \hat{\Omega}, t) + \sigma_t(r) \psi(r, \hat{\Omega}, t) = \frac{1}{4\pi} \sigma_s(r) \phi(r, t) + Q(r, t). \tag{1}
\]
Here the angular flux \( \psi(r, \hat{\Omega}, t) \) with units of particles per area per steradian per time is a function of position \( r \in D \) where \( D \) is the computational domain, direction \( \hat{\Omega}(\mu, \varphi) \) where \( \mu \) is the cosine of the polar angle and \( \varphi \) is the azimuthal angle, and time \( t \). Note that \( \hat{\Omega} \) is a unit vector. The total and isotropic scattering macroscopic cross-sections with units of inverse length are denoted as \( \sigma_t(r) \) and \( \sigma_s(r) \), respectively, \( c \) is the particle speed and \( S(r, t) \) is a prescribed source with units of particles per volume per time. We also write the scalar flux, \( \phi(r, t) \), as the integral of the angular flux
\[
\phi(r, t) = \int_{4\pi} \psi(r, \hat{\Omega}, t) \, d\hat{\Omega}. \tag{2}
\]
In this study we approximate the solution to Eq. (1) using the form
\[
\psi(r, \hat{\Omega}, t) \approx \sum_{i,j=1}^{r} X_i(r, t) S_{ij}(t) W_j(\hat{\Omega}, t); \tag{3}
\]
that is, we seek the best approximation with rank \( r \) to the solution of Eq. (1), where we have written \( X_i \) as an orthonormal basis for \( r \) and \( W_j \) as an orthonormal basis for \( \hat{\Omega} \) using the inner products
\[
\langle f, g \rangle_r = \int_D fg \, dr, \quad \langle f, g \rangle_{\hat{\Omega}} = \int_{4\pi} fg \, d\hat{\Omega}.
\]
Due to orthonormality we also have \( \langle X_i, X_j \rangle_r = \langle W_i, W_j \rangle_{\hat{\Omega}} = \delta_{ij} \). We also use \( \tilde{X} = \{X_1, X_2, ..., X_r\} \) and \( \tilde{W} = \{W_1, W_2, ..., W_r\} \) as ansatz spaces. The expansion in Eq. (3) is not unique and we add orthogonal constraints \( \langle X_i, \dot{X}_j \rangle_r = 0 \) and \( \langle W_i, \dot{W}_j \rangle_{\hat{\Omega}} = 0 \) as gauge conditions, which identify \( X \) and \( W \) in Grassmann
We now define orthogonal projectors using the bases:

$$P_{\bar{X}} g = \sum_{i=1}^{r} X_i \langle X_i g \rangle_r,$$

$$P_{\bar{W}} g = \sum_{j=1}^{r} W_j \langle W_j g \rangle_{\hat{\Omega}}.$$

We apply the projectors to define a split of the original equations into three steps and each of these is solved for a time step:

$$\partial_t \psi_1 (r, \hat{\Omega}, t) = P_{\bar{W}} \left( -\hat{\Omega} \cdot \nabla \psi(r, \hat{\Omega}, t) - \sigma_t(r, t) \psi(r, \hat{\Omega}, t) 
+ \frac{1}{4\pi} \sigma_s(r, t) \phi(r, t) + Q(r, t) \right), \quad (6)$$

$$\partial_t \psi_2 (r, \hat{\Omega}, t) = -P_{\bar{X}} P_{\bar{W}} \left( -\hat{\Omega} \cdot \nabla \psi(r, \hat{\Omega}, t) - \sigma_t(r, t) \psi(r, \hat{\Omega}, t) 
+ \frac{1}{4\pi} \sigma_s(r, t) \phi(r, t) + Q(r, t) \right), \quad (7)$$

$$\partial_t \psi_3 (r, \hat{\Omega}, t) = P_{\bar{X}} \left( -\hat{\Omega} \cdot \nabla \psi(r, \hat{\Omega}, t) - \sigma_t(r, t) \psi(r, \hat{\Omega}, t) 
+ \frac{1}{4\pi} \sigma_s(r, t) \phi(r, t) + Q(r, t) \right). \quad (8)$$

The $\psi_2$ step uses $\psi_1$ as an initial condition, and the $\psi_3$ step uses $\psi_2$ as an initial condition. It can be shown that the above evolution is contained in the low-rank manifold $\mathcal{M}_r$ if the initial value is in $\mathcal{M}_r$ because the right-hand side of each step remains in the tangent space $\mathcal{T}_r$.

The main advantage of this scheme comes from the fact that the only the low-rank components $X(r, t)$, $S(t)$, and $W(\hat{\Omega}, t)$ need to be stored during the time evolution rather than the full size solution $\psi(r, \hat{\Omega}, t)$. To demonstrate this we first formulate the projections explicitly from time $t_0$ to $t_0 + h$ where $h$ is the step size. The low-rank representation of $\psi(r, \hat{\Omega}, t_0)$ is given by the
initial condition

\[ \psi^{(0)}(r, \hat{\Omega}, t_0) = \sum_{i,j=1}^{r} X_i^{(0)}(r, t_0) S_{ij}^{(0)}(t_0) W_j^{(0)}(\hat{\Omega}, t_0) \]  

(9)

In the first projection the basis \( W_j \) does not change with time and is evaluated at the initial value \( W_j^{(0)}(\hat{\Omega}) \). We simplify the notation by writing \( K_j(r, t) = \sum_i X_i(r, t) S_{ij}(t) \), then (9) becomes

\[ \psi^{(0)}(r, \hat{\Omega}, t_0) = \sum_{j=1}^{r} K_j^{(0)}(r, t_0) W_j^{(0)}(\hat{\Omega}) \]  

(10)

We plug this solution into Eq. (6) and multiply by \( W_j^{(0)}(\hat{\Omega}) \) and integrate over \( \mu \) and \( \varphi \) to get

\[ \partial_t K_j = - \sum_{l=1}^{r} \langle \hat{\Omega} W_l W_j \rangle_{\hat{\Omega}} - \sigma_t K_j + \frac{1}{4 \pi} \sigma_s \sum_{l=1}^{r} K_l^{(0)}(W_l)_{\hat{\Omega}} \]

\[ + Q(W_j)_{\hat{\Omega}}. \]  

(11)

Equation (11) resembles the standard \( P_N \) equations, a point we will return to later. It is a system of advection problems coupled through the streaming term.

Notice that \( \psi \) has not been formulated in this equation.

We can then factor \( K_j^{(1)} \), which is the solution of Eq. (11) into \( X_i^{(1)} \) and \( S_{ij}^{(1)} \) using a QR decomposition. In the second step both the \( X_i \) and \( W_j \) are preserved. The initial condition to solve Eq. (12) are \( X_i^{(2)}(r) = X_i^{(1)}(r, t_0 + h) \), \( S_{ij}^{(2)}(t_0) = S_{ij}^{(1)}(t_0 + h) \), and \( W_i^{(2)}(\hat{\Omega}) = W_i^{(0)}(\hat{\Omega}) \). Then, we can perform similar calculations on Eq. (7) to get

\[ \frac{d}{dt} S_{ij} = \sum_{kl} \langle \nabla X_k X_l \rangle_r S_{kl} \langle \hat{\Omega} W_l W_j \rangle_{\hat{\Omega}} + \sum_k \langle \sigma_t X_k X_i \rangle_r S_{kj} 

\[ - \frac{1}{4 \pi} \sum_{kl} \langle \sigma_s X_k X_i \rangle_r S_{kl} \langle W_l \rangle_{\hat{\Omega}} \langle W_j \rangle_{\hat{\Omega}} - \langle X_i Q \rangle_r \langle W_j \rangle_{\hat{\Omega}}. \]  

(12)

We call the solution \( S_{ij}^{(2)} \). Equation (12) defines a set of \( r^2 \) ordinary differential equations. The solution is used to create an initial condition for Eq. (8), where \( X_i^{(3)}(r) = X_i^{(1)}(r, t_0 + h) \), \( S_{ij}^{(3)}(t_0) = S_{ij}^{(2)}(t_0 + h) \), and \( W_i^{(3)}(\hat{\Omega}, t_0) = W_i^{(0)}(\hat{\Omega}) \). Notice that \( X_i \) does not change with time in this step.
Writing $L_i = \sum_j S_{ij}(t)W_j(\hat{\Omega}, t)$ we can multiply Eq. (8) by a spatial basis function and integrate over space to get

$$
\partial_t L_i = -\hat{\Omega} \sum_k \langle \nabla X_k X_i \rangle_r L_k - \sum_k \langle \sigma_t X_k X_i \rangle_r L_k + \frac{1}{4\pi} \sum_k \langle \sigma_s X_k X_i \rangle_r (L_k)_{\hat{\Omega}}
$$

$$
+ \langle Q X_i \rangle_r, \quad (13)
$$

which evolves the solution in $\mu$ and $\varphi$ spaces. Upon factoring $L_i = S_{ij}^{(3)}(t)W_j^{(3)}(\hat{\Omega}, t)$ using a QR decomposition we can write the low-rank solution as $\psi(r, \hat{\Omega}, t_0 + h) = \sum_{i,j=1}^r X_i(1)(r, t_0 + h)S_{ij}^{(3)}(t_0 + h)W_j^{(3)}(\hat{\Omega}, t_0 + h)$.

3. Numerical Scheme

In this section the procedure outlined above of solving Eqs. (11), (12), and (13) is implemented in one and two spatial dimensions with a first-order explicit time integrator [25] and a finite volume discretization in space. For the angular basis, we use a spherical harmonics expansion. In this section, we describe the numerical method to solve the 2D problem in detail.

3.1. Discretization details

In the two dimensional system, we write the spatial variables as $x$ and $z$. The transport equation in this reduced geometry is

$$
\frac{1}{c} \frac{\partial \psi(x, z, \mu, \varphi, t)}{\partial t} + \mu \partial_z \psi(x, z, \mu, \varphi, t) + \sqrt{1 - \mu^2 \cos \varphi} \partial_x \psi(x, z, \mu, \varphi, t)
$$

$$
+ \sigma_t(x, z) \psi(x, z, \mu, \varphi, t) = \frac{1}{4\pi} \sigma_s(x, z) \phi(x, z, t) + Q(x, z, t). \quad (14)
$$

The projection system simplifies to

$$
\partial_t K_j = -\sum_{l=1}^r \partial_z K_l \langle \mu W_l W_j \rangle_{\hat{\Omega}} - \sum_{l=1}^r \partial_x K_l \left\langle \sqrt{1 - \cos \varphi^2} W_l W_j \right\rangle_{\hat{\Omega}} - \sigma_t K_j
$$

$$
+ \frac{\sigma_s}{2} \sum_{l=1}^r K_l \langle W_l \rangle_{\mu} \langle W_j \rangle_{\mu} + \frac{\langle W_j \rangle_{\mu}}{2} Q, \quad (15)
$$
\[
\partial_t S_{ij} = \sum_{kl} r \langle \partial_z X_k X_i \rangle_r S_{kl} \langle \mu W_l W_j \rangle_\Omega + \sum_{kl} r \langle \partial_x X_k X_i \rangle_r S_{kl} \langle \sqrt{1 - \cos^2 \varphi} W_l W_j \rangle_\Omega
\]
\[
+ \sum_k \langle \sigma_s X_k X_i \rangle_r S_{kj} - \frac{1}{2} \sum_{kl} \langle \sigma_s X_k X_i \rangle_r S_{kl} \langle W_l \rangle_\Omega \langle W_j \rangle_\Omega - \frac{1}{2} \langle X_i Q \rangle_r \langle W_j \rangle_\Omega,
\]

\text{(16)}

\[
\partial_t L_i = -\mu \sum_k \langle \partial_z X_k X_i \rangle_r L_k - \sqrt{1 - \cos^2 \varphi^2} \sum_k \langle \partial_x X_k X_i \rangle_r L_k - \frac{1}{2} \sum_k \langle \sigma_s X_k X_i \rangle_r L_k
\]
\[
+ \frac{1}{2} \sum_k \langle \sigma_s X_k X_i \rangle_r \langle L_k \rangle_\Omega + \frac{1}{2} \langle Q X_i \rangle_r.
\]

\text{(17)}

The bases we use are arise from a finite volume discretization in space with a constant mesh area \(\Delta x \Delta z\) and \(N_x \times N_z\) zones, and the truncated at \(N_l\) spherical harmonics in angle. To make orthonormal bases we define

\[
X_i(t, x, z) = \sum_{p=1}^{N_x} \sum_{q=1}^{N_z} Z_{pq}(x, z) u_{pqi}(t)
\]

\text{(18)}

\[
W_j(t, \mu, \varphi) = \sum_{l=0}^{N_l} \sum_{k=0}^{N_l} Y^k_l(\mu, \varphi) v_{lkj}(t)
\]

\text{(19)}

Note that \(Z_{pq}(x, z) = \frac{1}{\sqrt{\Delta x \Delta z}}\) with \(x \in [x_i - \frac{1}{2}, x_i + \frac{1}{2}]\) and \(z \in [z_i - \frac{1}{2}, z_i + \frac{1}{2}]\), where \(p\) and \(q\) are the cell index. The spherical harmonics are defined as

\[
Y^k_l(\mu, \varphi) = \sqrt{\frac{2l + 1}{4\pi} \frac{(l - k)!}{(l + k)!} P^k_l(\mu) e^{ik\varphi},}
\]

where \(P^k_l(\mu)\) is the associate Legendre polynomial. The negative \(k\) are not necessary here because of the recursion properties of the spherical harmonics \cite{27}. Here \(u_{pqi}\) and \(v_{lkj}\) are components of the time dependent tensor \(U(t) \in \mathbb{R}^{N_x \times N_z \times r}\) and \(V(t) \in \mathbb{R}^{N_l \times (N_l+1) \times r}\).

We also notice that the computations in Eqs. (18), (19) can be performed by the matrix multiplication instead of tensor operation. This is achieved by rearranging the matrices \(Z \in \mathbb{R}^{N_x \times N_z}\) and \(Y \in \mathbb{R}^{N_l \times (N_l+1)}\) into vectors and tensors \(U\) and \(V\) to matrices.
To make the notation consistent we denote the number of degrees of freedom in space as \( m = N_x N_z \) and the angular degrees of freedom as \( n = \frac{1}{2}(N_\ell + 1)(N_\ell + 2) \). In addition, the index of \( U \) and \( V \) conform to Eqs. (18) and (19).

Consequently the new ansatz spaces \( X \) and \( W \) have the form

\[
X = UZ = \begin{bmatrix}
  u_{111} & u_{112} & \ldots & u_{11r} \\
  \vdots & \vdots & \ddots & \vdots \\
  u_{N_x 11} & u_{N_x 12} & \ldots & u_{N_x 1r} \\
  u_{121} & u_{122} & \ldots & u_{12r} \\
  \vdots & \vdots & \ddots & \vdots \\
  u_{N_x N_z 1} & u_{N_x N_z 2} & \ldots & u_{N_x N_z r}
\end{bmatrix}
\begin{bmatrix}
  Z_{11} \\
  \vdots \\
  Z_{N_x 1} \\
  Z_{12} \\
  \vdots \\
  Z_{N_x N_z}
\end{bmatrix}
\]

\[
W = VY = \begin{bmatrix}
  v_{001} & v_{002} & \ldots & v_{00r} \\
  v_{011} & v_{012} & \ldots & v_{01r} \\
  v_{111} & v_{112} & \ldots & v_{11r} \\
  v_{021} & v_{022} & \ldots & v_{02r} \\
  \vdots & \vdots & \ddots & \vdots \\
  v_{Ni N_\ell 1} & v_{Ni N_\ell 2} & \ldots & v_{Ni N_\ell r}
\end{bmatrix}
\begin{bmatrix}
  Y_{00}^0 \\
  Y_{01}^0 \\
  Y_{11}^0 \\
  Y_{02}^0 \\
  \vdots \\
  Y_{Ni N_\ell}^0
\end{bmatrix}
\]

To solve Eqs. (18) and (19) we need to calculate spatial integration terms like \( \langle \partial_z X_k X_l \rangle_r \). Due to our use of finite volume method, the basis \( X_i \) is discontinuous and piecewise constant in space. We apply integration by parts and obtain

\[
\langle \partial_z X_k X_l \rangle_r = \left\langle \partial_z \left( \sum_{p} \sum_{q} Z_{pq} u_{pqk} \right) \sum_{p'} \sum_{q'} Z_{p'q'} u_{p'q'k} \right\rangle_r
\]

\[
= \sum_{p} \sum_{q} Z_{pq} u_{pqk} \left( \left\langle \partial_z Z_{p'q'} \sum_{p} \sum_{q} Z_{pq} u_{pqk} \right\rangle_r - \left\langle \partial_z Z_{p'q'} \sum_{p} \sum_{q} Z_{pq} u_{pqk} \right\rangle_r \right)
\]

\[
= \sum_{p} \sum_{q} \sum_{p'} \sum_{q'} Z_{pq} u_{pqk} \left( \left\langle u \right\rangle_{p,q+\frac{1}{2},k} - \left\langle u \right\rangle_{p,q-\frac{1}{2},k} \right)
\]

\[
\frac{2\Delta z}{2\Delta z}
\]

(20)

Here, \( \left\langle u \right\rangle_{p,q+\frac{1}{2},k} \) denotes the value at the cell boundary between the spatial cells \( p \) and \( p+1 \). We set the value at the cell boundary by the average of its left and right values, such as \( \left\langle u \right\rangle_{p,q+\frac{1}{2},k} = \frac{1}{2}(u_{p,q+1,k} + u_{p,q,k}) \).
For the angular terms, e.g., \( \langle \mu W_j W_{j'} \rangle_\Omega \), we can use write the integral as

\[
\langle \mu W_j W_{j'} \rangle_\Omega = \frac{1}{2\Delta z} \left( K_{p,q+1,j} - K_{p,q-1,j} \right) \langle \mu W_j W_i \rangle_\Omega \\
= \frac{1}{2\Delta z} \left( K_{p,q+1,j} - K_{p,q-1,j} \right) \left( V^T CV \right)_{jl} - \frac{1}{2\Delta z} \left( u_{p,q+1,i} - u_{p,q-1,i} \right) S_{ij} \left( V^T CV \right)_{jl} \\
= \frac{1}{\sqrt{\Delta z^2}} \sum_{i=1}^{N_x} \sum_{p=1}^{N_x} \sum_{q=1}^{N_x} \left( \frac{u_{p,q+1,i} - u_{p,q-1,i}}{2\Delta z} \right) S_{ij} \left( V^T CV \right)_{jl} \\
- \frac{1}{\sqrt{\Delta z^2}} \sum_{i=1}^{N_x} \sum_{p=1}^{N_x} \sum_{q=1}^{N_x} \left( \frac{u_{p,q+1,i} + u_{p,q-1,i} - 2u_{p,q,i}}{2\Delta z} \right) S_{ij} \left( V^T CV \right)_{jl}
\]

(22)

where \( \Sigma \) is a stabilization matrix that we take to be a diagonal matrix with the singular values of \( C \). Other stabilization terms could be used, including Lax-Friedrichs where \( V^T \Sigma V \) is replaced by a constant times an identity matrix. This method allows the spatial variables to be differentiated separately, so the same treatment can be applied to \( \partial_x K_i \langle \sqrt{1 - \cos \varphi^2} W_j W_i \rangle_\Omega \).
Additionally, the harmonic mean limiter is adopted to reconstruct this slope term $K_j$ for better accuracy. We define the slope of $z$ direction in the edge of the cell $(p,q)$ as

$$m_{p,q}^+ = \frac{K_{p,q,j} - K_{p,q-1,j}}{\Delta z}, \quad m_{p,q}^- = \frac{K_{p,q+1,j} - K_{p,q,j}}{\Delta z}.$$ 

Then the slope of this cell is

$$m_{p,q} = \begin{cases} 
2m_{p,q}^- m_{p,q}^+ & \text{if } m_{p,q}^+ m_{p,q}^- > 0 \\
0 & \text{otherwise}
\end{cases} \quad (23)$$

With the reconstructed slope

$$K_{p,q,j}^+ = K_{p,q,j} + \frac{\Delta z}{2} m_{p,q}, \quad K_{p,q,j}^- = K_{p,q,j} - \frac{\Delta z}{2} m_{p,q},$$

Eqs. (22) can be modified

$$\partial_z K_j \langle \mu W_j W_i \rangle_{\hat{\Omega}} = \frac{1}{\Delta z} (K_{p,q+\frac{1}{2},j} - K_{p,q-\frac{1}{2},j}) (\mu W_j W_i)_{\hat{\Omega}}$$

$$= \frac{1}{2\Delta z} \left( (K_{p,q+1,j}^+ + K_{p,q,j}^+ - K_{p,q-1,j}^- - K_{p,q,j}^-)(V^T CV)_{jl} \
- (K_{p,q+1,j}^- - K_{p,q,j}^- + K_{p,q,j}^+ + K_{p,q-1,j}^+)(V^T \Sigma V)_{jl} \right), \quad (24)$$

Spherical harmonics expansions can yield oscillatory or negative solutions [4]. To address this issue we implemented angular filtering [5, 28, 29] which can significantly increase the performance of $P_n$ method in solving radiative transfer equation by removing the oscillations. We implemented the Lanczos filter into our explicit solver by using an equivalent equation approach [29] and combined it with the low-rank approximation algorithm. The filtered equation has the form of

$$\frac{1}{c} \partial_t \psi(r, \hat{\Omega}, t) + \hat{\Omega} \cdot \nabla \psi(r, \hat{\Omega}, t) + \sigma_t(r) \psi(r, \hat{\Omega}, t) + \beta \sigma_f(r, \hat{\Omega}) \psi(r, \hat{\Omega}, t) = \frac{1}{4\pi} \sigma_s(r) \phi(r, t) + Q(r, t). \quad (25)$$

where the free parameter $\beta$ is the filter strength, $\sigma_t = \log \frac{\sin \frac{l}{\eta}}{l+1}$ and $\eta$ is the order of the $P_N$ expansion and $l$ is the index of $P_N$ moments.
3.3. Memory Reduction

The memory footprint required to compute the solution is based on storing the matrices $U$, $V$, and $S$. Therefore, the memory required is

$$\text{memory} = 2(mr + r^2 + nr),$$

where factor 2 assumes that we need to store the previous step solution as well as the new step. The full solution to this problem without splitting would require a memory footprint of $2mn$. Therefore, for $r \ll m, n$, there will be large memory savings.

3.4. Conservation

The low-rank algorithm we have described does not conserve the number of particles. This loss of conservation is a result of information lost in the algorithm when restricting the solution to low-rank descriptions. We have addressed this by globally scaling the solution after each time step to correct for any particles lost. We can do this because we know the number of particles that are absorbed, travel across the boundary, and born from sources. This correction will not preserve higher moments of the solution, and it only preserves the zeroth-order moment in space and angle. This issue has also been addressed in [30], where a correction term calculated by the imposed conservation law is added to each splitting step.

4. Numerical Results

We run the transport simulations with four test problems, including the plane source problem and Reed’s problem in 1D slab geometry in addition to the line source problem and lattice problem in 2D planar geometry. It should be noted that the full rank of the solution matrix only depends on the columns $n$ since the number of mesh zones $m$ is always larger than $n$, which is the number of angular basis functions. To find out the relations behind different low-rank cases, we fix the spatial resolution and vary the $n$ and the rank $r$ in the
following simulations. The CFL condition with the formula $CFL = \frac{\Delta t}{\Delta x}$ in 1D and $CFL = \min(\frac{\Delta t}{\Delta x}, \frac{\Delta t}{\Delta z})$ in 2D is set to 0.2. The conservation fix is applied to the plane and line source problems unless specified otherwise. Additionally, we used one simulation to demonstrate that the low-rank algorithm is compatible with the filter, other than that all the results are unfiltered. Our implementation is written in Matlab, and our particle speeds are set to $c = 1$.

(a) Low-rank solutions without scaling at $t=1$

(b) Low-rank solutions with scaling at $t=1$

Figure 1: Solutions to the plane source problem using the low rank method compared to the analytic solution. Numerical smearing errors are observed in both edges due to numerical dissipation [31]. More accurate results can be obtained with the fixed rank but higher $P_N$ order, which will be shown shortly.
Figure 2: Comparison of $P_7$ solutions of rank 4 with and without a filter to the analytic solution at $t=1$.

4.1. Plane source problem

The plane source problem describes a plane of isotropically moving particles emitted at $t=0$ in a purely scattering medium with no source, i.e., $\sigma_t = \sigma_s = 1$ and $Q = 0$. The only spatial variable in this slab geometry is $z$; the initial condition is given by a delta function as $\psi(z, \mu, t) = \delta(z)/2$. For the simulation parameters, we set the spatial resolution to be $\Delta z = 0.01$, which corresponds to the number of mesh zones $m = 300$ for the $t = 1$ solution and $m = 1200$ for $t = 5$. $P_{23}$ solutions with different rank are compared. When used, the filter strength $\beta$ is set to 50. The analytical benchmark solution that we compare to was given by Ganapol [32].

Figure 1 shows the solutions of varying rank and Legendre polynomial orders with and without the conservation fix where the zeroth moment is scaled. As can be seen in either case, the solution with rank 12, which is half of the full rank, matches the analytic solution to the scale of the graph in the middle part of the problem. It also agrees well with the full rank solution. The rank 8 solutions still capture the analytical solution well. However, the loss of conservation can be observed when the conservation fix is not applied. Rank 4 is not sufficient for accurate results and suffers more for the conservation lost. As shown in Figure 2, the low-rank solution can be improved by the filter: $P_7$ solutions of reduced...
rank improve when a filter is used. Figure 3 presents the solution at \( t = 5 \), at which even the rank 8 appears to be sufficient. At this later time, there are few remaining uncollided particles from the initial condition. Therefore, fewer angular degrees of freedom is needed.

For a more quantitative comparison, the root mean square (RMS) error of the numerical results with different \( n \) and \( r \) is shown in Figure 4. In this figure, the colors for the dotted lines correspond to the rank used in a calculation, and different values of the \( n \), the number of angular basis functions, are corresponding dots. For each color the value of \( n \) ranges from \( r \) to 100. The large points are the value of the error using the standard full rank method with \( r = n \). We can observe that the low-rank solution is more accurate than the full rank with the same memory usage. For example, the error of full rank solution \( n = 12 \) at \( t = 1 \) using with a memory footprint of 7200 is about 0.026. With the same memory, the error can be reduced to 0.013. We can also use 70% of the memory to achieve the same accuracy. Increasing the resolution and rank will contribute to the accuracy of solutions. Given the way we performed this study with a fixed spatial mesh and time step and the conservation fix we used, we can see some error stagnation in the low-rank solution at \( t = 5 \). Other numerical experiments indicate that increasing the number of spatial zones can further decrease the
4.2. Reed’s problem

The second test problem is Reed’s problem, which is a multi-material problem, and its set-up is detailed in Figure 5. Because Reed’s problem does not have an analytical solution, a numerical result with a high degree of angular basis and full rank, where $\Delta z = 0.01$ and $P_{99}$ (corresponding to $m = 1600$ and $n = 100$) is set as a benchmark for memory analysis. Figure 6 shows that the
rank 4 solutions differ in the vacuum regions \((z \in (3, 5)\) and \(z \in (11, 13)\)) and the scattering region with source \((z \in (2, 3)\) and \(z \in (13, 14)\)), but the rank 8 solution matches the \(P_{99}\) reference solution well.

It can be observed in Figure 6 that the low-rank solutions (solid lines with small dots) can give solutions with comparable errors to the full rank solutions (large dots) with much larger memory. For example, the rank 10 solutions obtain a solution error better than the full rank \(P_{19}\) solution with less memory.

4.3. Line source problem

The line source problem is a natural extension of the plane source problem to 2-D, where the plane source becomes a line. In this problem we have \(\sigma_t = \sigma_s = 1\), \(Q = 0\) and the initial condition \(\psi(x, z, \mu, \varphi, t) = \delta(x)\delta(z)\). We use a
computational domain of $[-1.5, 1.5] \times [-1.5, 1.5]$ for the simulation time $t = 1$, while the spatial grid is set to be $150 \times 150$.

The analytical solution from Ganapol [32] and the rank 210 solutions with $P_{19}$, $P_{29}$ and $P_{39}$ are shown in Figure 8 from which we can see that the $P_{15}$ solution which is full rank, has large oscillations. The results obtained with the same rank but more angular basis functions are much better, as we can see in Figure 8e where fixing the rank and increasing the expansion order improves the solution dramatically. Figure 9 demonstrates that increasing the angular resolution while fixing the rank improves the solution considerably.

Table 1: The quantitative comparison for the line source problem of memory footprints and errors with the same rank but different angular discretizations.

| Rank     | Memory | Error |
|----------|--------|-------|
| $P_9$    | 1625184| 0.2541|
| $P_{39}$ | 1681632| 0.0829|
| $P_{11}$ | 2487100| 0.1972|
| $P_{19}$ | 2571250| 0.0629|

In this figure, we note that the full rank $P_{15}$ solution has negative values, which are due to the oscillatory property of $P_N$ discretizations [4]. This non-
Figure 8: Solutions to the line source problem at $t = 1$ using rank 210 compared to the analytic solution.

A physical phenomenon can be alleviated by increasing the order of $P_N$ with low-rank approximation with only a modest increase in memory.

Figure 10 shows that memory saving is more significant in the 2D problem, where the number of spatial degrees of freedom is large. As we can see, the memory footprint is mostly dominated by rank. It indicates that the accuracy can be improved as we increase the $P_N$ order with few extra memory costs. For
Figure 9: Solutions to the line source problem at $t = 1$ using rank 136 compared to the analytic solution at the cut $z = 0$.

Figure 10: The comparison of errors for the line source problem with different memory usage are shown. Each dotted line represents the error with a fixed rank that varies the number of angular basis functions $n$. The bold dot denotes the full rank solution.

example, the error of the solution at rank 78 with the low-rank method is three times smaller than the full rank solution. It is also shown in Table 1 that only 3.4% extra memory is required for this accuracy increase. Alternatively, we can save 65% of the memory by adopting a low-rank solution at rank 78 rather than a full rank solution at rank 210.

4.4. Lattice problem

As described in Figure 11, the lattice problem is a $7 \times 7$ checkerboard with purely scattering zones $\sigma_t = \sigma_s = 1$, purely absorbing zones $\sigma_t = 10, \sigma_s = 0$, and...
Figure 11: The material layout in the Lattice problem. The blue zones are purely scattering region, the black are absorbing region and the yellow is also the scattering region with an isotropic source which is turned on at T= 0s. The checkerboard is surrounded by vacuum.

and an isotropic source at the center where $Q = 1$. In this problem, we use a spatial grid of size $210 \times 210$ for the computational domain $[0, 7] \times [0, 7]$.

Figure 12 shows that the solution with different rank agrees well to each other except the absorbing zones, where high-rank solutions such as rank 55 and 36 contain more details than the rank 21 and 10 solutions. Additionally, low-rank solutions converge to the full rank as we increase the rank, which leads to more memory usage. As we can see that even with 25% of the full rank memory the difference is still small.

5. Conclusion and Future Work

We have developed a practical algorithm to find the low-rank solution of the slab and planar geometry transport equation using explicit time integration. The method is based on projecting the equation to low-rank manifolds and numerically integrating with three steps. The numerical simulations show that on several test problems, the memory savings of the low-rank method can be on the order of a factor of 2-3. This study establishes a projection-based framework...
for the direct model decomposition of the radiation transport problems.

In future work will attempt to solve the conservation issues present in the low-rank method using a high-order low-order approach (such as quasi-diffusion), where the low-rank method is used only to create a closure. In this approach, the low-rank method is estimating a ratio of moments that should be insensitive to conservation issues. Furthermore, several research problems, including asymptotic preservation, the extension to energy-dependent transport equation should be explored, and other angular treatments, such as discrete ordinates.

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