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SOLUTION ALGORITHMS FOR A $P_{N-1}-$ EQUIVALENT S_N ANGULAR DISCRETIZATION OF THE TRANSPORT EQUATION IN ONE–DIMENSIONAL SPHERICAL COORDINATES

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ABSTRACT

Angular discretizations of the S_N transport equation in curvilinear coordinate systems may result in a streaming–plus–removal operator that is dense in the angular variable or that is not lower–triangular. We investigate numerical solution algorithms for such angular discretizations using relationships given by Chandrasekhar to compute the angular derivatives in the one–dimensional S_N transport equation in spherical coordinates with Gauss quadrature. This discretization makes the S_N transport equation $P_{N-1}-$ equivalent , but it also makes the sweep operator dense at every spatial point because the N angular derivatives are expressed in terms of the N angular fluxes. To avoid having to invert the sweep operator directly, we must work with the angular fluxes to solve the equations iteratively. We show how we can use approximations to the sweep operator to *precondition* the full $P_{N-1}-$ equivalent S_N equations. We show that these preconditioners affect the operator enough such that convergence of a Krylov iterative method improves.

Key Words: Spherical coordinates, discrete ordinates, transport methods, Krylov iterative methods

1. INTRODUCTION

It is possible that an angular discretization of the transport equation in curvilinear coordinate systems results in a streaming–plus–removal operator that is not lower–triangular, such that it cannot be inverted efficiently with a space–angle sweep. Our purpose is to define and test four variations of a solution algorithm specifically designed for such angular discretizations. In particular, we derive a set of $P_{N-1}-$ equivalent S_N equations using relationships given in [2] that express the angular derivatives at each quadrature point in terms of the angular fluxes at all the quadrature points. The result is that the angular–derivative matrix is dense in the number of quadrature points. It represents a worst–case for our proposed solution algorithms because direct solution of the sweep equations associated with the $P_{N-1}-$ equivalent S_N equations would require as much computational effort as it would for a direct solution of the full S_n equations. To avoid these high cost associated with directly inverting the sweep operator, it necessary to work with the angular fluxes rather than just the scalar fluxes when solving the problem

iteratively. While this is a drawback for problems with isotropic or mildly–anisotropic scattering because of the additional memory required, it is not for problems with highly anisotropic scattering.

We cast our solution algorithms as preconditioned Krylov iterative methods, with the expectation that Krylov methods will be significantly more efficient, and possibly more robust, than classical iterations. Each of the four preconditioners represents an approximation to the P_{N-1}– equivalent S_N sweep operator. The first and simplest preconditioner is obtained from the P_{N-1}– equivalent S_N sweep operator by neglecting that part of the discrete angular derivative operator corresponding to $(1-\mu^2)\dfrac{\partial\psi}{\partial\mu}$. This preconditioner consists of the slab–geometry sweep operator $\mu\dfrac{\partial\psi}{\partial r}+\sigma_t\psi$, which can be inverted efficiently. The second preconditioner is an approximate sweep operator obtained from the P_{N-1}– equivalent operator by neglecting the upper–triangular portion of the angular derivative matrix. Again, the inverse of this approximate sweep operator can be computed efficiently in one dimension because it is still lower triangular. The third preconditioner is the sweep operator obtained from a step discretization of the angular derivative term. The fourth is the sweep operator obtained from the WDD discretization for the angular derivative term. We show which of our preconditioners are candidates for further investigation by presenting convergence rates that are reasonable for some representative calculations. The important consideration of computational efficiency is not addressed presently.

2. P_{N-1}– EQUIVALENT S_N EQUATIONS

Using standard notation [3], with isotropic scattering and an isotropic distributed source, the one–dimensional transport equation in spherical coordinates is

$$\begin{gathered}\frac{\mu}{r^2}\frac{\partial(r^2\psi)}{\partial r}+\frac{1}{r}\frac{\partial}{\partial\mu}\left[\left(1-\mu^2\right)\psi\right]+\sigma_t(r)\psi(r,\mu)=\frac{\sigma_s(r)}{4\pi}\phi(r)+\frac{1}{4\pi}q(r),\\ \phi(r)=2\pi\int_{-1}^{1}\psi(r,\mu)\,d\mu.\end{gathered}\tag{1}$$

As shown in [2], it is possible to express derivatives of the angular flux $\psi'_m=\left.\dfrac{\partial\widetilde{\psi}}{\partial\mu}\right|_{\mu_m}$ in terms of the angular fluxes ψ_m through the following relationship

$$\int_{-1}^{1}Q_l(\mu)f'(\mu)d\mu=\int_{-1}^{1}P_l(\mu)f(\mu)d\mu,\tag{2a}$$

where

$$Q_l(\mu)=\frac{(1-\mu^2)}{l(l+1)}P'_l(\mu)\tag{2b}$$

and

$$\begin{gathered}Q'_l(\mu)=-P_l(\mu)\\ Q_l(\pm1)=0.\end{gathered}\tag{2c}$$

Using the S_N (Gauss) quadrature to express this relationship for $\psi(r)$

$$\sum_{m=1}^{N}w_mQ_l(\mu_m)\psi'_m(r)=\sum_{m=1}^{N}w_mP_l(\mu_m)\psi_m(r),\quad l=1,\ldots,N,\tag{3}$$

whcih gives an $(N \times N)$ operator that converts a vector of N discrete angular fluxes at position r to a vector of N derivatives at each of quadrature points. In other words,

$$\Psi'(r) = \mathbf{A}\Psi(r) \tag{4a}$$

where

$$\mathbf{A} = \mathbf{Q}^{-1}\mathbf{R} \tag{4b}$$

and

$$\begin{aligned} \mathbf{Q}_{i,j} &= Q_i(\mu_j)w_j \\ \mathbf{R}_{i,j} &= P_i(\mu_j)w_j. \end{aligned} \tag{4c}$$

Note that these relationships are valid only for Gauss quadratures because the integrands in (3) are polynomials of degree $2N-1$ for $l = N-1$, and the Gauss set is the only N–point set that is exact for polynomials of this degree. Also note that, as one would expect, the operator $\mathbf{A}$ is not invertible because the nodes of an N–point Gauss set are the roots of $P_N(\mu)$.

Because we can now represent the derivatives exactly (for a given quadrature) using (4a), it is easy to show that the following S_N equations are P_{N-1}– equivalent :

$$\begin{aligned} &\frac{\mu}{r^2}\frac{\partial(r^2\psi_m)}{\partial r} + \frac{1}{r}\left[\left(1-\mu_m^2\right)\sum_{m'=1}^{N}\mathbf{A}_{m,m'}\psi_{m'}(r) - 2\mu_m\psi_m(r)\right] \\ &+\sigma_t(r)\psi_m(r) - \sigma_s(r)\sum_{m'=1}^{N} w_{m'}\psi_{m'}(r) - q_m(r) = 0, \quad m = 1,\ldots,N. \end{aligned} \tag{5}$$

In vector form, (5) is

$$\mathbf{M}\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\Psi(r)\right) + \frac{1}{r}\left[\left(\mathbf{I}-\mathbf{M}^2\right)\mathbf{A} - 2\mathbf{M}\right]\Psi(r) + \sigma_t(r)\Psi(r) - \frac{\sigma_s(r)}{2}\mathbf{P}\Psi(r) - \frac{1}{2}q(r) = 0, \tag{6a}$$

where

$$\mathbf{P}_{i,j} = w_j,\ i = 1, N, \tag{6b}$$

$$\mathbf{M} = \underset{m=1,N}{\text{diag}}\ (\mu_m). \tag{6c}$$

3. NUMERICAL SOLUTION ALGORITHMS

Multiplying (6a) through by r^2, the P_{N-1}– equivalent S_N equations are written in matrix–vector form as

$$\left(\mathbf{L}_{\text{r}} + \mathbf{L}_{\text{a}} - \mathbf{S}\right)\overline{\psi} = \overline{q}, \tag{7}$$

where the operators have the following correspondence:

$$\mathbf{L}_{\text{r}}\overline{\psi} \rightarrow \mathbf{M}\frac{\partial}{\partial r}\left(r^2\Psi\right) + r^2\sigma_t(r)\Psi, \tag{8a}$$

$$\mathbf{L}_{\text{a}}\overline{\psi} \rightarrow r\left[\left(\mathbf{I}-\mathbf{M}^2\right)\mathbf{A} - 2\mathbf{M}\right]\Psi, \tag{8b}$$

$$\mathbf{S}\overline{\psi} \rightarrow r^2\frac{\sigma_s(r)}{2}\mathbf{P}\Psi, \tag{8c}$$

$$\overline{q} \rightarrow r^2\frac{1}{2}q. \tag{8d}$$

The operators are discretized in the space variable r using a linear–discontinuous spatial finite element method.

We can solve (7) with a Krylov method by multiplying through with the inverse of the full sweep operator and rearranging to find

$$\left[\mathbf{I} - \left(\mathbf{L}_{\mathrm{r}} + \mathbf{L}_{\mathrm{a}}\right)^{-1}\mathbf{S}\right]\overline{\psi} = \left(\mathbf{L}_{\mathrm{r}} + \mathbf{L}_{\mathrm{a}}\right)^{-1}\overline{q}. \tag{9}$$

This has the advantage that it can be written in terms of the scalar fluxes. However, a direct solution method is needed to compute compute the inverse, which would be as costly as directly inverting the full transport equation itself. Instead, we precondition (7) with approximations to the inverse of the sweep operator, $\widetilde{\mathbf{L}}^{-1}$, chosen with the understanding that they can be computed efficiently. The first approximate sweep preconditioner is obtained from (7) by neglecting the terms arising out of the angular derivatives in the $\mathrm{P}_{N-1}-$ equivalent S_N sweep operator, that is,

$$\widetilde{\mathbf{L}}^{-1} = \mathbf{L}_{\mathrm{r}}^{-1}. \tag{10}$$

With this preconditioner, the linear system that is solved iteratively is

$$\left[\mathbf{I} - \mathbf{L}_{\mathrm{r}}^{-1}\left(\mathbf{S} - \mathbf{L}_{\mathrm{a}}\right)\right]\overline{\psi} = \mathbf{L}_{\mathrm{r}}^{-1}\overline{q}, \tag{11}$$

The action of this operator on a vector can be computed efficiently with the standard S_N sweep algorithm because the preconditioner is lower triangular. The second preconditioner splits the angular derivative operator, $\mathbf{L}_{\mathrm{a}}$, into lower and upper triangular parts, $\mathbf{L}_{\mathrm{a}} = \mathbf{L}_{\mathrm{a}}^{\mathsf{L}} + \mathbf{L}_{\mathrm{a}}^{\mathsf{U}}$, and takes the approximate sweep operator to be

$$\widetilde{\mathbf{L}}^{-1} = \left(\mathbf{L}_{\mathrm{r}} + \mathbf{L}_{\mathrm{a}}^{\mathsf{L}}\right)^{-1}. \tag{12}$$

Substituting into (7) gives

$$\left[\mathbf{I} - \left(\mathbf{L}_{\mathrm{r}} + \mathbf{L}_{\mathrm{a}}^{\mathsf{L}}\right)^{-1}\left(\mathbf{S} - \mathbf{L}_{\mathrm{a}}^{\mathsf{U}}\right)\right]\overline{\psi} = \left(\mathbf{L}_{\mathrm{r}} + \mathbf{L}_{\mathrm{a}}^{\mathsf{L}}\right)^{-1}\overline{q}, \tag{13}$$

which may be solved iteratively. Again, computing the action of the operator with this preconditioner can be done efficiently because it is lower triangular.

The other two approximate sweep preconditioners corresponds to the sweep operator for the step and WDD angular discretization [1, 4], denoted by $\mathbf{L}_{\mathrm{STEP}}$ and $\mathbf{L}_{\mathrm{WDD}}$, respectively, with the same LD spatial discretization used for the $\mathrm{P}_{N-1}-$ equivalent S_N equations. Some extra care is required for the WDD preconditioner because the rank of the WDD angular discretization is $N+1$ while the rank of the $\mathrm{P}_{N-1}-$ equivalent S_N discretization is N. This is because the WDD discretization has an addition unknown in the form of the starting–direction flux. One way to make the ranks for the two discretizations the same is to simply add the WDD equation for the starting–direction flux to the $\mathrm{P}_{N-1}-$ equivalent S_N equations. This does not alter the $\mathrm{P}_{N-1}-$ equivalent S_N solution for the fluxes at the Gauss points, but it makes the rank of the modified system $N+1$. Another way would be to determine a projection from the N angular fluxes of the $\mathrm{P}_{N-1}-$ equivalent equations to the $N+1$ fluxes of the WDD equations along with a corresponding interpolation.

COMPUTATIONAL RESULTS

In this section, we will present a very limited set of measurements of convergence of the various preconditioners. A study of the numerical properties of all the algorithms and an investigation into the computational efficiencies of the implementation will be forthcoming.

We have implemented the fully discrete linear systems for homogeneous material properties, equal mesh spacing, and isotropic scattering in MATLAB. The data used for the first set of examples are $r_{\max} = 10$ cm, $N_{\text{cells}} = 128$, $\sigma_t = 10$ cm^{-1}, $\sigma_s = 9.999$ cm^{-1}, and $N = 8$ Gauss quadrature. We note that we observed the operators to be nonsymmetric, non–normal and, in general, not positive–definite, meaning we must use a Krylov iterative method suitable for nonsymmetric operators. The number of matvecs correspond to the number iterations for GMRES(m), but BiCGStab requires the application of the operator twice per iteration, so that the convergence history as a function of the number of matvecs allows for a fair comparison of computational effort. The WDD preconditioner was implemented by writing the WDD S_N equations in terms of the cell–edge angular fluxes and using a projection and interpolation from the angular cell–edges to the the angular cell midpoints, rather than by augmenting the the P_{N-1}–equivalent S_N equations with the starting direction angular flux equation as previously discussed. Projection from the angular cell–edge fluxes to the cell midpoints is just the WDD relation and represented by the operator $\mathbf{W}$ and the simplest approach would be to use to be the transpose of the projection operator, $\mathbf{W}^T$ for interpolation. It was expedient to do it this way in our MATLAB implementation, and it provides a baseline for comparison with a computer code implementation, where the WDD equations would not be written in terms of the angular cell–edge values and the augmented approach would be preferred.

Table I. Number of matvecs for convergence to relative residual 10^{-6} for $\mathbf{A} = \mathbf{L}_{\text{r}} + \mathbf{L}_{\text{a}} - \mathbf{MSD}$.

Method	Preconditioner				
	None	$\mathbf{L}_{\text{r}}^{-1}$	$(\mathbf{L}_{\text{r}} + \mathbf{L}_{\text{a}}^{\text{L}})^{-1}$	$\mathbf{W}\mathbf{L}_{\text{WDD}}^{-1}\mathbf{W}^T$	$\mathbf{L}_{\text{STEP}}^{-1}$
GMRES(20)	84688	6160	816	$\star$[a]	962
GMRES(30)	56189	2070	565	5765	842
GMRES(40)	61755	1041	280	4198	588
GMRES(50)	48488	993	248	3632	527
GMRES(60)	50503	713	235	2761	465
GMRES(70)	46986	743	203	2517	521
GMRES(80)	44538	621	145	3033	331
GMRES(90)	45180	621	174	2147	336
GMRES(100)	42979	476	170	2584	175
Full GMRES	1024	133	113	399	113
BiCGStab	17494	504	658	$\diamond$[b]	234

[a] Stagnated
[b] Diverged

Results are shown in Table I. It appears that an impractically large restart parameter is required to achieve a reasonable convergence rate given that we are working with the angular flux vectors. Because the operators are not positive definite, restarted GMRES can stagnate. Together with the fact that BiCGStab converges slowly (and can also stagnate or diverge), it is apparent that these solution algorithms need further preconditioning, ideally one which would make the operators positive definite, symmetric, or both, for a

range of problem parameters or in general. Nonetheless, the step–differencing preconditioner appears to be reasonably effective, it can be implemented efficiently, and does not need a starting–direction calculation. An augmented approach to using the WDD preconditioner may change the results presented. In any case, the effect on convergence is enough to warrant further investigation of these solution algorithms, including investigating computational efficiency and alternative angular discretizations of the transport equation in higher–dimensional curvilinear coordinates.

Closing Remarks

We have seen that specific approximation to the transport equation for the angular flux preconditioned by several possible specific approximations to the streaming–plus–removal operator. This could be a useful technique anytime the action of $\mathbf{L}^{-1}$ on a vector is difficult to compute, such as in the application we presented here. But it could also be considered a general approach to solving the transport equation. To follow this idea a bit further, consider the transport equation without reference to any particular coordinate system or any spatial or angular discretization, and which may include energy dependence,

$$(\mathbf{L} - \mathbf{S})\,\psi = q. \tag{14}$$

The operator $\mathbf{L}$ corresponds to a streaming–plus–removal operator and $\mathbf{S}$ corresponds to a redistribution operator, which could redistribution in energy, such as a fission operator. We speculate that *any* reasonable approximation to $\mathbf{L}^{-1}$ could be used to precondition (14), perhaps even one developed from a completely different transport model. An exotic example might be one in which (14) corresponds to a P_N angular approximation with discontinuous finite element spatial discretization. The approximate sweep operator inverse could be applied with a monte carlo method, a low–order S_N discretization or an incomplete LU decomposition of $\mathbf{L}$ itself. In any case, the goal is to choose an approximation whose inverse, or whose action on a vector, can be computed efficiently and whose effect on the spectrum of (14) is such that the convergence rate improves to point where the overall efficiency of a Krylov iterative method solution is acceptable. There are obviously myriad possibilities; whether there are specific combinations that are computationally feasible is an open and interesting question.

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