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Angular Dependent Rebalance Factor Method for Solving the S_N Transport Equations in $X-Y$ Geometry

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Abstract

The angular dependent rebalance (ADR) factor method is extended to the two-dimensional neutron transport problems and applied to acceleration of three nodal transport methods (i.e., constant-linear (C-L), simplified linear-discontinuous (SLD), and bilinear discontinuous (BLD)) and three non-nodal spatial differencing schemes (i.e., step scheme (SS), step characteristic (SC), and constant-constant (C-C)) where the spatial distributions of the angular flux are assumed to be flat in mesh interior and mesh edges. In ADR, the rebalance factor is defined as the ratio of the angular fluxes of the same phase point in two iterates and it is angular dependent. In this paper, the S_2 approximation for the angular dependency of the rebalance factor is used. The resulting S_2-like lower-order equation is solved by three iterative methods (four-cyclic (FC), conjugate gradient (CG), and bi-conjugate gradient stabilized (Bi-CGSTAB) methods). The numerical tests show that the ADR method can be used effectively for all tested transport methods.

1. Introduction

To reduce the computational burden of multidimensional neutron transport calculations, a number of coarse-mesh nodal spatial differencing schemes have been devised for solving the transport equations. As with the discrete ordinates approximation of angular variable, the nodal transport methods requires the use of an iterative scheme for evaluation of the scattering source term. Since the convergence of this scattering source iteration is extremely slow for optically thick systems characterized by the scattering ratio close to unity, an acceleration scheme must be used to speed up the convergence of the iteration procedure. The lack of an acceleration technique has limited the usefulness of nodal S_N methods. Therefore, acceleration of the convergence of nodal transport methods has received increased attention recently. In the area of acceleration of the nodal transport methods, to our knowlege, three methods are most effective. The first is Khalil's approach[1] in which the lower-order equation (diffusion model) is derived from the spatially continuous diffusion equation by applying spatial approximations that are P_1 expansions of the corresponding approximations made in solving the transport equation. He applied successfully the method to C-L nodal transport method[2] in $X-Y$ gemometry problems. The second is the boundary projection approach developed by Lawrence[3] and by Adams[4], independently. Lawrence successfully applied his double-P_0 acceleration to several nodal transport methods in one, two, and three dimensions.

The third is the transport synthetic acceleration (TSA) method[5] developed by Ramone and Adams. It avoids the "consistent differencing" issue because the lower-order equation can be discretized exactly like higher-order transport equation.

In this paper, the ADR method[6,7,8] is extended to the discrete ordinates transport equations in $X-Y$ geometry. The ADR method was first derived with DP_N expansion of the rebalance factor for the generally discretized transport equations in slab geometry. Since the ADR method uses the projected transport equation onto a coarse angular space with angular dependent rebalance factor as the lower-order equation, the ADR method avoids "consistent differencing" and the extension to any transport method in various geometries is very easy. At present, the S_2 approximation for the angular dependency of the rebalance factor is tested in $X-Y$ geometry. The S_2-like lower-order equation obtained by integrating the rebalance equation over each octant is solved by the conjugate gradient (CG) method[9] for symmetric lower-order operator, by the bi-conjugate gradient stabilized (Bi-CGSTAB) method[9] for unsymmetric lower-order operator. For comparison, the lower-order equation is also solved by the four-cyclic iterative method for all spatial differencing schemes.

2. Theory and Methodology

2.1. Derivation of the Lower-Order Equation

To describe the ADR method in $X-Y$ geometry, the general discretized form of the nodal transport methods is written in the following vector form for mesh i,j :

$$\begin{aligned}\vec{\psi}_{i,j,m}^{out,l+1/2} &= \mathbf{A}_{i,j,m}\vec{\psi}_{i,j,m}^{in,l+1/2} + \mathbf{B}_{i,j,m}(\sigma_{s,i,j}\vec{\phi}_{i,j}^{l} + \vec{s}_{i,j}),\\ \vec{\psi}_{i,j,m}^{l+1/2} &= \mathbf{C}_{i,j,m}\vec{\psi}_{i,j,m}^{in,l+1/2} + \mathbf{D}_{i,j,m}(\sigma_{s,i,j}\vec{\phi}_{i,j}^{l} + \vec{s}_{i,j}),\end{aligned} \tag{1}$$

where $\vec{\psi}_{i,j,m}^{out}$ includes the outgoing angular flux moments, $\vec{\psi}_{i,j,m}^{in}$ incoming angular flux moments, $\vec{\psi}_{i,j,m}$ interior angular flux moments, $\vec{\phi}_{i,j}$ interior scalar flux moments, and $\vec{s}_{i,j}$ interior inhomogeneous source moments. From now on, the indices i,j are omitted for simplicity. The next step is introduction of a nonlinear rebalance factor. The factor is the ratio of the new flux iterate to the previous iterate in the same phase point. Similarly to the one-dimensional case, it is anticipated that the new iterate satisfies the balance equation and the rebalance factor becomes unity on convergence. The S_2 approximation for the rebalance factor is given by

$$f_{\gamma,p}^{out\ or\ in}(\mu,\eta) = \frac{\psi_p^{out\ or\ in,l+1}(\mu,\eta)}{\psi_p^{out\ or\ in,l+1/2}(\mu,\eta)} = \begin{cases} f_{\gamma,p}^{out\ or\ in} & ,\Omega(\mu,\eta) \in \ octant\ \gamma \\ 0 & ,\ otherwise, \end{cases} \tag{2}$$

where the index p represents a component of the vector. If all iteration indices in Eq.(1) are changed to $l+1$ and Eq.(2) is substituted into the equation, the following equation is obtained :

$$\begin{aligned} f_{\gamma,p}^{out}\psi_{m,p}^{out,l+1/2} &= \sum_q A_{m,p,q} f_{\gamma,q}^{in}\psi_{m,q}^{in,l+1/2} + \sum_q B_{m,p,q}(\sigma_s\phi_q^{l+1} + s_q),\\ \psi_{m,p}^{l+1} &= \sum_q C_{m,p,q} f_{\gamma,q}^{in}\psi_{m,q}^{in,l+1/2} + \sum_q D_{m,p,q}(\sigma_s\phi_q^{l+1} + s_q),\end{aligned} \tag{3}$$

where q is the dummy index representing a component of the vector.

To obtain a lower-order equation, Eq.(3) is first multiplied by weighting functions $g_x(\mu,\eta)$ for x-direction edge and $g_y(\mu,\eta)$ for y-direction edge, respectively. In this paper, $g_x(\mu,\eta)=\mu$ and $g_y(\mu,\eta)=\eta$ are used. Then, the equation is integrated for angular variables over each octant. The resulting equation can be written in the following vector form :

$$\begin{aligned}\vec{f}_\gamma^{out} &= \mathbf{U}_\gamma \vec{f}_\gamma^{in} + \mathbf{V}_\gamma(\sigma_s\vec{\phi}^{l+1}+\vec{s}),\\ \vec{\phi}_\gamma^{l+1} &= \mathbf{X}_\gamma \vec{f}_\gamma^{in} + \mathbf{Y}_\gamma(\sigma_s\vec{\phi}^{l+1}+\vec{s}),\ \gamma=1,2,3,4,\end{aligned} \tag{4}$$

where

$$U_{\gamma,p,q} = \frac{\sum_{m\in\ octant\ \gamma} w_m g(\mu_m,\eta_m) A_{m,p,q}\psi_{m,q}^{in,l+l/2}}{\sum_{m\in\ octant\ \gamma} w_m g(\mu_m,\eta_m)\psi_{m,p}^{out,l+1/2}}, \tag{5}$$

$$V_{\gamma,p,q} = \frac{\sum_{m\in\ octant\ \gamma} w_m g(\mu_m,\eta_m) B_{m,p,q}}{\sum_{m\in\ octant\ \gamma} w_m g(\mu_m,\eta_m)\psi_{m,p}^{out,l+1/2}}, \tag{6}$$

$$\begin{aligned}X_{\gamma,p,q} &= \sum_{m\in\ octant\ \gamma} w_m C_{m,p,q}\psi_{m,q}^{in,l+1/2},\\ Y_{\gamma,p,q} &= \sum_{m\in\ octant\ \gamma} w_m D_{m,p,q},\end{aligned} \tag{7}$$

and

$$\vec{\phi}^{l+1} = \sum_{\gamma=1}^{4}\vec{\phi}_\gamma. \tag{8}$$

Eq.(1) and Eq.(4) compose the ADR method for general nodal S_N transport method. The lower-order equation (i.e., Eq.(4) resembles the S_2 equation and is difficult to solve by direct inversion.

2.2. Conjugate Gradient Method and Bi-CGSTAB Method for ADR

Since the lower-order equation of the ADR method resembles the S_2 equation, the convergence of the scattering source iteration (SI) for solving the lower-order equation can be extremely slow for highly scattering dominant problems. More efficient method than the scattering source iteration method is the four-cyclic iterative scheme[6,7] with an optimal estimate of overrelaxation factor. However, this method is also slow for highly scattering dominant problems. Therefore, we proposes the conjugate gradient method for symmetric positive definite lower-order operator (e.g., DD, SS, and SC) and the Bi-CGSTAB method for nonsymmetric lower-order operator. In general, the lower-order operators of the nodal transport methods are not symmetric. To apply the Krylov subspace methods, the lower-order equations must be rewritten as a linear operator form. The lower-order operator ($\mathbf{M_{lower}}$)is defined as

$$\begin{aligned}(\mathbf{I}-\mathbf{M})\vec{\phi} &= \mathbf{M}_s\vec{s},\\ \mathbf{M}_{lower} &= \mathbf{M}_s^{-1}(\mathbf{I}-\mathbf{M}).\end{aligned} \tag{9}$$

and rewritten as

$$\begin{aligned} \mathbf{T}\vec{\phi} &= \vec{b}, \\ \mathbf{T} &= \mathbf{I} - \mathbf{M}, \\ \vec{b} &= \mathbf{M_s}\vec{s}. \end{aligned} \tag{10}$$

In Eq.(9), the linear operator $\mathbf{M}$ representing sweeping with the scattering source is given by

$$\begin{aligned} \vec{f}_\gamma^{out} &= \mathbf{U}_\gamma \vec{f}_\gamma^{in} + \mathbf{V}_\gamma(\sigma_s\vec{x}), \\ \vec{x}_\gamma &= \mathbf{X}_\gamma \vec{f}_\gamma^{in} + \mathbf{Y}_\gamma(\sigma_s\vec{x}), \ \gamma = 1,2,3,4, \\ \mathbf{M}\vec{x} &= \sum_{\gamma=1}^{4} \vec{x}_\gamma, \end{aligned} \tag{11}$$

and the linear operator $\mathbf{M_s}$ represents sweeping with the inhomogeneous source. The conjugate gradient method for the lower-order equation (i.e., Eq.(10)) of the ADR method is described by

$$\begin{aligned} &\text{Step 1}: && k = 0, \\ &\text{Step 2}: && \vec{r}^{(0)} = \vec{d}^{(0)} = \vec{b} - \mathbf{T}\phi^{(0)}, \\ &\text{Step 3}: && \alpha = \frac{< \vec{r}^{(k)}, \vec{r}^{(k)} >}{< \vec{d}^{(k)}, \mathbf{T}\vec{d}^{(k)} >}, \\ &\text{Step 4}: && \vec{\phi}^{(k+1)} = \vec{\phi}^{(k)} + \alpha\vec{d}^{(k)}, \\ &\text{Step 5}: && \textit{Check Convergence}, \\ &\text{Step 6}: && r^{(k+1)} = r^{(k)} + \alpha\mathbf{T}\vec{d}^{(k)}, \\ &\text{Step 7}: && \beta = \frac{< \vec{r}^{(k+1)}, \vec{r}^{(k+1)} >}{< \vec{r}^{(k)}, \vec{r}^{(k)} >}, \\ &\text{Step 8}: && d^{(k+1)} = r^{(k+1)} + \beta\vec{d}^{(k)}, \\ &\text{Step 9}: && k = k + 1, \\ &\text{Step 10}: && \textit{Go To } 2. \end{aligned}$$

In the above procedure, for symmetry of the lower-order operator, the inner product represented by $< \cdot >$ must be defined by

$$< \vec{u}, \vec{v} >= \sum_{ij} \sigma_{s,i,j} u_{i,j} v_{i,j} h_i^x h_j^y, \tag{12}$$

where i represents x-direction mesh index, j y-drection mesh index, h_i^x the x-direction mesh size, and h_j^y the y-direction mesh size. The Bi-CGSTAB method for nonsymmetric lower-order

operator are described by

Step 1 : $k = 0$,

Step 2 : $\vec{r}^{(0)} = \vec{b} - \mathbf{T}\vec{\phi}^{(0)}$,

$and\ \rho^{(0)} = \alpha = \omega^{(0)},\ \vec{v} = \vec{p} = 0,\ \rho^{(1)} = < \vec{r}^{(0)}, \vec{r}^{(0)} >$,

Step 3 : $k = k + 1$,

Step 4 : $\beta = \dfrac{\rho^{(k)}\alpha}{\rho^{(k-1)}\omega}$,

Step 5 : $\vec{p} = \vec{r}^{(k-1)} + \beta(\vec{p} - \omega\vec{v})$,

Step 6 : $\vec{v} = \mathbf{T}\vec{p}$,

Step 7 : $\alpha = \dfrac{\rho^{(k)}}{< \vec{r}^{(0)}, \vec{v} >}$,

Step 8 : $\vec{s} = \vec{r}^{(k-1)} - \alpha\vec{v},\ \vec{t} = \mathbf{T}\vec{s}$,

Step 9 : $\omega = \dfrac{< \vec{t}, \vec{s} >}{< \vec{t}, \vec{t} >},\ \rho^{(k+1)} = -\omega < \vec{r}^{(0)}, \vec{t} >$,

Step 10 : $\vec{\phi}^{(k)} = \vec{\phi}^{(k-1)} + \alpha\vec{p} + \omega\vec{s}$,

Step 11 : *Check Convergence*,

Step 12 : $\vec{r}^{(k)} = \vec{s} - \omega\vec{t}$,

Step 13 : *Go To* 3.

In the above procedure, the inner product represented by $< \cdot >$ must be defined by

$$< \vec{u}, \vec{v} >= \sum_{ij} u_{i,j} v_{i,j} \tag{13}$$

At present, any preconditioning is not applied to the CG method and to the Bi-CGSTAB method. For CG and Bi-CGSTAB, the initial guess is the resulting flux ($\psi^{l+1/2}$) of the higher-order transport calculation.

3. Numerical Analysis and Results

For verification of the ADR method, the ADR method was applied to two benchmark problems and numerically analyzed. In all calculations, a pointwise relative maximum error is used as a stopping criterion of the iteration and the uniform distribution is used as the initial guess. Although the estimations of the spectral radius and the number of iterations are important in a view of theoretical aspect, the estimation of effectiveness is not practical if the lower-order equation is not solved effectively. In this paper, the effectiveness of the ADR method is estimated in terms of the number of iterations and the speedup of the computing time with respect to the scattering source iteration (SI) method.

3.1. Two-Dimensional Version of McCoy-Larsen Problem

The first problem is a two-dimensional version of McCoy-Larsen problem (benchmark problem I) that consists of a uniform, isotropically scattering $8cm \times 8cm$ rectangular box, with a scattering ratio c of 0.98, two reflecting boundaries at the left edge and at the bottom

edge, and two vacuum boundaries at the right edge and at the top edge. The problem is divided into 8×8 meshes and the total cross section σ is variable (i.e., $0.01 \leq \sigma \leq 6.0$). The uniform source is distributed in the left-bottom region. In Table 1, the number of iterations required to achieve a pointwise relative maximum error of 10^{-4} in the scalar flux is given. In this calculation, S_8 angular quadrature set is used for the ADR method and the uniform distribution of scalar flux is used as an initial guess. However, the other methods except the ADR method used the solution of the diffusion equation as an initial guess. The results in Table 1 show that ADR gives nearly the same number of iterations as the interface-current synthetic acceleration (ICSA)[3] and the interface-current diffusion-synthetic acceleration (ICDSA)[1,3] for C-L nodal transport method, and gives significant reduction in the number of iterations for C-L, BLD, and SLD in comparison with SI.

To test ADR for more scattering dominant problems, the scattering ratio (c) is increased to 0.999. Table 2 shows the number of iterations required to achieve a pointwise relative maximum error of 10^{-4} and the speedup with Bi-CGSTAB for solving the lower-order equation for this problem. The term "speedup" means the computing time ratio of ADR to SI. In Table 2, the speedup of ADR increases rapidly as the total cross section increases (i.e., as the mesh size increases) and the speedup is significant. This aspect makes the ADR method very effective as the acceleration of the nodal S_N transport methods.

Table 1: Comparison of the number of iterations for benchmark problem I

σ	C-L				BLD		SLB	
	ICSA	ICDSA	ADR	SI	ADR	SI	ADR	SI
0.01			4	7	4	7	4	7
0.1			5	23	7	23	5	23
1.0	4	5	4	215	5	215	4	215
2.0	4	4	4	354	5	355	4	353
4.0	4	4	4	520	5	528	4	519
6.0	4	4	4	648	5	677	4	646

Table 2: Comparison of the speedup for benchmark problem I ($c = 0.999$, Bi-CGSTAB)

σ	CL	BLD	SLD
	ADR(S_8)	ADR(S_8)	ADR(S_8)
1.0	30.6(4[a],326[b])	26.3(4,326)	27.0(4,326)
2.0	58.2(4,775)	54.2(4,775)	55.2(4,775)
4.0	93.6(4,1521)	104.6(4,1525)	93.6(4,1521)
6.0	170.3(2,2162)	144.0(4,2172)	125.9(4,2162)

[a]Number of iterations with ADR, [b]Number of iterations with SI

Next, to compare the speedups of CG and four-cyclic iteration methods, the ADR method is applied to three non-nodal transport methods (i.e., SS, SC, C-C) where the lower-order operator is symmetric. The speedup and number of iterations required to achieve a pointwise

maximum relative error of 10^{-5} are given in Table 3. The results show that the ADR method with CG is very effective in comparison with SI.

Table 3: Comparison of the iterations and speedup for SS, SC and C-C

σ	SS		SC		C-C	
	CG	FC	CG	FC	CG	FC
1.0	22.3(4,204)	8.4(4)	22.0(4,268)	11.0(4)	18.6(5,282)	10.3(5)
2.0	39.5(4,479)	12.2(4)	50.8(4,618)	16.9(4)	53.0(4,645)	16.3(4)
4.0	104.3(3,948)	20.9(3)	93.0(4,1134)	23.3(4)	126.3(4,1155)	21.1(4)
6.0	145.0(3,1311)	24.2(3)	163.0(3,1488)	27.2(3)	164.3(3,1502)	27.4(3)

3.2. The Iron-Water Benchmark Problem

The effectiveness of the ADR method is tested for a realistic situation. For this purpose, the iron-water benchmark problem (benchmark problem II)[1] is chosen. This is a diagonally symmetric, isotropically scattering, two-dimensional model shielding problem. This problem is solved using S_8 angular quadrature set and 20×20 mesh division and with a convergence criterion of 10^{-5}. The results for three non-nodal methods are given in Table 4. The results in Table 4 show that the ADR method with CG are very effective in comparison with SI. The results for nodal methods with Bi-CGSTAB are given in Table 5. The speedup is nearly 60 for all tested nodal S_N methods and the number of iterations is very significantly reduced in comparison with that of SI.

Table 4: Comparison of the iterations and speedup for SS, SC and C-C

items	SS(948[a],172.1[b])		SC(1143,207.4)		C-C(1171,211.4)	
	CG	FC	CG	FC	CG	FC
Number of iterations	4	4	4	4	4	4
Computing time (sec)	3.2	10.5	3.8	12.0	3.8	12.1
Speedup	53.8	16.4	54.6	17.3	55.6	17.5

[a]Number of iterations with SI

[b]Computing time with SI on ULTRA SUN 1 computer

Table 5: Comparison of the speedup for benchmark problem II

items	CL		SLD		BLD	
	ADR	SI	ADR	SI	ADR	SI
Number of iterations	6	2089	6	2103	6	2406
Computing time (sec)	30.9	1833.2	32.0	1845.5	135.6	8269.6
Speedup	59.3	1.0	57.7	1.0	60.9	1.0

4. Conclusions

The ADR method was successfully extended to the two-dimensional discrete ordinates transport equations and applied to acceleration of three nodal transport methods (C-L, SLD, and BLD) and three non-nodal spatial differencing schemes (SS, C-C, SC). To derive the lower-order equation of the ADR method, the angular dependency of the rebalance factor was approximated by S_2 unlike DP_N approximation for one-dimensional case. The resulting lower-order equation looks like S_2 transport equation. The lower-order equation was solved by the four-cyclic, CG, and Bi-CGSTAB methods. The numerical tests show that the ADR method can be used effectively for the discrete-ordinates transport equations in $X-Y$ geometry.

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