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# A New Acceleration Method of Additive Angular Dependent Rebalance with Extrapolation for Discrete Ordinates Transport Equation

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# Abstract

A new extrapolation method is developed and applied to the additive angular dependent rebalance (AADR) acceleration for discrete ordinates neutron transport calculations. With this extrapolation, the convergence of AADR solution for distinct discretizations between the high-order and low-order equations is remarkably improved and thus the "inconsistent discretization problem" is resolved. Fourier analysis is also performed to find the optimal extrapolation and weighting parameters, which give the smallest spectral radius. The numerical tests demonstrate that the AADR with extrapolation works well as predicted by the Fourier analysis.

# 1. Introduction

It has been known that linear acceleration methods, for convergence, require the low-order preconditioning equation to be discretized consistently with the discretization of the high-order transport sweep [1]. On the other hand, nonlinear methods do not, for rapid convergence, require the low-order equation to be discretized consistently with the high-order equation.

To avoid the above consistency requirement, an extrapolation concept is considered for the additive angular dependent rebalance (AADR) method [2][3][4] which is a linear form of ADR [5][6]. An extrapolation concept was used in the diffusion synthetic acceleration (DSA) method by Miller and Larsen [7]. But, a different extrapolation is considered in this study. The new extrapolation applied to AADR affects the convergence of the solution drastically and it provides stability with better performance of AADR with inconsistent discretization.

Fourier analyses as well as numerical tests for various cases are performed and the optimal parameters, which give the smallest spectral radius, are also found from Fourier analysis.

In Section 2, the basic equations of AADR are derived and their Fourier analyses are performed. Section 3 shows the derivation of inconsistent discretization of AADR with several

cases of spatial difference schemes. The numerical tests and results are given in Section 4, and finally, Section 5 provides conclusions.

#### 2. Derivation of AADR with Extrapolation

Basic equations of the additive angular dependent rebalance (AADR) with DP<sub>0</sub>-like rebalance will be given as follows. The high-order equation, which provides angular flux ( $\psi^{l+1/2}$ ), is given as

$$\mu \frac{d\psi^{l+1/2}}{dx} + \sigma \psi^{l+1/2} = \sigma_s \phi^l + q(x),$$
(1)

where *l* is an iteration index. The scalar flux  $(\phi^{l+1/2})$  is obtained by integrating angular flux over angular domain:

$$\phi^{l+1/2} = \frac{1}{2} \int_{-1}^{1} \psi^{l+1/2} d\mu.$$
(2)

The low-order equation, which gives the rebalance factors (  $f_{\pm}^{l+1}$  ), are derived as

$$k \frac{df_{+}^{l+1}}{dx} + \sigma f_{+}^{l+1/2} = \sigma_{s}(\phi^{l+1} - \phi^{l}), \quad \mu > 0,$$
(3)

$$-k \ \frac{df_{-}^{l+1}}{dx} + \sigma \ f_{-}^{l+1/2} = \sigma_s(\phi^{l+1} - \phi^l), \quad \mu < 0, \tag{4}$$

where k is a weighting parameter which is defined as

$$k = \int_{0}^{1} \mu W(\mu) d\mu \Big/ \int_{0}^{1} W(\mu) d\mu \,, \tag{5}$$

and  $W(\mu)$  is a weighting function. Finally, the scalar flux is updated with the previous scalar flux which is the result of the high-order equation and rebalance factors which are the solution of low-order equation:

$$\phi^{l+1} = \phi^{l+1/2} + \frac{f_+^{l+1} + f_-^{l+1}}{2}.$$
(6)

The optimal weighting parameter can be found from Fourier analysis.

An extrapolation concept for AADR is first considered with scalar flux  $\phi^{l+1}$ . We may modify Eq.(6) as

$$\phi^{l+1} = \alpha(\phi^{l+1/2} + \frac{f_{+}^{l+1} + f_{-}^{l+1}}{2}) + (1 - \alpha)\phi^{l}, \qquad (7)$$

where  $\alpha$  is an extrapolation parameter. This idea was used by Miller and Larsen [7] to get better performance of the diffusion synthetic acceleration (DSA). But when applied to AADR, the

method does not work. So a new extrapolation concept with  $\phi^{l+1/2}$  (not with  $\phi^{l+1}$ ) is devised in this paper. Thus, Eq.(2) is replaced by

$$\phi^{l+1/2} = \alpha \frac{1}{2} \int_{-1}^{1} \psi^{l+1/2} d\mu + (1-\alpha)\phi^{l}.$$
(8)

Fourier analysis is then performed to investigate the efficiency of the extrapolation. Let us define Fourier ansatz as

$$\psi^{l+1/2} = A \,\omega^{l} Exp(j\lambda x),$$

$$\phi^{l} = B \omega^{l} Exp(j\lambda x),$$

$$\phi^{l+1/2} = D \omega^{l} Exp(j\lambda x),$$

$$f_{\pm}^{l+1/2} = F_{\pm} \omega^{l} Exp(j\lambda x),$$
(9)

with several assumptions, without loss of generality, as

 $\sigma = 1, \quad \sigma_s = c, \quad q(x) = 0. \tag{10}$ 

Then, Eq. (1) becomes

$$(j\lambda\mu + 1)A = cB,\tag{11}$$

and Eq. (8)

$$D = \frac{\alpha}{2} \int_{-1}^{1} \frac{cB}{j\lambda\mu + 1} d\mu + (1 - \alpha)B.$$
 (12)

Low-order equations (3) and (4) are also expressed as

$$(j\lambda k+1)F_{+} = c(\omega-1)B, \tag{13}$$

$$(-j\lambda k+1)F_{-} = c(\omega-1)B.$$
(14)

Using the above two Eqs. (13) and (14), we obtain

$$F_{+} + F_{-} = \frac{(\omega - 1)c}{1 + \lambda^{2}k^{2}}B.$$
(15)

Finally, using Eqs. (11) and (15), Eq. (5) becomes

$$\omega B = \frac{\alpha}{2} \int_{-1}^{1} \frac{cB}{j\lambda\mu + 1} d\mu + \frac{(\omega - 1)c}{1 + \lambda^2 k^2} B + (1 - \alpha)B,$$
(16)

and arranging for eigenvalue ( $\omega$ ), then we obtain

$$\omega(1 - \frac{c}{1 + \lambda^2 k^2}) = \frac{\alpha}{2} \int_{-1}^{1} \frac{c}{1 + \lambda^2 \mu^2} d\mu - \frac{c}{1 + \lambda^2 k^2} + (1 - \alpha).$$
(17)

Multiplying the denominator on both sides of Eq. (17), Eq. (17) can be expressed as

$$\omega(1+\lambda^2k^2-c) = \frac{1}{2} \int_{-1}^{1} \frac{c(\alpha\lambda^2k^2+\alpha-1-\lambda^2\mu^2)+(1-\alpha)(1+\lambda^2k^2)(1+\lambda^2\mu^2)}{1+\lambda^2\mu^2} d\mu.$$
(18)

Finally, the eigenvalue is expressed in the following inequality as

$$\omega \leq \frac{1}{2} \int_{-1}^{1} \frac{1 + \frac{(1 - \alpha)\lambda^2 k^2 - \alpha}{\lambda^2 k^2} \lambda^2 \mu^2}{1 + \lambda^2 \mu^2} d\mu,$$
(19)

and the spectral radius ( $\rho$ ), maximum of the eigenvalues, is obtained in an analytic form:

$$\rho = \left| \frac{1}{2} \int_{-1}^{1} \frac{1 + A(\alpha, \lambda) \lambda^2 \mu^2}{1 + \lambda^2 \mu^2} d\mu \right| = \left| A(\alpha, \lambda) + \frac{(1 - A(\alpha, \lambda)) \arctan(\lambda)}{\lambda} \right|, \tag{20}$$

where

$$A(\alpha,\lambda) = \frac{(1-\alpha)\lambda^2 k^2 - \alpha}{\lambda^2 k^2}.$$
(21)

Fig. 1 shows spectral radii for various extrapolation parameters from continuous Fourier analysis. We can find optimal  $\alpha$  in this figure, which provides smallest spectral radius, 0.0864, when  $\alpha$  approaches about 1.2. Fig. 2 depicts spectral radii of AADR with and without extrapolation for various weighting parameters.



Fig. 1. Spectral radius for various extrapolation parameters from continuous Fourier analysis.



Fig. 2. Spectral radius for various weighting parameters from continuous Fourier analysis.

## 3. Inconsistent Discretization of AADR

Linear acceleration methods including AADR are required to use consistent discretizations between the high-order and low-order equations for stable convergence. This means that the convergence may be poor, if different spatial schemes are used for the high-order and low-order equations.

In this study, it is shown by the Fourier analysis and numerical tests that AADR with extrapolation can mitigate this inconsistent discretization problem. We have chosen four cases of AADR with step difference (SD) scheme and diamond difference (DD) scheme. If some complicated algebraic manipulations are performed, the spectral radius can be obtained from discrete Fourier analysis. The spectral radii of the four cases are derived as: a) AADR0 (DD-DD):

$$\rho = \left| c\alpha \sum_{n=1}^{N/2} \frac{w_n [\{ -(2\mu_n / \Delta_i)^2 + (2k / \Delta_i)^2 \} \cos^2(\tau)]}{(2\mu_n / \Delta_i)^2 (2k / \Delta_i)^2 \sin^2(\tau) + (2k / \Delta_i)^2 \cos^2(\tau)} + (1 - \alpha) \right|,$$
(22)

b) AADR1 (DD-SD):

$$\rho = \left| c\alpha \sum_{n=1}^{N/2} \frac{w_n [-(2k/\Delta_i + 1)(2\mu_n/\Delta_i)^2 \sin^2(\tau) + \{(2k/\Delta_i + 1)2k/\Delta_i - (2\mu_n/\Delta_i)^2\}\cos^2(\tau)]}{(2\mu_n/\Delta_i)^2 (2k/\Delta_i + 1)(2k/\Delta_i)\sin^2(\tau) + (2k/\Delta_i + 1)(2k/\Delta_i)\cos^2(\tau)} + (1-\alpha) \right|, \quad (23)$$

c) AADR2 (SD-DD):

$$\rho = \left| c \alpha \sum_{n=1}^{N/2} \frac{w_n [(2\mu_n / \Delta_i + 1)(2k / \Delta_i)^2 \sin^2(\tau) + \{-(2\mu_n / \Delta_i + 1)2\mu_n / \Delta_i + (2k / \Delta_i)^2\} \cos^2(\tau)]}{(2\mu_n / \Delta_i + 1)^2 (2k / \Delta_i)^2 \sin^2(\tau) + (2k / \Delta_i)^2 \cos^2(\tau)} + (1 - \alpha) \right|, \quad (24)$$

d) AADR3 (SD-SD):

$$\rho = \left| c\alpha \sum_{n=1}^{N/2} \frac{w_n \{ (2k/\Delta_i + 1)(2\mu_n/\Delta_i + 1)(2k/\Delta_i - 2\mu_n/\Delta_i) \} \sin^2(\tau)}{(2\mu_n/\Delta_i + 1)^2 (2k/\Delta_i + 1)(2k/\Delta_i) \sin^2(\tau) + (2k/\Delta_i + 1)(2k/\Delta_i) \cos^2(\tau)} + c\alpha \sum_{n=1}^{N/2} \frac{w_n \{ (2k/\Delta_i + 1)2k/\Delta_i - (2\mu_n/\Delta_i + 1)2\mu_n/\Delta_i \} \cos^2(\tau)}{(2\mu_n/\Delta_i + 1)^2 (2k/\Delta_i + 1)(2k/\Delta_i) \sin^2(\tau) + (2k/\Delta_i + 1)(2k/\Delta_i) \cos^2(\tau)} + (1-\alpha) \right|,$$
(25)

where DD-SD means that the diamond difference scheme is applied for high-order equation and the step difference scheme for low-order equation.

Spectral radii for various cases of AADR without extrapolation are given in Fig. 3. In this figure, the weighting parameter (k) is set to 0.53 and scattering ratio (c) is given as unity. The spectral radii of consistently discretized AADR (DD-DD, SD-SD) are very small for various mesh sizes. But in the case of inconsistent discretization (DD-SD, SD-DD), the spectral radii approach around unity for large mesh sizes, which will take a large number of iterations or may not converge. With optimal extrapolation parameter ( $\alpha$ ) and optimal weighting parameter (k), the spectral radii of AADR1 (DD-SD) are depicted in Figs. 4 and 5. Note that the spectral radii are very small for large mesh sizes if optimal parameters are used in inconsistently discretized AADR.



Fig. 3. Spectral radius for various mesh sizes ( $k=0.53, \alpha=1.0, c=1.0$ ).



Fig. 4. Spectral radius for inconsistently discretized AADR1 (DD-SD).



Fig. 5. Spectral radius with various extrapolation for AADR1 (DD-SD) ( $\sigma\Delta$ =10).

# 4. Numerical Tests and Results

As a test problem, a slab geometry problem with optically thick medium is selected as shown in Fig. 6. The problem is 100 cm wide and mesh size is chosen as 10 cm.  $S_{16}$  Gauss-Legendre quadrature is used, and convergence criterion is given as 1.0E-9.

Vacuum  

$$Q = 1.0 \ \text{\#/cm sec}$$
 Vacuum  
 $\sigma = \sigma_{s} = 1 \text{ cm}^{-1}$  Vacuum  
0 cm 100 cm

Fig. 6. Configuration of test problem.

Table I shows number of iterations and computing time for various cases of AADR. AADR with extrapolation shows better results than that of AADR without extrapolation. All optimal parameters are found from Fourier analysis and the numerical results are in good agreement with those of discrete Fourier analysis.

The solutions of inconsistently discretized AADRs converge to those of high-order solvers, but in the case of non-linear acceleration methods, the solutions approach those of low-order solvers. Thus, when AADR with extrapolation is applied realistic problems, we had better choose a highly accurate scheme as the solver of high-order equation and a simple scheme such as step difference scheme as the solver of low-order equation. In this study, the preconditioned bi-conjugate gradient stabilized (PBi-CGSTAB) algorithm with "transport sweep incomplete factorization (TSIF)" is used to solve the low-order equation.

			1 0	
	AADR0	AADR1	AADR2	AADR3
	$(DD^{a}-DD^{b})$	(DD-SD)	(SD-DD)	(SD-SD)
Source Iteration	39171 °	39171	6549	6549
	0.9997 <sup>d</sup>	0.9997	0.9986	0.9986
	$(32.2 \text{ sec})^{e}$	(32.2 sec)	(2.67 sec)	(2.67 sec)
AADR	10	566	98	7
without	0.0908	0.9701	0.8422	0.0348
Extrapolation	(0.03 sec)	(1.42 sec)	(0.13 sec)	(0.03 sec)
	α=1.00	α=1.00	α=1.00	α=1.00
	k=0.55	k=1.86	k=1.22	k=0.51
	(W= µ +1.17)	(W= µ -0.44)	(W= µ –0.38)	(W= µ +7.83)
AADR	8	6	5	6
with	0.0245	0.0264	0.0105	0.0111
Extrapolation	(0.02 sec)	(0.02 sec)	(0.02 sec)	(0.03 sec)
	α=1.24	α=-9.0	α=11.4	α=1.24
	k=0.63	k=-4.30	k=5.70	k=0.63
	(W= µ +0.14)	(W= µ -0.52)	(W= µ -0.48)	(W= µ +0.14)

Table I. Number of Iterations and Computing Time

<sup>a</sup>: Solver for high-order equation, <sup>d</sup>: Numerical spectral radius, <sup>b</sup>: Solver for low-order equation, <sup>c</sup>: Number of iterations, <sup>e</sup>: Calculation on SUN-ULTRA1 system.

## 5. Conclusions

A new extrapolation concept is applied to the AADR acceleration method, resulting in remarkable improvement in convergence and the inconsistent discretization problem resolved.

Continuous and discrete Fourier analyses show that AADR with extrapolation provides better results. The spectral radius of S<sub>2</sub>-like AADR without extrapolation is less than 0.1865c, but if extrapolation is considered, the spectral radius is less than 0.0864c. Even with inconsistent discretizations, the AADR with extrapolation works well and provides sufficiently fast convergence. Optimal parameters ( $\alpha$ ,k) can be obtained from Fourier analysis and they are demonstrated by numerical results.

As a conclusion, AADR (a linear acceleration method) with new extrapolation concept does not always require the low-order equation to be discretized consistently with the discretization of the high-order transport sweep as in the case of DSA.

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#### References

- 1. R.E. Alcouffe, "Diffusion Synthetic Acceleration Methods for the Diamond-Differenced Discrete-Ordinates Equations," *Nucl. Sci. Eng.*, **64**, 344 (1977).
- C.J. Park and N.Z. Cho, "A Linear Multiple Balance Method with High Order Accuracy for Discrete Ordinates Neutron Transport Equations," *Annals of Nuclear Energy*, 28, 1499 (2001).
- C.J. Park and N.Z. Cho, "The Additive Angular Rebalance Acceleration Method for Solving Neutron Transport Equations in X-Y Geometry," *Proceedings of the Korean Nuclear Society Spring Meeting*, May 2001, Cheju (Full Paper in CD-ROM).
- 4. N.Z. Cho and C.J. Park, "An Additive Angular-Dependent Rebalance Method for Neutron Transport Equations," *Trans. Am. Nucl. Soc.*, **84**, 222 (2001).
- S.G. Hong and N.Z. Cho, "A Rebalance Approach to Nonlinear Iteration for Solving the Neutron Transport Equations," *Annals of Nuclear Energy*, 24, 147 (1997).
- S.G. Hong and N.Z. Cho, "Angle-Dependent Rebalance Factor Method for Nodal Transport Problems in X-Y Geometry," *Trans. Am. Nucl. Soc.*, 79, 139 (1998).
- W.F. Miller, Jr. and E.W. Larsen, "Modified Diffusion Synthetic Acceleration Algorithms," *Nucl. Sci. Eng.*, 93, 403 (1986).