Nuclear Mathematical and Computational Sciences: A Century in Review, A Century Anew
Gatlinburg, Tennessee, April 6-11, 2003, on CD-ROM, American Nuclear Society, LaGrange Park, IL (2003)

ACCELERATION TECHNIQUE FOR MONOTONOUS NUMERICAL SCHEMES FOR BOLTZMAN TRANSPORT EQUATION

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ABSTRACT

A new simple and robust acceleration technique has been developed for monotonous iterations, where monotony is assumed in terms of scalar flux or scattering source. The basic idea of acceleration is to use maximal extrapolation preserving pointwise monotony of iterations. The extrapolation parameter is derived from a Neumann series analysis. The new acceleration technique has the following attractive features: (a) theoretically secured convergence; (b) accurate estimation of upper or lower bound solution is available optionally at any iteration; (c) the estimation monotonously converges to the accurate solution; (d) any iteration improves accuracy of estimation at any node. The new approach shows better efficiency against Aitken's method. The requirement of monotony is not restrictive in practice. Numerical scheme can be monotonous in terms of scalar flux, in spite of absence of this property for angular flux iterations. In that case the source iteration can be accelerated. The areas of application of new approach are not bounded to transport theory calculations. It can be applied, for example, for source acceleration in a transient fixed source problem encountered in multigroup nonstationary diffusion calculations.

Key Words: Monotonous Acceleration Scheme, Fixed Source Problem

1. INTRODUCTION

Some of the neutronic package still uses the simple and effective flux convergence acceleration technique [1](page 3-49), [2] (page 224), originating from the Aitken's Δ^2-method. This method was developed for scalar equations [3], and latter it was implemented for linear and non-linear systems. The TORT code manual refers to this acceleration method as Error Mode Extrapolation Technique, which consists of flux or source extrapolation under the assumption that the sequence $\{\phi_n\}$ converges towards ϕ^* like a geometric sequence:

$$\phi^* = \phi_n + (\phi_{n+1} - \phi_n) + (\phi_{n+2} - \phi_{n+1}) + \ldots \approx \phi_n + (\phi_{n+1} - \phi_n) + \rho(\phi_{n+1} - \phi_n) + \rho^2(\phi_{n+1} - \phi_n) + \ldots$$

Hence, the improved flux approximation can be obtained as a sum of geometric sequence.

$$\phi^* \approx \phi_n + \frac{1}{1-\rho_n}(\phi_{n+1} - \phi_n),$$

$$\rho_n = \|\phi_{n+1} - \phi_n\| / \|\phi_n - \phi_{n-1}\|.$$

where, ρ is the estimation of the spectral radius. The advantage of this method is its simplicity and efficiency. Unfortunately this method is not always robust. It is robust only in case of stabilization of ρ_n during the iterations, which leads to no acceleration until getting convergent estimation of the spectral radius. There are some empirical recommendations [2] on how accurate the estimation of spectral radius should be. At the same time, there is no theoretical prescription for a general case about what accuracy of the spectral radius estimation should be used to guarantee convergence and robust acceleration.

Fortunately, there are particular cases of the monotonous scheme, when it is possible to get consistent a lower estimation of spectral radius on the basis of any three sequent monotonous iterations [4,5]. We started from this fact to derive the robust acceleration technique. We found, that the extrapolation based on the lower estimation of the spectral radius leads to the maximal extrapolation, which preserves pointwise monotony of iterations. This secures convergence and robustness of acceleration.

2. DESCRIPTION OF ACCELERATION TECHNIQUE.

First let us introduce necessary definitions and key facts.

Let **R** is N×N matrix. The matrix **R** is called nonnegative if $\mathbf{R}_{i,j} \geq 0$ for $\forall i, j \in [1, N]$.We write $\mathbf{R} \geq \mathbf{0}$. The matrix **R** is called positive if $\mathbf{R}_{i,j} > 0$ for $\forall i, j \in [1, N]$. We write $\mathbf{R} > \mathbf{0}$. We define nonnegative and positive vectors by the similar rules and notations. We write $\vec{x} \geq \vec{y}$ if $\vec{x} - \vec{y} \geq \vec{0}$.Similarly, we write $\vec{x} > \vec{y}$ if $\vec{x} - \vec{y} > \vec{0}$.
Let $\rho(\mathbf{R})$ be the spectral radius of matrix R.

Suppose we have iteration processes

$$\vec{u}^{(n+1)} = \mathbf{R}\vec{u}^{(n)} + \vec{q}\,; \tag{1}$$

$$\vec{z}^{(n+1)} = \mathbf{R}\vec{z}^{(n)} + \vec{q} \tag{2}$$

and the following conditions hold:

$$\mathbf{R} \geq \mathbf{0}, \rho(\mathbf{R}) < 1,\ \vec{q} \geq \vec{0}. \tag{3}$$

It can easily be checked that:

(a) if $\vec{u}^{(1)} \geq \vec{u}^{(0)}$ then $\vec{u}^{(1)} \leq \vec{u}^{(2)} \leq ... \leq \vec{u}^{(n)} \leq ... \leq \vec{x}^*$, where $\vec{x}^* \overset{def}{=} (\mathbf{E} - \mathbf{R})^{-1}\vec{q}$. ;

(b) if $\vec{z}^{(1)} \leq \vec{z}^{(0)}$ then $\vec{x}^* \leq ... \leq \vec{z}^{(n)} \leq ... \leq \vec{z}^{(1)}$;

(c) if $\vec{x}^* \geq \vec{u}^{(0)}$ then $\vec{u}^{(0)} \leq \vec{u}^{(1)} \leq ... \leq \vec{u}^{(n)} \leq ... \leq \vec{x}^*$;

(d) if $\vec{x}^* \leq \vec{z}^{(0)}$ then $\vec{x}^* \leq ... \leq \vec{z}^{(n)} \leq ... \leq \vec{z}^{(1)} \leq \vec{z}^{(0)}$;

(e) if $\vec{q} \geq \vec{0}$ and $\vec{u}^{(0)} = \vec{0}$ then $\vec{u}^{(0)} \leq \vec{u}^{(1)} \leq ... \leq \vec{u}^{(n)} \leq ... \leq \vec{x}^*$.

In the above considerations we assume that

$$\vec{u}^{(1)} \geq \vec{u}^{(0)} \tag{4}$$

and

$$\vec{z}^{(1)} \leq \vec{z}^{(0)}. \tag{5}$$

By definition, put

$$\alpha_{n+1} \overset{def}{=} Max\left\{t : \mathbf{R}(\vec{u}^{(n+1)} - \vec{u}^{(n)}) \equiv (\vec{u}^{(n+2)} - \vec{u}^{(n+1)}) \geq t \cdot (\vec{u}^{(n+1)} - \vec{u}^{(n)})\right\}; \quad n = 0,1,... \tag{6}$$

Let us show that $\alpha_n \le \alpha_{n+1} \le \rho(\mathbf{R})$.

Combining $\vec{u}^{(n+2)} = \mathbf{R}\vec{u}^{(n+1)} + \vec{q}$ and $\vec{u}^{(n+1)} = \mathbf{R}\vec{u}^{(n)} + \vec{q}$ we get $\mathbf{R}(\vec{u}^{(n+1)} - \vec{u}^{(n)}) = (\vec{u}^{(n+2)} - \vec{u}^{(n+1)})$. Multiplying both sides $(\vec{u}^{(n+1)} - \vec{u}^{(n)}) \ge \alpha_n \cdot (\vec{u}^{(n)} - \vec{u}^{(n-1)})$ by nonnegative matrix **R**, we get $(\vec{u}^{(n+2)} - \vec{u}^{(n+1)}) \ge \alpha_n \cdot (\vec{u}^{(n+1)} - \vec{u}^{(n)})$. Recalling the definition of a_{n+1} we obtain $\alpha_n \le \alpha_{n+1}$.

It is proven by [4],[5] (page 81) that: if $\vec{x} \ge \vec{0}$, $\mathbf{R} \ge \mathbf{0}$, $\mathbf{R}\vec{x} \ge \xi\vec{x}$ then it is true lower estimation $\rho(\mathbf{R}) \ge \xi$ for spectral radius $\rho(\mathbf{R})$. Taking into account (6) we conclude $\alpha_{n+1} \le \rho(\mathbf{R})$. This completes the proof.

The main result of this paper is given by the following proposition.

Proposition 1.

Suppose the iteration process (1) satisfies (3) and (4). Then

$$\vec{u}^{(n+1)} \le \vec{u}_{extr}^{(n+1)} \le \vec{x}^* \qquad (7)$$

where

$$a_n = Max\left\{t : (\vec{u}^{(n+1)} - \vec{u}^{(n)}) \ge t \cdot (\vec{u}^{(n)} - \vec{u}^{(n-1)})\right\}$$

$$\vec{x}^* = \mathbf{R}\vec{x}^* + \vec{q}\,.$$

$$\vec{u}_{extr}^{(n+1)} = \vec{u}^{(n)} + \frac{1}{1-\alpha_n}\left(\vec{u}^{(n+1)} - \vec{u}^{(n)}\right) \qquad (8)$$

$\vec{u}_{extr}^{(n+1)}$ -extrapolated value.

Proof.

Taking into account

$$\vec{x}^* = \mathbf{R}\vec{x}^* + \vec{q} \text{ and } 0 \le \alpha_n \le \alpha_{n+1} \le \rho(\mathbf{R}) < 1$$

we can write

$$\vec{x}^* = \vec{u}^{(n)} + (\mathbf{E} - \mathbf{R})^{-1}(\vec{q} + \mathbf{R}\vec{u}^{(n)} - \vec{u}^{(n)}) = \vec{u}^{(n)} + (\mathbf{E} - \mathbf{R})^{-1}(\vec{u}^{(n+1)} - \vec{u}^{(n)}) =$$

$$= \vec{u}^{(n)} + \sum_{k=0}^{\infty}\mathbf{R}^k(\vec{u}^{(n+1)} - \vec{u}^{(n)}) \ge \vec{u}^{(n)} + \sum_{k=0}^{\infty}\alpha_{n+1}^k(\vec{u}^{(n+1)} - \vec{u}^{(n)}) \ge$$

$$\ge \vec{u}^{(n)} + \sum_{k=0}^{\infty}\alpha_n^k(\vec{u}^{(n+1)} - \vec{u}^{(n)}) = \vec{u}^{(n)} + \frac{1}{1-\alpha_n}(\vec{u}^{(n+1)} - \vec{u}^{(n)}) \ge \vec{u}^{(n+1)}$$

This concludes the proof.

Corollary. Inequality (7) shows possibility of acceleration iterations (1) by using précised extrapolated value $\vec{u}_{extr}^{(n+1)}$ instead of $\vec{u}^{(n+1)}$. Monotony of accelerated iterations follows from (7) and property (c). Accelerated iterations are lower estimations of accurate solution. Convergence follows from convergence $\vec{u}^{(n)} \to \vec{x}^*$. and inequality (7).

Put by definition

$$\beta_{n+1} \overset{def}{=} Min\left\{t : \mathbf{R}(\vec{u}^{(n+1)} - \vec{u}^{(n)}) \equiv (\vec{u}^{(n+2)} - \vec{u}^{(n+1)}) \le t \cdot (\vec{u}^{(n+1)} - \vec{u}^{(n)})\right\}; \quad n = 0,1,... \qquad (9)$$

As far $\beta_n \cdot (\vec{u}^{(n)} - \vec{u}^{(n-1)}) - (\vec{u}^{(n+1)} - \vec{u}^{(n)}) \ge 0,\ \ \mathbf{R} \ge 0 \quad \Rightarrow$

$$\Rightarrow \mathbf{R}\left[\beta_n \cdot (\vec{u}^{(n)} - \vec{u}^{(n-1)}) - (\vec{u}^{(n+1)} - \vec{u}^{(n)})\right] = \beta_n \cdot (\vec{u}^{(n+1)} - \vec{u}^{(n)}) - (\vec{u}^{(n+2)} - \vec{u}^{(n+1)}) \geq \vec{0}$$

Hence $\beta_n \geq \beta_{n+1}$.

Proposition 2. Suppose the iteration process (1) satisfies (3) and (4). Then there is number N such that $\beta_N < 1$.

Proof. Inequality immediately follows from convergence β_n to the spectral radius. •

The next proposition gives answer how begin monotonously decreasing sequence of upper estimation of accurate solution.

Proposition 3. Suppose the iteration process (1) satisfies (3), (4) and $\beta_n < 1$.

Then

$$\vec{z}_0 \geq \vec{x}^*,$$

where

$$\vec{z}_0 = \vec{u}^{(n)} + \frac{1}{1-\beta_n}(\vec{u}^{(n+1)} - \vec{u}^{(n)})$$

Proof.

Taking into account

$$\vec{x}^* = \mathbf{R}\vec{x}^* + \vec{q} \text{ and } \rho(\mathbf{R}) \leq \beta_{n+1} \leq \beta_n < 1$$

we can write

$$\vec{x}^* = \vec{u}^{(n)} + (\mathbf{E} - \mathbf{R})^{-1}(\vec{q} + \mathbf{R}\vec{u}^{(n)} - \vec{u}^{(n)}) = \vec{u}^{(n)} + (\mathbf{E} - \mathbf{R})^{-1}(\vec{u}^{(n+1)} - \vec{u}^{(n)}) =$$

$$= \vec{u}^{(n)} + \sum_{k=0}^{\infty} \mathbf{R}^k (\vec{u}^{(n+1)} - \vec{u}^{(n)}) \leq \vec{u}^{(n)} + \sum_{k=0}^{\infty} \beta_{n+1}^k (\vec{u}^{(n+1)} - \vec{u}^{(n)}) \leq$$

$$\leq \vec{u}^{(n)} + \sum_{k=0}^{\infty} \beta_n^k (\vec{u}^{(n+1)} - \vec{u}^{(n)}) = \vec{u}^{(n)} + \frac{1}{1-\beta_n}(\vec{u}^{(n+1)} - \vec{u}^{(n)}) = \vec{z}^{(0)}$$

This concludes the proof.

Proposition 3 gives the answer to how to get upper estimation $\vec{z}^{(0)}$ for accurate solution $\vec{x}^*$.Vector $\vec{z}^{(0)}$ can be used as initial guess for monotonously decreasing sequence of upper estimations. The next proposition gives the acceleration technique for upper estimations.

Proposition 4. Suppose the iteration process (2) satisfies (3) and (5). Then

$$\vec{x}^* \leq \vec{z}_{extr}^{(n+1)} \leq \vec{z}^{(n+1)}$$

where

$$\overline{a}_n = Max\left\{t : (\vec{z}^{(n)} - \vec{z}^{(n+1)}) \geq t \cdot (\vec{z}^{(n-1)} - \vec{z}^{(n)})\right\}$$

$$\vec{x}^* = \mathbf{R}\vec{x}^* + \vec{q}.$$

$$\vec{z}_{extr}^{(n+1)} = \vec{z}^{(n)} + \frac{1}{1-\overline{\alpha}_n}\left(\vec{z}^{(n+1)} - \vec{z}^{(n)}\right) \quad (10)$$

$\vec{z}_{extr}^{(n+1)}$ -extrapolated value.

The proof is omitted, because it repeats the proof of proposition 1.

Remark 1. Convergence of the accelerated procedure immediately follows from its monotony and inequality (7). The left part of inequality (7) shows, that acceleration is robust.

Remark 2. In practice, we use the following formula for calculation β_{n+1}

$$\beta_{n+1} = \underset{k}{Min}\left\{(u_k^{(n+2)} - u_k^{(n+1)})/(u_k^{(n+1)} - u_k^{(n)})\right\},$$

where k is the node index. In order to avoid numerical instability due to round off error, we have to exclude from consideration nodes k such that

$$\left|(u_k^{(n+2)} - u_k^{(n+1)})/u_k^{(n+1)}\right| < \varepsilon$$

where ε is the prescribed small value (~1.e-8).

3. NUMERICAL RESULTS

The acceleration technique has been examined for two numerical schemes:

(1) finite-difference diffusion equation for a 2D square region, SSOR-type iteration method, the proposed acceleration scheme is used for flux iterations;
(2) S4 WDD scheme for square region, scattering is isotropic, the proposed acceleration scheme is used for source iterations.

The reference solution in the both cases was generated with a tight convergence criteria. In order to provide the proper termination criteria of iteration process, the accuracy of examined iterations has been checked against the reference solution. The results are summarized in tables 1 and 2.The both of tables show gain in number of iterations

Table I. Iteration reduction factors in diffusion problem

	Case 1	**Case 2**	**Case 3**	**Case 4**
Spectral radius	0.9592	0.9784	0.9882	0.9981
New method	4.89	6.46	8.05	10.94
Aitken’s method	3.67	4.20	3.00	4.15

Table II. Iteration reduction factors in S4 calculation

	Case 1	**Case 2**	**Case 3**	**Case 4**
Spectral radius	0.908	0.911	0.9792	0.9880
New method	3.51	3.54	4.19	4.57
Aitken’s method	2.62	2.32	3.27	3.15

Another test was performed for the acceleration of the fixed-source problem encountered in the subgroup formulation of the DeCART code [6]. In an application to a whole-core 2D calculation for the SMART reactor, the fixed source problem was solved for the lower resonance group in 45 group calculation. Reference solution was generated with a tight convergence criterion (the relative change of scalar flux $<10^{-10}$). Flux extrapolation has been performed at 3, 6, 9 etc iterations. Figure 1 compares the error reduction behaviors of the accelerated and unaccelerated cases. This figure shows the robust error reduction in the both cases, as predicted by the theory. The spectral radius of iterations is about 0.74. This is a well-convergent problem, without any acceleration. If we assume, that the acceleration technique suppress mainly the error in the first eigenmode, then the efficiency of the acceleration should be dependent on the ratio $(1-|\lambda_1|)/(1-|\lambda_0|)$. That is why the efficiency of acceleration in this problem is not so good, unlike in the previous cases.

We have modified scattering/absorption ratio of the previous problem, in order to obtain a larger spectral radius of about 0.98. The results are given at Figure 2. In contrast to the original case giving the flux error against the reference solution, Figure 2 shows the error in terms of relative flux change in two successive iterations. It explains the non-monotonic trend. This figure shows about two times better efficiency of acceleration compared to the original case.

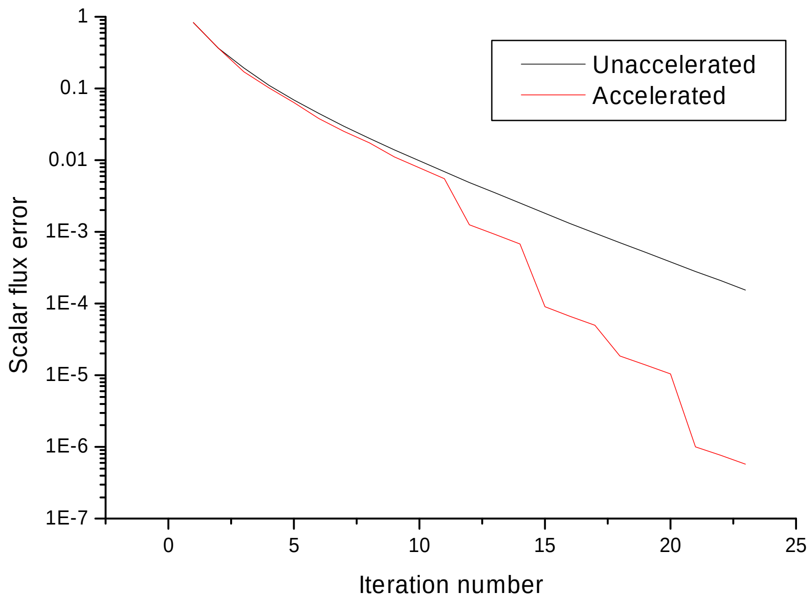

Figure 1. Convergence rate for accelerated and un accelerated cases in the full-core MOC calculation, spectral radius = 0.74.

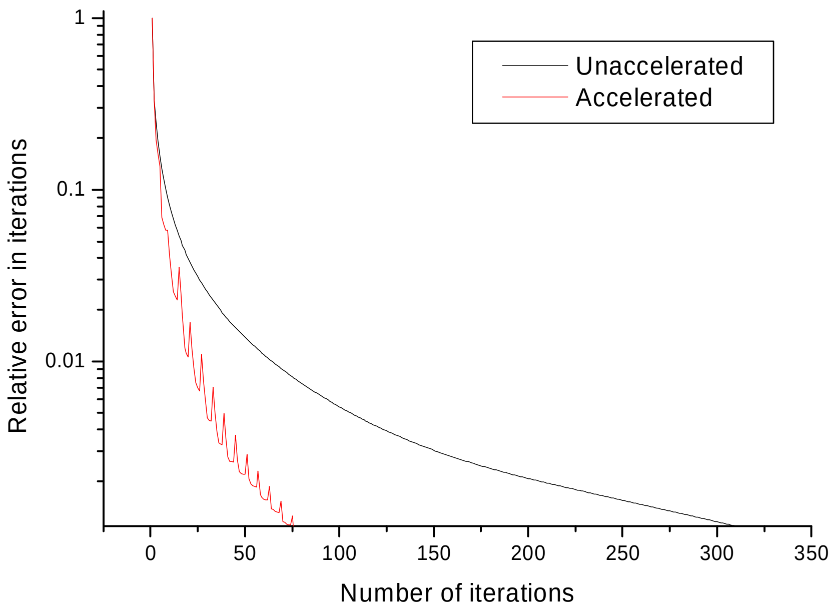

Figure 2. Convergence rate for accelerated and non accelerated case in modified problem, spectral radius = 0.98 .

CONCLUSION

A new simple and robust acceleration technique has been developed for monotonous iteration methods for the solution of fixed source problems. The monotony is assumed with respect to scalar flux or scattering source. It is essentially less restrictive requirement, than monotony with respect to angular flux. New acceleration technique has the following attractive features: (a) theoretically secured convergence; (b) accurate estimation of upper or lower bound solution is available optionally at any iteration; (c) the estimation monotonously converges to the accurate solution; (d) any iteration improves accuracy of estimation at any node; (e) the acceleration technique is very simple to program and the extrapolation causes only a negligible computational overhead other than the increase in storage to store two previous iterates of scalar fluxes

REFERENCES

1. W.A Roades, D.B.Simpson. *The TORT three-dimensional discrete ordinates neutron / photon transport code (TORT version-3),* ORNL report ORNL/TM-13221, (1997).
2. R. J. Stamml'er, M.J.Abbate. *Methods odf steady Tate Reactor Physics in Nuclear Design,* Academic Press Inc, London, (1983).
3. J.Stoer, R. Bulirich. *Introduction to numerical analysis,* Springer-Verlag, New-York, (1992)
4. Krasnoselskii M.A., Lifshitz E.A., Sobolev A.V. *Positive linear system,* "Nauka", Moscow, Russia, (1985). /in Russian/.
5. Krasnoselskii M., Vainikko G., Zabreiko P.,Rutitzkii Ja. and Stecenko V. *Approximate solution of operator equations.* Moscow, "Nauka", 1969. (in Russian) or translation in German (Krasnoselskii M., Vainikko G., Zabreiko P.,Rutitzkii Ja. and Stecenko V. Naherungsverfahren zur Losung von Operatorgleichungen. Akademic-Verlag, Berlin)
6. H. G. Joo, et. al. *Dynamic Implementation of the Equivalence Theory in the Heterogeenous Whole Core Transport Calculation.* Paper in CDROM, PHYSOR 2002, Seoul, Korea, Oct. 7-10, 2002.
7. Marvin L.Adams, Edward W. Larsen. *Fast Iterative Methods For Discrete-Ordinates Particle Reansport Calculations.* "Pergamon, Elsevier Science Ltd", Great Britan, Progress in Nuclear Energy, Vol. 40, No., 1 pp. 3-159, 2002