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Krylov sub-space methods for *K*-eigenvalue problem in 3-D neutron transport

Anurag Gupta [a,*], R.S. Modak [b]

[a] *Reactor Physics Design Division, Bhabha Atomic Research Centre, Mumbai 400085, India*
[b] *Theoretical Physics Division, Bhabha Atomic Research Centre, Mumbai 400085, India*

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Abstract

The *K*-eigenvalue problem in nuclear reactor physics is often formulated in the framework of Neutron Transport Theory. The fundamental mode solution of this problem is usually obtained by the power iteration method. Here, we are concerned with the use of a Krylov sub-space method, called ORTHOMIN(1), to obtain a more efficient solution of the *K*-eigenvalue problem. A *Matrix-free* approach is proposed which can be easily implemented by using a transport code which can perform fixed source calculations. The power iteration and ORTHOMIN(1) schemes are compared for two realistic 3-D multi-group cases with isotropic scattering: an LWR benchmark and a heavy water reactor problem. In both the schemes, within-group iterations over self-scattering source are required as intermediate procedures. These iterations are also accelerated using another Krylov method called conjugate gradient method. The overall work is based on the use of Sn-method and finite-differencing for discretisation of transport equation.

1. Introduction

The solution of *K*-eigenvalue problem is frequently required for the analysis of fission based systems such as nuclear reactors. The prime interest is to evaluate

* Corresponding author.
E-mail address: anurag@apsara.barc.ernet.in (A. Gupta).

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the fundamental mode eigenvalue (K_{eff}) and the associated shape of neutron flux. The problem is formulated using either the neutron transport theory or its approximate form called diffusion theory. In the present paper, we are concerned with the use of Krylov sub-space methods for an efficient solution of this problem in transport theory. The K-eigenvalue equation can be written as:

$$\Omega \cdot \nabla\psi + \Sigma_t(\mathbf{r}, E)\psi - \int \mathrm{d}E' \int \mathrm{d}\Omega'\, \Sigma_s(\mathbf{r}, E' \to E, \Omega' \to \Omega)\psi' = (\chi(E)/4\pi K) \int \mathrm{d}E' \int \mathrm{d}\Omega' \nu\Sigma_f(\mathbf{r}, E')\psi'. \quad (1)$$

Here, ψ stands for ψ ($\mathbf{r}$, E, Ω) and ψ' for ψ' ($\mathbf{r}$, E', Ω'). These are energy and space-dependent angular fluxes. It obeys appropriate boundary conditions. For numerical solution, the energy E is usually discretised by multi-group approximation. The variables $\mathbf{r}$ and Ω are also discretised by some means. Here, we consider finite differencing in space and the well-known discrete ordinates (S_n) method for direction along with the use of Diamond Difference scheme. After such a discretisation, Eq. (1) reduces to a set of coupled algebraic equations, which can be formally expressed as:

$$A\mathbf{x} = \lambda B\mathbf{x} \quad (2)$$

A and B are square matrices of order $N{\cdot}M{\cdot}G$, where N is the total number of meshes, M is the number of directions and G is the number of groups. The coefficient matrix B stands for neutron production by fission while A represents all terms on left hand side (LHS) of Eq. (1). $\mathbf{x}$ is a vector containing the M angular fluxes in G groups and N meshes. λ stands for $(1/K)$. This is often called as "generalised" eigenvalue problem because coefficient matrices occur on both the sides of equation. If matrix on one of the side is an identity matrix, then it reduces to a simple matrix eigenvalue problem. Usually, Eq. (2) is solved by the well-known power iteration (PI) method, which makes use of certain inner–outer iterations. The procedure involves repeated solution of a fixed source problem within each energy group which, in turn, involves the well-known mesh-angle sweeping procedure (Lewis and Miller, 1984).

Several attempts have been made (Adams and Larsen, 2002) to obtain a more efficient solution of Eq. (2) using methods such as shifted PI, coarse mesh rebalancing and Chebyschev acceleration. The present work is also an attempt to achieve this by using the Krylov sub-space methods. The idea of using the ORTHOMIN(1) method was inspired by Suetomi and Sekimoto's work on the same problem in diffusion theory. In what follows, earlier work by Suetomi and Sekimoto (1991) is briefly described followed by description of present work.

1.1. Earlier work on diffusion theory

It may be noted that in case of finite-differenced multi-group neutron diffusion theory also, the K-eigenvalue equation can be represented by Eq. (2). However, the order of matrices A and B would be $N \cdot G$ since only total flux is involved in diffusion theory and directional fluxes do not occur. It is well-known that, analogous to the transport case, in diffusion theory also, Eq. (2) is usually solved by the PI method

which involves an inner–outer iteration scheme (Duderstadt and Hamilton, 1976). The fission source and K-value are updated after each outer iteration. A single outer iteration itself involves solution of external source problems in each energy group which is often obtained iteratively. In all this solution procedure, explicit construction of matrices A and B is not required. In the more common multi-group case, A and B are, in general, non-symmetric.

As an improvement over the above solution procedure, Suetomi and Sekimoto (1991) have proposed the use of a Krylov sub-space method called "ORTHOMIN(1)". The exact algorithm is listed in Appendix A. The method is briefly as follows. With a guess vector $\mathbf{x}$, a residual vector $\mathbf{r}$ is defined as:

$$\mathbf{r} = \rho(\mathbf{x})B\mathbf{x} - A\mathbf{x}, \tag{3}$$

where ρ $(\mathbf{x})$ itself is given by

$$\rho(\mathbf{x}) = \frac{(A\mathbf{x}, B\mathbf{x})}{(B\mathbf{x}, B\mathbf{x})}. \tag{4}$$

The Euclidean norm of $\mathbf{r}$ is defined as $(\mathbf{r}, \mathbf{r})^{1/2}$. A gradient method is employed to iteratively minimise this norm by successively improving the guess vector $\mathbf{x}$. As the norm of $\mathbf{r}$ (and hence $\mathbf{r}$ itself) tends to zero, it can be seen from Eq. (3) that the iterate $\mathbf{x}$ satisfies following equation:

$$A\mathbf{x} = \rho(\mathbf{x}) \cdot B\mathbf{x}$$

so that $\mathbf{x}$ tends to eigenvector and ρ tends to eigenvalue λ as iterations proceed.

As can be seen from the actual algorithm given in Appendix A, the main operation repetitively needed is the multiplication of matrices A and B with a known vector and certain scalar products of vectors; for which routines can be developed. It is interesting to note that this approach does not involve two separate levels of iteration: inner and outer. It has been shown by Suetomi and Sekimoto that the ORTHOMIN(1) method can be much more efficient than the usual PI method.

1.2. Present work

The idea is to apply the ORTHOMIN (1) method to the K-eigenvalue problem in transport theory. A straightforward way to do this is to develop programs for explicit construction of matrices A and B for any given problem so that their products with any given vectors can be computed, as needed by the algorithm. To save memory, the matrices can be stored in sparse format. Sparse algebra routines can be used to execute the algorithm efficiently. However, such an approach needs substantial development work for realistic 3-D problems. Moreover, some problems may arise in cases prone to negative flux fix-ups. Some techniques need to be worked out to overcome the negative flux problem.

Here, a quite different approach is presented which is easy to implement. It makes use of conventional transport codes (based on inner–outer iterations) which can solve fixed source problems to implement the ORTHOMIN(1) method. No explicit construction of any matrix (or computation of matrix–vector product) is required.

The plan of this paper is as follows. In Section 2, the proposed matrix-free approach to implement the ORTHOMIN(1) method is described. It will be seen that, just like the conventional PI scheme, this approach also needs the within-group external source calculations. For further efficiency, another Krylov method called the conjugate gradient (CG) method is used here to accelerate these source calculations. This particular work on CG method is simply an extension of our earlier work on 1-D and 2-D problems (Gupta and Modak, 2002) to 3-D problems and is only briefly described in Section 3. Section 4 briefly describes the code ATES3 developed to implement the conventional PI scheme as well as ORTHOMIN(1) method with the option of using CG method for source calculations in a group. Section 5 gives numerical results for an light water reactor (LWR) benchmark and a heavy water reactor case, which involve isotropic scattering. Section 6 gives conclusions and possible extension of the work.

2. The proposed matrix-free scheme

The discretised K-eigenvalue problem given by Eq. (2) is cast in terms of fission sources as vectors. Let N_F be the number of meshes which contain fissionable material. It may be noted that in general, $N_F < N$ (=total number of meshes) because there will be no fissionable material in regions such as reflector. Then the eigenvector $\mathbf{f}$ can be considered to be made up of N_F elements which are the fission source densities in the N_F meshes. The K-eigenvalue problem can be written as

$$P\mathbf{f} = K\mathbf{f}, \tag{5}$$

where P is a square matrix of order N_F called "fission matrix". The concept of fission matrix can be found in standard texts (e.g. Wachspress, 1966). It should be noted that the order of the coefficient matrix in Eq. (5) is much less than that in Eq. (2). This reduction is possible because fission source is always isotropic and has a fixed energy spectrum irrespective of the energy and direction of neutron causing fission. This problem has N_F eigenvalues and eigenvectors. If f_i denotes ith eigenvector with eigenvalue K_i, one can write:

$$P\mathbf{f}_i = K_i\mathbf{f}_i. \tag{6}$$

Assuming that all eigenvalues are real, one can order them as $K_1 > K_2 \geqslant K_3 \geqslant \cdots \geqslant K_{N_F}$. Then K_1 denotes the fundamental eigenvalue, usually referred to as K-eff.

It is easy to see that the ORTHOMIN(1) algorithm for problem $A\mathbf{x} = \lambda B\mathbf{x}$, listed in Appendix A, can be directly used to solve Eq. (5) by simply replacing A by P and B by an identity matrix. Now the main requirement is that one should be able to evaluate the product of matrix P with the vector $\mathbf{x}$ occurring in the algorithm. This can be done without explicitly constructing P by making use of standard transport codes based on inner–outer iterations, which have a capability to perform an external source calculation. It may be mentioned that such an approach to evaluate effect of P on a vector has been employed (Modak and Jain, 1996; Modak et al., 1995) earlier.

The precise procedure to evaluate $P\mathbf{x}$ from $\mathbf{x}$ is as follows:

Step-1: Let $\mathbf{x} = x_1, x_2, \ldots, x_{N_F}$ be the given vector. It is assumed that each of the N_F meshes in the reactor model contains a steady external source of neutrons. The source in ith mesh emits x_i neutrons per unit volume per unit time isotropically. The energy distribution of the emitted neutrons is as per the fission spectrum χ_g.

Step-2: The fission production cross sections $(\nu\Sigma^i_{fg})$ for all meshes i and energy group g are set to zero. All other cross-sections are unchanged. Thus, we consider a non-multiplicative case.

Step-3: Using a standard S_n-method transport code, the total flux in all groups and meshes resulting due to the external source (specified in Step-1) in the non-multiplying system are found out. This involves source calculation in each energy group, where the source consists of the specified external source and group-to-group scattering source. Let ϕ_{ig} denote the computed total flux in ith mesh and gth group.

Step-4: Using the actual production cross-section $\nu\Sigma^i_{fg}$ and the just computed fluxes ϕ_{ig}, the ith element of $P\mathbf{x}$ can be written as

$$(P\mathbf{x})_i = \Sigma_g \upsilon \Sigma^i_{fg} \phi_{ig}. \tag{7}$$

Using Eq. (7) for all values of i, the full vector $P\mathbf{x}$ is obtained.

On physical grounds, it can be seen from the above procedure that if $\mathbf{x}$ is any given source vector, $P\mathbf{x}$ is the fission source vector in next generation. The eigenvalue K can be understood as the ratio of neutrons in successive generations.

The algorithm ORTHOMIN(1) can be implemented to solve Eq. (5) by writing a small routine which calls a standard S_n code repetitively to evaluate $P\mathbf{x}$ from $\mathbf{x}$ as explained in Steps 1–4 above. No explicit construction of matrices such as A, B or P is required. It is seen that in the scheme described above the ORTHOMIN(1) method is effectively being used to replace the outer iterations in PI scheme which update the fission source vector and K-value. The convergence properties and hence the performance of PI method and the ORTHOMIN (1) method are expected to differ.

3. The within-group source problem

As mentioned in step 3 in the earlier section, the solution of an external source problem is necessary to evaluate $P\mathbf{x}$ from $\mathbf{x}$ to implement the ORTHOMIN(1) method. The solution of an external source problem is also required in the usual PI scheme implemented via inner–outer iterations. In this section, acceleration of this computation is discussed.

The overall external source problem involves solution of within-group source problem for each group. The within-group source problem for group g can be written as:

$$\Omega \cdot \nabla \psi_g(\mathbf{r}, \Omega) + \Sigma_{t,g}(\mathbf{r}) \psi_g(\mathbf{r}, \Omega) - \Sigma_{s,g\to g}(\mathbf{r}) \int f(\mathbf{r}, \Omega' \to \Omega) \psi_g(\mathbf{r}, \Omega')\, \mathrm{d}\Omega' = q_g(\mathbf{r}, \Omega), \tag{8}$$

where $\psi_g(\mathbf{r}, \Omega)$ is angular flux in group g, $\Sigma_{s,g \to g}$ is self scattering cross-section and f is scattering function. $q_g(\mathbf{r}, \Omega)$ is the sum of neutron sources arising from scattering from other groups and fission/specified external source. Eq. (8) is solved by employing iterations over the self scattering source, called the source iterations (SI). As is well known (Lewis and Miller, 1984), these iterations converge slowly for thick highly scattering medium.

The use of diffusion synthetic acceleration (DSA) to accelerate these iterations is well-known. In this scheme, after a source iteration, a *corrective equation* is setup which is a diffusion equation (Ramone et al., 1997) in terms of total flux ϕ. It can be solved more easily than transport equation and the computed flux is used to correct the isotropic scattering source term. However, it is found that in many practical cases with strong spatial heterogeneity the DSA scheme fails. This is because the differencing schemes for the transport and diffusion cases are not consistent. Also, implementing DSA in a transport code usually requires significant additional coding effort.

It is possible to set up the corrective equation as a transport equation in a scheme called as transport synthetic acceleration (TSA) (Ramone et al., 1997). This avoids the *consistent differencing issues*. A lower S_N-quadrature order is chosen so that corrective equation can be solved easily. Moreover, the corrective equation is always considered to have only *isotropic scattering*. This equation with isotropic scattering can be formally expressed in terms of total flux ϕ and solved more efficiently by employing the conjugate gradient (CG) method. Ramone et al. (1997) have used such a scheme with step characteristic and finite element methods. Gupta and Modak (2002) have applied the scheme in case of spatial finite differencing along with the diamond difference approximation. This case is often prone to generate negative fluxes. Yet, the scheme was shown to work efficiently for some 1-D and 2-D source problems in Cartesian geometry. The overall scheme is as follows.

The problem is basically solved by SI-method, which includes negative flux fix-up procedure. However, after a few source iterations, the corrective TSA equation is solved. This corrective equation is solved using a quadrature set of order lower than the original problem. The CG method is used to solve it. In fact, only a *limited* number of CG-iterations (say, 5) are used to solve it approximately. There is no negative flux fix-up while solving the corrective equation. The overall procedure is found to be more efficient than solving the problem by SI-iterations alone. This has been explained in detail along with some applications for 2-D problems in our earlier work (Gupta and Modak, 2002). In the present studies, this scheme is applied to solve Eq. (8) needed in the overall procedure to solve K-eigenvalue problem and the performance is compared with the simple SI-method. The present work forms generalisation of CG based TSA scheme to 3-D problems.

It may be mentioned that, for isotropic problems, the CG-method can replace the source iterations directly without employing the TSA. However, this is possible in the cases which are not prone to occurrence of negative fluxes. Hence, here the TSA(CG) method is used which is more robust than using CG method directly. The CG algorithm to solve a linear system of equations $A\mathbf{x} = \mathbf{b}$ can be seen in Saad (1996).

4. The code ates3

A multi-group neutron transport code ATES3, based on Sn-method with diamond differencing, has been developed by the authors to implement the above mentioned schemes. It can handle Cartesian *XYZ* geometry problems with spatial heterogeneity and general group-to-group scattering. Both, vacuum and reflective boundary conditions can be used on any side. However, reflective boundary conditions cannot be given on opposite faces. At present the isotropic scattering option is operational. It can analyse *K*-eigenvalue problem as well as external source problems. The within-group inner iterations are optionally accelerated with the use of CG-methods: either directly, or indirectly through transport synthetic acceleration (TSA) scheme. For the *K*-eigenvalue problem two options are available: the conventional PI procedure and the more efficient Krylov sub-space method called ORTHOMIN(1). The code is written in a modular form in Fortran-90/95 language.

5. Numerical results

Various schemes were compared by analysing two different problems in *XYZ* geometry. All the computations were done in double precision using a Pentium-III 667 MHz processor with 256 MB of RAM. For neutron directions and weights, fully symmetric quadrature sets were used. *K*-eigenvalue calculations are carried out for the following computational schemes:

Scheme-1: Standard PI scheme with inner–outer iterations is employed. The within group source calculations are carried out by simple ''source iterations'' (SI) over self-scattering term.

Scheme-2: Same as Scheme-1, but the within group source calculations are carried out using TSA and CG method is used to solve the corrective TSA equations: the corrective TSA equations are approximately solved after every 5 source iterations using only 5 CG iterations.

Scheme-3: Instead of PI, the ORTHOMIN(1) method was used as given in Section 2. For the within group source calculations, the TSA(CG) method was used as in Scheme-2.

5.1. Convergence criteria

Three types of convergence criteria were applied to the group-flux, net fission source density and the *K*-value. They are designated by ϵ_s, ϵ_f,ϵ_k, respectively.

1. For the within-group source iterations, relative point-wise convergence of group flux in successive iterations n and $n+1$, the criterion is as follows (with subscript i for the mesh):

$$\max_i \frac{\phi_{gi}^{(n+1)} - \phi_{gi}^{(n)}}{\phi_{gi}^{(n+1)}} < \varepsilon_s. \tag{9a}$$

2. The relative point-wise convergence ϵ_f of fission source in successive outer iterations is defined in a fashion analogous to ϵ_s.
3. The relative convergence criterion for eigenvalue in successive outer iterations is

$$\frac{K^{(n+1)} - K^{(n)}}{K^{(n+1)}} < \varepsilon_K. \tag{9b}$$

It may be mentioned that it is difficult to decide how tightly the inner iterations must be converged. If they are converged more tightly than necessary, a substantial computer time may be wasted but if they are not converged tightly enough, the procedure may become unstable. One has to rely on experience and intuition. (Lewis and Miller, 1984, page 94). Hence the results are presented for different values of ε_s ranging from 10^{-3} to 10^{-8} for the LWR core. For the heavy water reactor case, the value of ϵ_s cruder than 10^{-5} are found to be inadequate and are not considered.

5.2. Results for LWR benchmark

This is a 2-energy-group LWR benchmark (Takeda and Ikeda, 1991) with a fuel region at the centre surrounded by reflector. There are two shut-off rods/void positions. A 1/8th core is simulated as the problem is symmetric in all three directions. The problem is simulated using $25 \times 25 \times 25$ mesh structure, each mesh being 1.0 cm in all directions. The results given here are for the core with all SRs withdrawn. The calculations are done with S_8 symmetric quadrature set.

Table 1 gives the computed K-eigenvalues and CPU times for the three schemes for different convergence criteria for the LWR case. The reference K-value given by Takeda and Ikeda (1991) is also shown in the table. The K-values computed using various schemes agree with the reference value. Comparison of scheme 1 and 2 shows that the TSA (CG) offers more benefit over SI for tighter value of ϵ_s. This is because for tighter ϵ_s, large number of within-group iterations are required and the TSA(CG) scheme helps in reducing them.

The last column in Table 1 presents results for scheme-3. It is seen that the accuracy of K-eigenvalue obtained by ORTHOMIN(1) increases as ε_s decreases. This is expected because when ε_s is small, the computation of $P\mathbf{x}$ (repeatedly needed in the ORTHIMIN(1) algorithm) is sufficiently accurate, leading to accurate K-value. This behaviour is in contrast with the PI method employed in Schemes 1 and 2, where the accuracy of computed K-value does not depend on ε_s. Nevertheless, the ORTHOMIN(1) offers some benefit in CPU time over the other schemes.

It may be noted that for $\varepsilon_s = 10^{-3}$, the computation of matrix–vector product $P\mathbf{x}$ is inaccurate. As a result, the K-value converges to a different answer as seen in Table 1. Hence, the corresponding CPU time cannot be used to estimate any trends.

Fig. 1 shows the variation of point wise fission source convergence with the CPU time for the three schemes. The utility of TSA and ORTHOMIN(1) is clearly seen.

Table 1
Computed K-eff and CPU times for various schemes for LWR case (reference K-value with S_8 quadrature = 0.9772 ± 0.0001)

Convergence criteria			K-eff		
			Scheme-1	Scheme-2	Scheme-3
ε_s	ε_f	ε_K	PI with (SI)	PI with TSA(CG)	ORTHOMIN(1) with TSA(CG)
10^{-3}	10^{-8}	10^{-8}	0.97717785	0.97717791	0.97401180
			875 s	877 s	263 s
10^{-5}	10^{-8}	10^{-8}	0.97717791	0.97717791	0.97716278
			1502 s	685 s	167 s
10^{-7}	10^{-8}	10^{-8}	0.97717791	0.97717791	0.97717766
			3003 s	580 s	297 s
10^{-8}	10^{-8}	10^{-8}	0.97717790	0.97717788	0.97717789
			4120 s	671 s	374 s

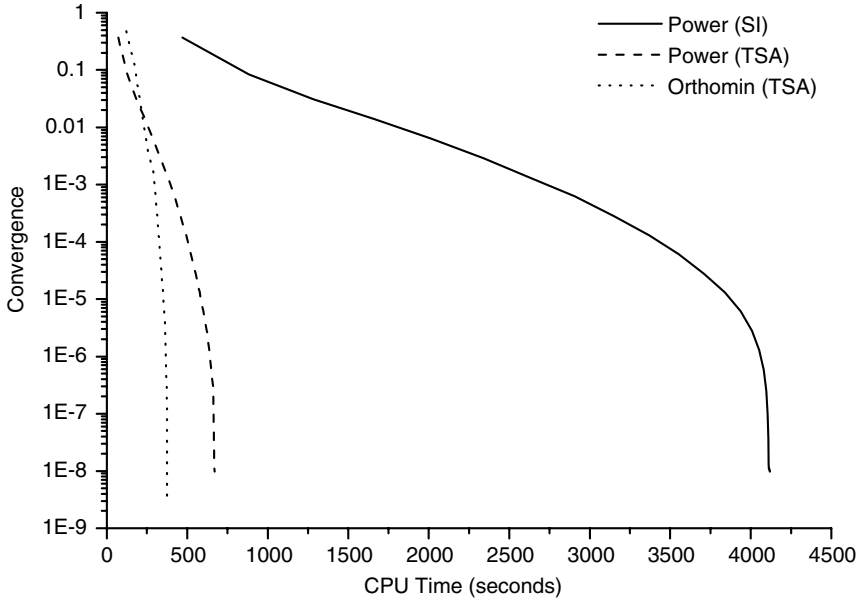

Fig. 1. Point wise fission-source convergence against CPU time for LWR case ($\varepsilon_s = \varepsilon_f = \varepsilon_K = 10^{-8}$).

6. Results for the proposed critical facility for AHWR

The critical facility (CF) is a heavy water moderated experimental research reactor to be used for testing advanced heavy water reactor (AHWR) fuel lattices. The core consists of two types of homogenised fuel lattice regions surrounded by D_2O reflector. There are six shut-off rod/void positions. An adjuster rod is also put just outside the fuel region. The whole core is simulated using $48 \times 48 \times 24$ mesh structure

with vacuum on all boundaries. These calculations are done with four energy-groups and using S_4 symmetric quadrature set. The details on geometry and material cross sections can be found in a report elsewhere (Gupta and Modak, 2004).

The results for various schemes with different convergences are presented in Table 2. Two value of ε_s were tried: 10^{-5} and 10^{-6}. For $\varepsilon_s = 10^{-5}$, the TSA (CG) seems to be faster than SI-scheme by about three times. For $\varepsilon_s = 10^{-6}$, the SI-based Scheme-1 does not converge even after 6 h, whereas the TSA(CG) scheme converges in 4752 s.

The last column in Table 2 gives results for ORTHOMIN(1) scheme. It can be seen that CPU times needed for ORTHOMIN(1) are much smaller than the other

Table 2
Computed *K*-eff and CPU times for various schemes for CF(AHWR) case

Convergence criteria			*K*-eff		
			Scheme-1	Scheme-2	Scheme-3
ε_s	ε_f	ε_K	PI with (SI)	PI with TSA(CG)	ORTHOMIN(1) with TSA(CG)
10^{-5}	10^{-6}	10^{-6}	1.00153294	1.00153335	1.00158444
			17379 s	6375 s	1862 s
10^{-6}	10^{-6}	10^{-6}	1.00145453[a]	1.00153041	1.00153459
			>6 h	4752 s	2963 s

[a] Did not converge, unconverged $\varepsilon_f = 0.94 \times 10^{-3}$.

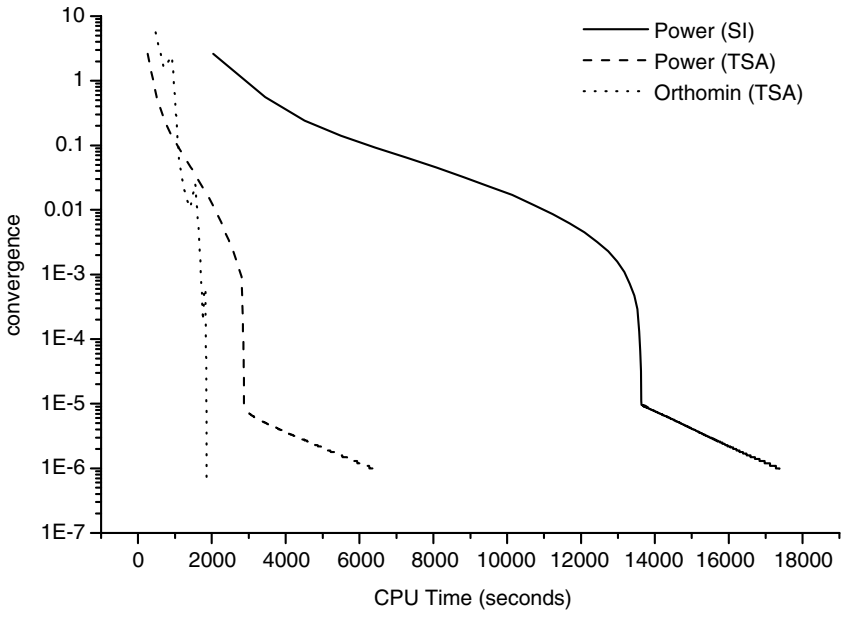

Fig. 2. Point wise fission-source convergence against CPU time for CF(AHWR) case ($\varepsilon_s = 10^{-5}$, $\varepsilon_f = \varepsilon_K = 10^{-6}$).

schemes. Again, the K-value is more accurate for the tighter value of ε_s as in the LWR case.

In Fig. 2, the variation of point wise fission source convergence with the CPU time for the three schemes is given.

7. Conclusion and discussion

The ORTHOMIN(1) method has been earlier shown to be an efficient alternative to the PI method for the fundamental mode solution of K-eigenvalue problem in neutron diffusion theory. In the present work, the ORTHOMIN(1) method is applied to the K-eigenvalue problem in transport theory. It was possible to apply the method in a manner exactly analogous to the earlier work in diffusion theory. This requires explicit construction of relevant coefficient matrices so that their product with vector can be evaluated. While this would be easy for simple problems, such as 1-D homogeneous one-energy-group problems, it is considerably complicated for realistic multi-group 3-D cases. Hence, an alternative procedure to implement the ORTHOMIN(1) method is suggested and tested in this paper. In this procedure, the eigenvalue problem is cast in terms of fission source densities (rather than the group fluxes) as eigenvectors. This leads to a simple eigenvalue problem for the fission matrix P. The matrix P is not known explicitly. However, it is shown that the effect of P on a vector can be computed using transport codes having option for external source calculations. This is enough to apply the ORTHOMIN(1) method. The method is then compared with the PI method.

Another aspect studied in the report is as follows. Both ORTHOMIN(1) as well as PI method require solution of fixed source problem in an energy group. Usually this is obtained by simple *Source Iterations* (SI). In the present report, another Krylov method CG was employed via the TSA. Utility of TSA(CG) over the SI-method is also analysed.

For numerical analysis, realistic 3-D multigroup models of LWR and CF(AHWR) were chosen. The TSA(CG) is seen to be more efficient than the SI-method. In case of CF(AHWR), the speed-up of TSA(CG) over the SI-method is substantially higher than for the LWR case. This is expected because heavy water has much larger ratio of scattering to absorption cross-section and hence needs very large number of SI, which are reduced by the use of CG-method.

The ORTHOMIN(1) method is found to be faster than the PI method. The advantage is more for the CF(AHWR) case. This may be because the LWR core is small. Hence, the eigenvalue separation between fundamental and next higher mode may be large. In such a situation, the PI method itself converges relatively faster and hence the advantage of ORTHOMIN(1) may be less. Another observation is that the K-value computed by ORTHOMIN(1) is more accurate for tighter convergence of iterations over the self-scattering source (or small ε_s). This may be because the ORTHOMIN(1) needs accurate evaluation of product of P with a vector. From the procedure to evaluate this product described in Section 2, it is clear that evaluation of $P\mathbf{x}$ is based on source calculations and hence it needs a fine value of ε_s.

It is planned to extend the work reported here for variety of cases including problems with anisotropic scattering. It should be mentioned that the more direct approach of implementing ORTHOMIN(1) by generating coefficient matrices may be more efficient than the approach followed in this paper. This aspect may be investigated. It is easy to see that various ways to implement the ORTHOMIN(1) method are applicable to the diffusion theory case also. In fact, such studies for 3-D cases have been carried out and will be reported later.

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Appendix A. The ORTHOMIN(1) algorithm to solve $Ax = \lambda Bx$

1. Choose $\mathbf{x}_0$
2. $$\lambda_0 = \frac{(A\mathbf{x}_0, B\mathbf{x}_0)}{(B\mathbf{x}_0, B\mathbf{x}_0)},$$
3. $\mathbf{r}_0 = \lambda_0\ B\mathbf{x}_0 - A\mathbf{x}_0$,
4. $\mathbf{s}_0 = \mathbf{r}_0$
5. For $i = 0,1,\ldots$, until convergence, Do
6. $$\alpha_i = \frac{\{(\mathbf{r}_i, A\mathbf{s}_i) - \lambda_i(\mathbf{r}_i, B\mathbf{s}_i)\}}{\{(A\mathbf{s}_i, A\mathbf{s}_i) - 2\lambda_i(A\mathbf{s}_i, B\mathbf{s}_i) - \lambda_i^2(B\mathbf{s}_i, B\mathbf{s}_i)\}}$$
7. $\mathbf{x}_{i+1} = \mathbf{x}_i + \alpha_i\ \mathbf{s}_i$,
8. $$\lambda_{i+1} = \frac{(A\mathbf{x}_{i+1}, B\mathbf{x}_{i+1})}{(B\mathbf{x}_{i+1}, B\mathbf{x}_{i+1})},$$
9. $\mathbf{r}_{i+1} := \lambda_{i+1}\ B\mathbf{x}_{i+1} - A\mathbf{x}_{i+1}$,
10. $$\beta_i = \frac{-[(A\mathbf{r}_{i+1}, A\mathbf{s}_i) - \lambda_{i+1}\{(A\mathbf{r}_{i+1}, B\mathbf{s}_i) + (A\mathbf{s}_i, B\mathbf{r}_{i+1})\} + \lambda_{i+1}^2(B\mathbf{r}_{i+1}, B\mathbf{s}_i)]}{[(A\mathbf{s}_i, A\mathbf{s}_i) - 2\lambda_{i+1}(A\mathbf{s}_i, B\mathbf{s}_i) - \lambda_{i+1}^2(B\mathbf{s}_i, B\mathbf{s}_i)]}$$
11. $\mathbf{s}_{i+1} := \mathbf{r}_{i+1} + \beta_i\ \mathbf{s}_i$
12. End Do.

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