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60 *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. The present report is 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: an LWR benchmark and the AHWR critical facility. The within-group iterations over self-scattering source are required in the solution of K-eigenvalue problem. They are also accelerated using another Krylov method called conjugate gradient method. In this work, the discretisation of transport equation is based on finite-differencing and Sn-method and isotropic scattering is considered.

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3-डी बहुवर्ग न्यूट्रॉन परिवहन में K-आइगेन मान समस्या हेतु क्रायोलोव उपांतरिक्ष विधियां

अनुराग गुप्ता * एवं आर.एस. मोडक +
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सार

नाभिकीय रिएक्टर भौतिकी में K-आइगेनमान समस्या अक्सर न्यूट्रॉन परिवहन सिद्धांत के ढाँचे में संरूपित रहती है । इस समस्या का मूल विधा समाधान साधारणतया घात- पुनरावृत्ति विधि से किया जाता है । यह रिपोर्ट ओर्थोमिन(1) नामक क्रायोलोव उपांतरीक्ष विधि का प्रयोग करते हुये K- आइगेनमान समस्या के अधिक प्रभावशाली समाधान निकालने के बारे में है । यहाँ पर एक आव्यूह-मुक्त विधि प्रस्तावित है जिसे नियत स्रोत गणना करने वाले न्यूट्रॉन परिवहन कोड का प्रयोग करते हुये आसानी से लागू किया जा सकता है । घात पुनरावृत्ति तथा ओर्थोमिन (1) योजनाओं की तुलना वास्तविक त्रि-डी आयामी बहुवर्गीय -LWR बेंच मार्क तथा AHWR क्रांतिक सुविधा के लिए की गयी है । आइगेन समस्या के समाधान हेतु स्वत: प्रकीर्णन स्रोत पर वर्गांतर्गत पुनरावृत्तियां जरूरी होती हैं । कांजूगेट ग्रेडिएन्ट विधि नामक अन्य क्रायलोव विधि का प्रयोग करते हुये उनको त्वरित किया गया । इस कार्य में परिवहन समीकरण का विविक्तीकरण परिमित अंतरणों पर आधारित है तथा Sn-विधि और समदैशिक प्रकीर्णन का उपयोग किया गया है ।

Krylov Sub-space Methods for K-Eigenvalue Problem in 3-D Multigroup Neutron Transport

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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. The present report is 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: an LWR benchmark and the AHWR Critical Facility. The within-group iterations over self-scattering source are required in the solution of K-eigenvalue problem. They are also accelerated using another Krylov method called Conjugate Gradient method. In this work, the discretisation of Transport Equation is based on finite-differencing and Sn-method and isotropic scattering is considered.

Krylov Sub-space Methods for K-Eigenvalue Problem in 3-D Multigroup Neutron Transport

1. INTRODUCTION

The solution of K-eigenvalue problem is commonly required for the analysis of fission based systems such as nuclear reactors. The prime interest is to evaluate the fundamental mode eigenvalue (K_{eff}) and the associated shape of neutron flux. The problem is usually solved using either the neutron transport theory or its approximate form called diffusion theory depending on the application. Here, we are concerned with the problem in the transport theory. The use of Krylov sub-space methods for an efficient solution of this problem is considered. The k-eigenvalue problem in transport theory can be written as:

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

Here, angular flux ψ stands for $\psi(\mathbf{r}, E, \Omega)$ and ψ' for ψ' $(\mathbf{r}, E', \Omega')$. The flux obeys appropriate boundary condition. 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, the Eqn.(1) reduces to a set of coupled algebraic equations, which can be formally expressed as:

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

where A and B are square matrices of order N.M.G where N is the total number of meshes, M is the number of directions and G is the number of groups. B stands for neutron production by fission while A represents all terms on left hand side (LHS) of Eqn.(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 a unit matrix, then it reduces to a simple matrix eigenvalue problem. Eqn.(2) is usually solved by using the power iteration method to find the fundamental mode. This involves solution of fixed source problem in each group which includes the well-known mesh-angle sweeping procedure (Lewis and Miller, 1984). Several attempts have been made (Adams and Larsen, 2002) to obtain an efficient solution of Eqn.(2) such as shifted power iteration, coarse mesh rebalancing and Chebyschev acceleration. The present work is also an attempt in this direction. Some of the ideas were inspired by the work carried out by Suetomi and Sekimoto 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.

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 Eqn.(2). However, the order of matrices A and B would be N.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, Eqn.(2) is usually solved by the power iteration 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 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 $\rho(\mathbf{x})$ is given by

$$\tilde{n}(\mathbf{x}) = \frac{(A\mathbf{x}, B\mathbf{x})}{(B\mathbf{x}, B\mathbf{x})} \tag{4}$$

The Euclidean norm of $\mathbf{r}$, defined as $(\mathbf{r}\ ,\ \mathbf{r})^{1/2}$ is iteratively minimised by a gradient method. As the norm of $\mathbf{r}$ and hence $\mathbf{r}$ itself tends to zero, it can be seen from Eqn.(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 algorithm, 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 that the ORTHOMIN(1) method can be much more efficient than the usual power iteration method.

Present Work:

The idea is to apply the ORTHOMIN (1) method for K-eigenvalue problem in transport theory. A straightforward way is to develop programs for explicit construction of matrices A and B for any given problem so that their products with vectors can be computed. The matrices can be stored in sparse format. Sparse algebra routines can be used to execute the algorithm. However, this approach needs substantial development work for realistic 3-D

problems. Moreover, there may be problems in cases prone to negative flux fix-ups. Some techniques need to be worked out to overcome this 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) to implement the ORTHOMIN(1) method. No explicit construction of any matrix (or computation of matrix-vector product) is required. The plan of this report 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 power iteration scheme, this approach also needs the within-group external source calculations. A Krylov method called the conjugate gradient (CG) method will be used to accelerate these source calculations. This work on CG method is an extension of our earlier work on 1-D and 2-D problems (Gupta and Modak, 2002) to 3-D problems and is described in section 3. Section 4 briefly describes the code ATES3 developed to implement the conventional power iteration scheme as well as ORTHOMIN(1) method with option of using CG method for source calculations in a group. Section 5 gives numerical results for LWR and CF(AHWR) test cases which involve only 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 Eqn.(2) is cast in terms of fission sources as vectors. This is based on the definition of K-eff as ratio of fission sources in successive generation. 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

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

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 dimension of the coefficient matrix in Eqn.(5) is much less than in Eqn.(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 i^{th} eigenvector with eigenvalue K_i, one can write:

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

Assuming that all eigenvalues are real, one can order them as $K_1 > K_2 \geq K_3 \geq \ldots \geq K_{N_F}$. 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 the appendix A, can be directly used to solve Eqn.(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 **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 has been earlier employed (Modak and Jain, 1996; Modak et.al., 1995). The precise procedure to evaluate P**x** from **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 i^{th} 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 Sn-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 i^{th} mesh and g^{th} group.

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

$$(\mathrm{P}\,\mathbf{x})_i = \sum_g \upsilon\Sigma^i_{fg}\ \phi_{ig} \qquad (7)$$

Using Eqn.(7) for all values of *i*, the full vector P**x** is obtained.

On physical grounds, it can be seen from the above procedure that if **x** is any given source vector, P**x** is the fission source vector in next generation. The algorithm ORTHOMIN(1) can be implemented to solve Eqn.(5) by writing a small routine which calls a standard Sn code repetitively to evaluate P**x** from **x**. 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 which update the fission source vector and K-value to implement the conventional power iteration. The convergence properties and hence the performance of power iteration and 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**x** to implement the ORTHOMIN(1) method. It is also required in the

usual power iteration scheme implemented via inner-outer iterations. In this section, acceleration of this computation is discussed.

The within-group source problem can be written as:

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

$\psi_g(\mathbf{r}, \Omega)$ is angular flux in group g, $\Sigma_{s,gg}$ 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. Eqn.(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 as a Diffusion Equation in terms of total flux Φ. It can be solved more easily than transport equation and the computed flux is used to correct the scattering source term. However, it is found that in many practical cases with sharp 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 equations in transport formulation 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 can be chosen for easier solution of corrective equation. Moreover, the corrective equation is always considered to have only *isotropic scattering*. This equations can be solved more efficiently by employing the Conjugate Gradient (CG) method. The overall scheme is as follows.

The problem is basically solved by SI-method, which includes negative flux fix-up. However, after a few source iterations, the corrective TSA equation is solved. This corrective equation is in low-order quadrature set and a *limited* number of CG-iterations are used to solve it without employing the negative flux fix-up. 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 work is generalised to 3-D problems and the performance is compared with the simple SI-method.

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 (Saad, 1996) to solve a linear system of equations $\mathbf{A}\mathbf{x} = \mathbf{b}$ is listed in Appendix B.

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 as well as external source problems. The within-group inner iterations are 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 Power Iteration 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

The various schemes were compared by analysing two different problems in XYZ geometry. All the computations were done in S_4 symmetric quadrature set on a Pentium-III 667 Mhz processor with 256 MB of RAM. Basically, K-eigenvalue calculations are carried out for the following three computational schemes:

Scheme-1: Standard Power Iteration (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 Transport Synthetic Accelerations (TSA) and Conjugate Gradient (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 Power iterations, 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.

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):

$$\max_i \frac{\Phi_{gi}^{(n+1)} - \Phi_{gi}^{(n)}}{\Phi_{gi}^{(n+1)}} < \varepsilon_s \qquad (9a)$$

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

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

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 CF(AHWR) core, the value of ε_s cruder than 10^{-5} are found to be inadequate and are not considered.

Results for LWR benchmark

It is a 2-energy-group light water reactor benchmark (Takeda and Ikeda, 1991) with a fuel region at the centre surrounded by reflector. There are two shut-off rods/void positions. A $1/8^{th}$ core is simulated as the problem is symmetric in all three directions. The problem is simulated using 25×25×25 mesh structure, each mesh being 1.0 cm in all directions. The results given here are for the core with all SR's withdrawn. The calculations are done with S_4 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. 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 the 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 may be because when ε_s is small, the computation of $\mathbf{Px}$ needed in the algorithm is sufficiently accurate. This behaviour is in contrast with the Power Iteration method employed in Schemes 1 and 2. Nevertheless, the ORTHOMIN(1) offers some benefit in CPU times over the other schemes.

Results for the AHWR Critical Facility

The Critical Facility (CF) is a heavy water moderated experimental research reactor to be used for testing AHWR fuel lattices. The core consists of two types of fuel regions surrounded by D_2O reflector. There are six shut-off rod/void positions. An adjuster rod is put just outside the fuel region as shown in Figure-1 (a & b). Due to the adjuster rod, core symmetry is lost and a full core simulation has to be performed. The whole core is simulated using 48×48×24 mesh structure with vacuum on all boundaries. These calculations are done with 4 energy-

groups and using S_4 symmetric quadrature set. More details on geometry and cross section can be found in earlier studies (Gupta and Modak, 2003) where quarter core could be used as adjuster rod is absent.

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 3 times. For $\varepsilon_s = 10^{-6}$, the Scheme-1 does not converge even after 6 hours. where as the TSA(CG) scheme converges in 4752 seconds.

The last column in the table gives results for ORTHOMIN(1) scheme. It can be seen that CPU times needed for ORTHOMIN(1) are much smaller than the other schemes. Again, the result is accurate for the tighter value of ε_s.

6. CONCLUSION AND DISCUSSION

The ORTHOMIN(1) method has been earlier shown to be an efficient alternative to the Power Iteration 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 is 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 has been suggested and tested here. 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. The ORTHOMIN(1) has been implemented in this way and compared with the Power Iteration method.

Another aspect studied in the report is as follows. Both ORTHOMIN(1) as well as Power Iteration 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 scheme 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 Source Iterations, which are reduced by the use of CG-method.

The ORTHOMIN(1) method is found to be faster than the power iterations. 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 power iteration method 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 ε_s for iterations over the self-scattering source. 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 3, it is clear that this needs a fine value of ε_s.

It is planned to extend the work reported here for variety of cases such as 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 report. 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.

7. ACKNOWLEDGEMENTS

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APPENDIX A

The ORTHOMIN(1) Algorithm to Solve $Ax = \lambda Bx$

1. choose $\mathbf{x}_0$
2. $\lambda_0 = \dfrac{(A\mathbf{x}_0, B\mathbf{x}_0)}{(B\mathbf{x}_0, B\mathbf{x}_0)}$,
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,…,until convergence, Do:
6. $\alpha_i = \dfrac{\{(\mathbf{r}_i, A\mathbf{s}_i) - \lambda_i(\mathbf{r}_i, B\mathbf{s}_i)\}}{\{(A\mathbf{s}_i, A\mathbf{s}_i) - 2\lambda_i(A\mathbf{s}_i, B\mathbf{s}_i) - \lambda_i^2(B\mathbf{s}_i, B\mathbf{s}_i)\}}$
7. $\mathbf{x}_{i+1} := \mathbf{x}_i + \alpha_i \mathbf{s}_i$,
8. $\lambda_{i+1} = \dfrac{(A\mathbf{x}_{i+1}, B\mathbf{x}_{i+1})}{(B\mathbf{x}_{i+1}, B\mathbf{x}_{i+1})}$,
9. $\mathbf{r}_{i+1} := \lambda_{i+1} B\mathbf{x}_{i+1} - A\mathbf{x}_{i+1}$,
10. $\beta_i = \dfrac{-[(A\mathbf{r}_{i+1}, A\mathbf{s}_i) - \lambda_{i+1}\{(A\mathbf{r}_{i+1}, B\mathbf{s}_i) + (A\mathbf{s}_i, B\mathbf{r}_{i+1})\} + \lambda_{i+1}^2(B\mathbf{r}_{i+1}, B\mathbf{s}_i)]}{[(A\mathbf{s}_i, A\mathbf{s}_i) - 2\lambda_{i+1}(A\mathbf{s}_i, B\mathbf{s}_i) - \lambda_{i+1}^2(B\mathbf{s}_i, B\mathbf{s}_i)]}$
11. $\mathbf{s}_{i+1} := \mathbf{r}_{i+1} + \beta_i \mathbf{s}_i$
12. End Do

APPENDIX B

The Standard CG Algorithm to Solve $Ax = b$

1. Compute $r_0 := b - Ax_0$, $p_0 := r_0$.
2. For j = 0,1,……,until convergence, Do:
3. $\alpha_j := (r_j, r_j) / (Ap_j, p_j)$
4. $x_{j+1} := x_j + \alpha_j p_j$
5. $r_{j+1} := r_j - \alpha_j Ap_j$
6. $\beta_j := (r_{j+1}, r_{j+1}) / (r_j, r_j)$
7. $p_{j+1} := r_{j+1} + \beta_j p_j$
8. End Do

APPENDIX C

The Fully Symmetric S_4 Quadrature Set Used

Level	μ	*Point Weight*
1	0.35002121	0.041666
2	0.86889029	

APPENDIX D

Notations and Abbreviations

$\psi(\mathbf{r}, E, \Omega)$	:	Angular flux in direction Ω at $\mathbf{r}$ with energy E.
$\Sigma_t(\mathbf{r},E)$	:	Total macroscopic cross section
$\nu\Sigma_f(\mathbf{r}, E')$	:	Fission production cross section
$\Sigma_s(\mathbf{r}, E' \rightarrow E, \Omega' \rightarrow \Omega)$	:	Differential scattering cross section
$\chi(E)$	:	Fission spectrum
$\psi_g(\mathbf{r}, \Omega)$	:	Angular Flux in the energy group *g*
$\Sigma_{t,g}(\mathbf{r})$	:	Total cross section for group *g*
$\Sigma_{s,gg}(\mathbf{r})$	:	Within-group scattering cross section
$f(\mathbf{r}, \Omega' \rightarrow \Omega)$	:	Scattering function
$q_g(\mathbf{r}, \Omega)$	:	Source in a group *g*
N	:	Total number of meshes
N_f	:	Number of meshes containing fissionable material
G	:	Total number of groups
K	:	Multiplication eigenvalue
λ	:	1 / K
P	:	Fission Matrix
f	:	Mesh-wise fission source densities vector
$\varepsilon_s, \varepsilon_f, \varepsilon_k$	:	Convergence criteria
$\Phi_{gi}^{(n)}$	:	Total flux in group *g* and mesh *i* at n^{th} iteration
PI	:	Power Iterations
SI	:	Source Iterations
CG	:	Conjugate Gradient
TSA	:	Transport Synthetic Acceleration
TSA(CG)	:	CG based TSA

TABLE-1

Comparison of various computational schemes for LWR case

(Numbers in bold indicate CPU time taken)

Convergence Criteria			K-eff		
			Scheme-1 *Power Iterations with (SI)*	**Scheme-2** *Power Iterations with TSA(CG)*	**Scheme-3** *ORTHOMIN(1) with TSA(CG)*
ε_s	ε_f	ε_K			
10^{-3}	10^{-8}	10^{-8}	0.97683389 **316 sec**	0.97683390 **297 sec**	0.97370545 **114 sec**
10^{-5}	10^{-8}	10^{-8}	0.97683390 **475 sec**	0.97683390 **234 sec**	0.97681963 **68 sec**
10^{-7}	10^{-8}	10^{-8}	0.97683390 **918 sec**	0.97683390 **211 sec**	0.97683371 **125 sec**
10^{-8}	10^{-8}	10^{-8}	0.97683388 **1277 sec**	0.97683387 **252 sec**	0.97683388 **158 sec**

TABLE-2

Comparison of various computational schemes for CF(AHWR) case

(Numbers in bold indicate CPU time taken)

Convergence Criteria			K-eff		
			Scheme-1 Power Iterations with (SI)	**Scheme-2** Power Iterations with TSA(CG)	**Scheme-3** ORTHOMIN(1) with TSA(CG)
ε_s	ε_f	ε_K			
10^{-5}	10^{-6}	10^{-6}	1.00153294 **17379 sec**	1.00153335 **6375 sec**	1.00158444 **1862 sec**
10^{-6}	10^{-6}	10^{-6}	1.00145453† ***> 6 hrs***	1.00153041 **4752 sec**	1.00153459 **2963 sec**
	10^{-8}	10^{-8}		1.00153441* **> 6000 sec**	1.00153455 **2980 sec**

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

*Did not converge, unconverged $\varepsilon_f = 0.4 \times 10^{-6}$.

Figure-1(a)

Schematic diagram showing horizontal (XY) cross-section of the Critical Facility

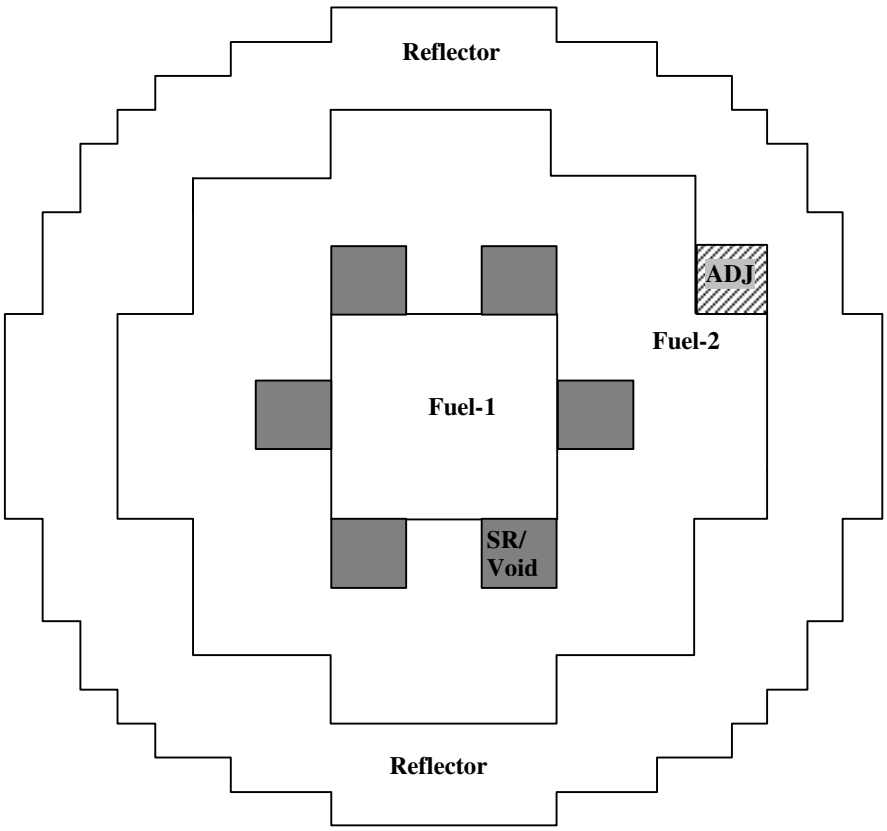
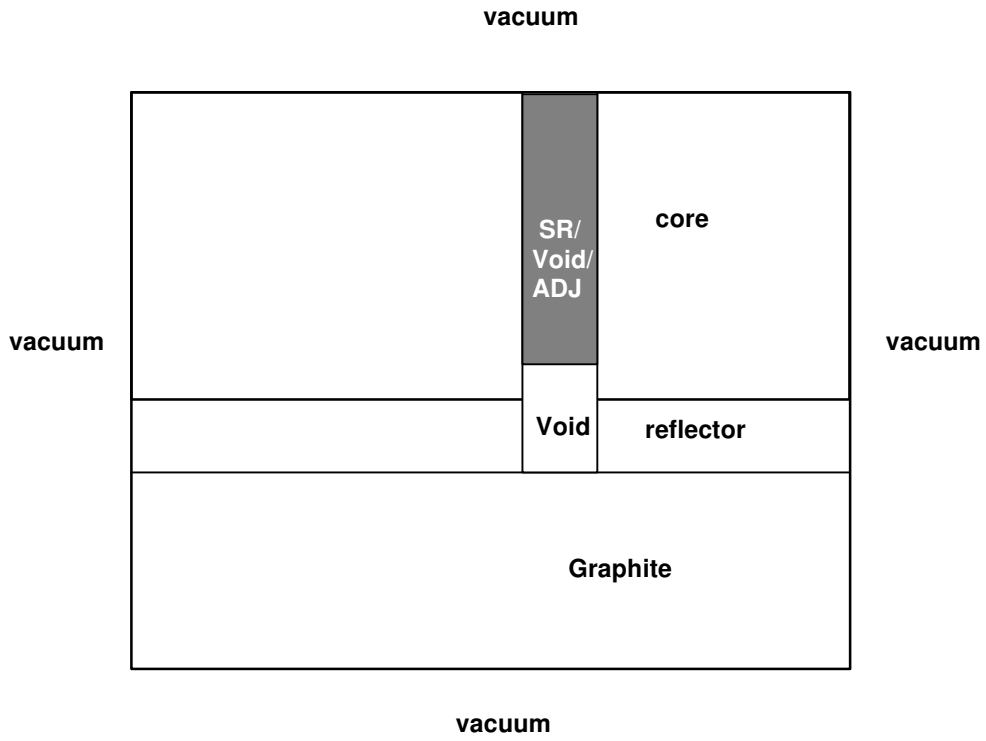


Figure-1(b)

Schematic diagram showing vertical (XY) cross-section of Critical Facility (only one reactivity device shown)



Nuclear Data Used in CF(AHWR) Case

A. Fission Spectrum

0.75000 0.25000 0.00000 0.00000

B. Transport And Fission Cross Sections (cm^{-1})

Σ_t	$\nu\Sigma_f$	Σ_t	$\nu\Sigma_f$
1-REFERENCE CORE		2-SHUT-OFF ROD	
1.25998E-01	7.07594E-03	1.38706E-01	0.00000E+00
2.80706E-01	9.90751E-05	2.76262E-01	0.00000E+00
2.62942E-01	5.67375E-04	2.59271E-01	0.00000E+00
3.90290E-01	5.40365E-03	3.86726E-01	0.00000E+00
3-REFLECTOR		4-AHWR CORE	
1.54344E-01	0.00000E+00	9.87713E-02	1.17296E-03
3.23939E-01	0.00000E+00	2.10247E-01	2.99718E-04
2.75888E-01	0.00000E+00	1.78728E-01	3.18981E-03
4.09758E-01	0.00000E+00	2.43648E-01	1.37307E-02
5-GRAPHITE		6-GUIDE TUBE	
1.65726E-01	0.00000E+00	1.05265E-01	0.00000E+00
3.97491E-01	0.00000E+00	2.45775E-01	0.00000E+00
4.03495E-01	0.00000E+00	2.62945E-01	0.00000E+00
4.34822E-01	0.00000E+00	3.77983E-01	0.00000E+00

C. Scattering Cross sections (cm^{-1})

1-REFERENCE CORE

GROUPS	1=>	2=>	3=>	4=>
1	6.18932E-02	0.00000E+00	0.00000E+00	0.00000E+00
2	6.12050E-02	2.50787E-01	0.00000E+00	0.00000E+00
3	3.44825E-06	2.91040E-02	2.44438E-01	5.36027E-05
4	6.32047E-13	7.00155E-08	1.66313E-02	3.85937E-01

2-SHUT-OFF ROD

GROUPS	1=>	2=>	3=>	4=>
1	5.63723E-02	0.00000E+00	0.00000E+00	0.00000E+00
2	8.21936E-02	2.41236E-01	0.00000E+00	0.00000E+00
3	1.29559E-06	3.49625E-02	2.40861E-01	2.63748E-05
4	0.00000E+00	5.41831E-08	1.80788E-02	3.83955E-01

3-REFLECTOR

GROUPS	1=>	2=>	3=>	4=>
1	6.03854E-02	0.00000E+00	0.00000E+00	0.00000E+00
2	9.38997E-02	2.84855E-01	0.00000E+00	0.00000E+00
3	2.75020E-06	3.90840E-02	2.57052E-01	4.81041E-05
4	0.00000E+00	9.43943E-08	1.88318E-02	4.09666E-01

4-AHWR CORE

GROUPS	1=>	2=>	3=>	4=>
1	5.46349E-02	0.00000E+00	0.00000E+00	0.00000E+00
2	4.33502E-02	1.91050E-01	0.00000E+00	0.00000E+00
3	2.27514E-06	1.85051E-02	1.66790E-01	1.22585E-04
4	5.50861E-16	4.48954E-08	8.59724E-03	2.33361E-01

5-GRAPHITE

GROUPS	1=>	2=>	3=>	4=>
1	1.44383E-01	0.00000E+00	0.00000E+00	0.00000E+00
2	2.12941E-02	3.91116E-01	3.17293E-05	0.00000E+00
3	0.00000E+00	6.30334E-03	3.68984E-01	6.57852E-05
4	0.00000E+00	0.00000E+00	3.42398E-02	4.33358E-01

6-GUIDE TUBE

GROUPS	1=>	2=>	3=>	4=>
1	4.09184E-02	0.00000E+00	0.00000E+00	0.00000E+00
2	6.43459E-02	2.32547E-01	1.41385E-05	0.00000E+00
3	0.00000E+00	1.29338E-02	1.77224E-01	2.07889E-06
4	0.00000E+00	2.89616E-04	8.56855E-02	3.77847E-01