On the Accelerated Sub-Critical Multiplication (ASCM) Scheme in code ATES3 for Sub-critical ADS Analysis

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Abstract. The present paper is concerned with a 3-D Cartesian geometry deterministic neutron transport code "ATES3" developed in BARC [1,2], India, with emphasis on its capabilities relevant to sub-critical ADS (Accelerator Driven Systems). It is a finite difference Discrete Ordinates (S_n) code which can handle anisotropic scattering of any order. It can solve static K-eigenvalue problem and external source problem in a Nuclear Reactor. The code is equipped with conventional methods of solution as well as the modern Krylov Sub-space methods. The code can find the quantity K_s (often called K-source) which is of primary importance to ADS.

The solution of external source problem in a sub-critical state is the main calculation needed for ADS analysis. It is obtained by the usual within-group source iterations and the fission source (or outer) iterations. One of the concerns is that the fission source iterations converge very slowly if K_{eff} is close to unity. In order to improve the convergence, an acceleration scheme called ASCM (Accelerated Sub-Critical Multiplication) has been incorporated in ATES3 and is found to work very well [3]. The ASCM scheme is explained. The code has been used for neutronic analysis of a sub-critical experiment in PFBR [4]. It was also used to compute K_s and flux distribution in IAEA ADS Benchmarks [5,6]. The effect of using transport-corrected cross-sections from WIMS Library on the convergence of source iterations in S_n-method is discussed. Further planned work on ATES3 is described.

Keywords: Subcritical Reactor, Acceleration schemes, Neutron Transport

INTRODUCTION

A code called ATES3 (Anisotropic-scattering based Transport Equation Solver in 3D) was developed [2] in Cartesian geometry primarily for steady state neutronics problems in conventional critical reactors. The subcritical source option in it can be used for ADS analysis. This paper presents a brief description of the code with emphasis on its capabilities relevant to ADS. The fission source iteration method for external source problem in a sub-critical medium and its effective acceleration by ASCM is discussed. Some issues related to WIMS library are mentioned.

MAIN FEATURES OF CODE ATES3

The code ATES3 is a modular computer program developed using Fortran-90/95 to solve the time-independent, multigroup discrete ordinates form of the Neutron Transport equation in XYZ Cartesian geometry. It uses finite differencing in space and the discrete ordinates (Sn) method for directions. It has user friendly input preparation and is well documented. It uses multi energy group and fine energy groups representations. It can solve K-eigenvalue and external source problem in multiplying and non-multiplying medium. It handles anisotropic scattering to any order. The code has options for conventional as well as advanced Krylov subspace schemes and options for selective flux printing / flux dumping, Re-start etc. ATES is validated against international benchmarks [1,2].

EXTERNAL SOURCE PROBLEM

The fission source iterations

The external source problem can be written using integro-differential form of the multi-group Neutron Transport equation as :

$$\begin{aligned} &\Omega \cdot \nabla \Psi_g(r,\Omega) + \sigma_g \Psi_g(r,\Omega) \; = \\ &\int \sigma_{g\to g}(\Omega' \to \Omega) \Psi_g(r,\Omega') \, d\Omega' \; + \; Q_g^{tot} \end{aligned} \tag{1}$$

where group g varies from 1 to G and Q^{tot} denotes the sum of all sources except the self scattering source, namely fission source, scattering source from other groups and external source. Eq.(1) can be written in a compact form as:

$$\mathrm{T}\ \Psi_g = \mathrm{S}\ \Psi_g + \mathrm{Q}_g \tag{2}$$

The set of all G equations in Eq.(1) can be written by rearranging terms as:

$$M\,\Psi = F\Psi + \mathrm{Q} \tag{3}$$

Where F is fission source operator, Q is the external source and M stands for all other terms of transport equation. Eq.(3) is solved by the fission source iterations shown as:

$$M\,\Psi^{n+1} = F\Psi^{n} + \mathrm{Q} \tag{4}$$

The superscript *n* denotes iteration number.

For above equation, $M^{-1}F$ is the "iteration matrix". The asymptotic rate of convergence of iterations depends on spectral radius $Sp(M^{-1}F) = K_{eff}$. If K_{eff} is very close to 1, the iterations converge very slowly.

Let ERRFS denote the maximum relative point wise error in successive fission sources given by:

$$\mathrm{ERRFS} = max_i \left\{ \frac{abs(F\Phi_i^{n+1} - F\Phi_i^{n})}{F\Phi_i^{n+1}} \right\} \tag{5}$$

where *i* stands for element number of fission source vector $F\Phi$, Φ being the total flux.

A small positive number EPSFS is chosen (here 10^{-5} and 10^{-6}). Iterations are stopped when ERRFS become smaller than EPSFS.

To solve Eq.(4), one needs to obtain effect of M^{-1} on vector $F\,\Psi$. This is obtained by solving $M\,\mathbf{x} = F\,\Psi$. This involves solution of Eq.(2) in each energy group, which is obtained by the "source iterations". The convergence criterion for source iterations is analogous to EPSFS and is chosen to be 10^{-5} in present paper. The source iterations involve "sweeping" a spatial region for each direction using principle of directional evaluation.

The ASCM method

An acceleration scheme called ASCM (Accelerated Sub-Critical Multiplication) has been suggested as an option in the well-known 3-D S_n-method based neutron transport code TORT [8]. The ASCM method can be briefly described as follows.

After a few fission source iterations as shown in Eq. (4), a scaling factor "f" is evaluated in every subsequent iteration using following formula:

$$f = \frac{1}{1 - \frac{\langle F\Psi^{n+1}\rangle - \langle F\Psi^{n}\rangle}{\langle Q\rangle}} \tag{6}$$

The $\langle F\Psi^{n}\rangle$ stands for sum of all the elements of vector $F\Psi^{n}$ weighted by corresponding mesh volume. After computing 'f', all the fluxes (and fission sources) are multiplied by 'f' before starting next iteration. This corrects the overall flux level and fission source convergence is improved. As the iterations proceed, 'f' tends to unity because $F\Psi^{n+1}$ tends to $F\Psi^{n}$. A derivation of the scaling factor f based on overall neutron balance has been given in a recent paper [9].

NUMERICAL RESULTS ON ASCM

There exists a realistic 3-D two energy group LWR K_{eff} benchmark problem by Takeda [7] with two states of the reactor: control rod (CR) Out and In. The sub-criticalities are about 23 and 38 mk, which is a typical value for ADS. It can be modeled by a uniform 25×25×25 mesh structure for the 1/8th core. We have designed a test-case for ADS by considering an external fast source of unit strength kept in the central 8 meshes of the full core. The flux distribution is found for both cases (CR In and Out) with and without ASCM with EPSFS=10^{-5} and 10^{-6}. Table 1 shows that a speed-up by an order of magnitude can be obtained. In the case with CR out, K_{eff} is closer to unity and hence the speed-up is larger. From Table 2 it is seen that the K-source is larger than K_{eff} as expected from the fact that the source is located in a high importance region. Table 3 gives fluxes obtained at selected meshes for all the cases. It may be noted that the fluxes obtained with ASCM for EPSFS=10^{-5} are as good as those obtained without ASCM for EPSFS=10^{-6}.

TABLE 1. Effect of ASCM on run time

Case	Method	EPSFS	Outer Iterations	CPU Time (sec)
CR Out	No ASCM	10^{-5}	348	616
		10^{-6}	446	938
	With ASCM	10^{-5}	17	22
		10^{-6}	15	30
CR In	No ASCM	10^{-5}	232	401
		10^{-6}	286	602
	With ASCM	10^{-5}	18	21
		10^{-6}	16	29

TABLE 2. Computed Eigenvalues

Case	K-eff	K-Source
CR-Out	0.97673	0.98576
CR-IN	0.96235	0.97724

TABLE 3. Thermal flux in selected meshes for LWR test case

Mesh (i, j, k)	No ASCM		With ASCM	
	10^{-5}	10^{-6}	10^{-5}	10^{-6}
1, 1, 1	1.33994×10^{-1}	1.33642×10^{-1}	1.33599×10^{-1}	1.33601×10^{-1}
1, 25, 1	2.95803×10^{-2}	2.94387×10^{-2}	2.94228×10^{-2}	2.94226×10^{-2}
25, 1, 1	3.37564×10^{-2}	3.35987×10^{-2}	3.35818×10^{-2}	3.35809×10^{-2}
1, 25, 25	1.37256×10^{-3}	1.36586×10^{-3}	1.36508×10^{-3}	1.36510×10^{-3}
1, 1, 25	2.91665×10^{-2}	2.90271×10^{-2}	2.90113×10^{-2}	2.90112×10^{-2}
5, 5, 5	7.21138×10^{-2}	7.18062×10^{-2}	7.17717×10^{-2}	7.17711×10^{-2}
25, 25, 25	8.64964×10^{-5}	8.60742×10^{-5}	8.60260×10^{-5}	8.60263×10^{-5}

CONCLUSION AND DISCUSSION

The code ATES3, primarily developed for critical reactors, is useful for ADS analysis also. For the test case, ASCM provides a speed-up by over an order of magnitude. In most realistic analysis with finer groups and meshes and anisotropic scattering, CPU times increase drastically and ASCM would be very useful. In case of thermal systems, it is possible to use the transport corrected 172-group WIMS Library cross-sections [10]. For fine groups, sometimes the self-scattering cross-section becomes negative and large in magnitude. This creates difficulties in convergence of source iterations. However, usually reasonable results are obtained.

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