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CONJUGATE GRADIENT METHOD TO SOLVE 3-D NEUTRON TRANSPORT EQUATION WITH ISOTROPIC SCATTERING

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ABSTRACT

The utility of Conjugate Gradient (CG) method for the efficient solution of 3-D (xyz-geometry) S_n-equations based on Diamond Difference Scheme is demonstrated for problems with isotropic scattering. The K-eigenvalue problem is analysed for two international benchmark problems which model a small LWR and a FBR cores. A computer code 'ATES3' is being developed which has option of using CG method to solve the Transport Equation. It is also being parallelised.

Key Words: Neutron Transport, Conjugate Gradient, Diamond Difference

1. INTRODUCTION

Recently, the Conjugate Gradient like methods are being extensively studied for Neutron Transport problems in Nuclear Reactors [1]. The reason is that these methods have a potential of being much more efficient than the conventional methods and are also suitable for parallelisation. Most of the studies [2] [3] [4] are concerned with Discrete Ordinate methods for 2-D problems although many other aspects such as spatial heterogeneity, anisotropic scattering and sophisticated methods of spatial discretisation are considered. Here, the CG-method is studied for 3-D Cartesian xyz-geometry problems for a small LWR and FBR [5] benchmarks. These cases are multi-group K-eigenvalue problems. The spatially finite-differenced S_n-method is considered with Diamond Difference Scheme [6]. These studies are based on a computer code ATES3 (Anisotropic Transport Equation Solver for 3D problems) which has option of using CG-method.

The plan of the paper is as follows. Section 2 gives a brief description of the use of CG-method. Section 3 gives the results for the test cases. Section 4 gives conclusions.

2. METHOD OF ANALYSIS

It is well known that the solution of a multi-group K-eigenvalue problem is often obtained by solving repeatedly several mono-energetic (one group) external source problems. The external source consists of contribution form fission and group-to-group scattering to the particular group for which the problem is being solved. Such a one group source problem can be written as:

$$\Omega \cdot \nabla \Psi(r,\Omega) + \Sigma_t \Psi(r,\Omega) - \Sigma_s \int f_{scat}(r,\Omega' \rightarrow \Omega) \Psi(r,\Omega') d\Omega' = q(r,\Omega) \tag{1}$$

Here ψ (r, Ω) denotes angular flux at a point r in a direction Ω. q (r, Ω) is the space and direction dependent known external source. Σ_t and Σ_s are the macroscopic total and scattering cross-sections while f is scattering function. The equation is solved in the presence of appropriate boundary conditions. For isotropic scattering, f equals unity and the above equation can be written as:

$$T\,\psi = \gamma L\psi + q \tag{2}$$

where the operators T, γ and L have appropriate meaning. $L\psi$ equals the total flux ϕ. T is streaming plus collision operator. γ denotes effect of multiplying by scattering cross-section Σ_s. Denoting LT^{-1} by κ and iteration number by n, the simple SI-method method can be described as [4]:

$$\phi^{n+1} = \kappa \gamma \phi^n + \kappa q \tag{3}$$

For the application of CG-method, Eq.(3) is written as:

$$(I - \kappa \gamma)\,\phi = \kappa q \tag{4}$$

This represents a set of linear equations to which the CG-method can be applied. The main features of the procedure are:

[i] The use of standard CG-method for Eq.(4) requires that the coefficient matrix be Symmetric Positive Definite (SPD). If scattering cross-section Σ_s varies with space or mesh volumes are unequal ($I - \kappa\gamma$) is not SPD. However, the standard CG-method can be used if all inner products occurring in the algorithm are volume integrations weighted by scattering cross-sections [7].

[ii] The effect of the operator κ (= LT^{-1}) on another vector needs to be evaluated repeatedly in the CG-methods. This is achieved by the well-known mesh-angle sweeps based on principle of Directional Evaluation [4] [6].

[iii] It is known that Diamond Difference Scheme can occasionally lead to negative fluxes. As mentioned in the earlier studies of 2-D problems [4], the CG-method can be directly used to solve the finite difference need S_n-equation provided the problem is not prone to the negative

fluxes. It was also mentioned [4] that this is often true for the K-eigenvalue problem due to the presence of widely distributed fission source. In the 3-D problem presented here. also, the CG-method could be directly used and leads to substantial benefit over the Simple Source iterations (SI) method.

3. ANALYSIS OF TEST CASES

3.1. LWR Benchmark

This is a 3-D 2- group small light water reactor benchmark [5]. The $1/8^{th}$ reactor model extends upto 25 cms in each direction. It contains core, reflector and control rod. The S_4 symmetric quadrature set was used. There are 25 uniform meshes in each direction. The problem was solved using SI and CG-methods.

It should be mentioned that, in the present work no acceleration scheme is employed to reduce the number of outer iterations. The CG-method is used to reduce the number of inner iterations required per outer iterations.

Table-I gives the computed K-eigenvalue (with and without control rod) and CPU times for CG and SI-methods. For the results presented, the number of outer iterations required to solved the K-eigenvalue problem are same for the CG and SI-methods. In order to get similar K-eigenvalues with the two methods, however, the flux convergence for the SI-method needs to be tighter. The ratio of overall CPU times for the problems are a fair indication of the speed-up obtained by the CG-method over the SI-method. This applies to the next test case presented subsequently.

The convergence criteria ε and ε_k on flux and K-eigenvalue respectively are defined as:

$$\max_i \frac{\Phi_i^{(j)} - \Phi_i^{(j-1)}}{\Phi_i^{(j)}} < \varepsilon \tag{5}$$

$$\frac{K^{(n)} - K^{(n-1)}}{K^{(n)}} < \varepsilon_K \tag{6}$$

where j, n denote inner and outer iteration numbers and i denotes mesh point. As seen from table-I, a more stringent point flux convergence is required for SI-method to get result comparable with CG-method. This is also applicable to table-II related to the FBR benchmark discussed subsequently.

Table I. Results of LWR benchmark

Case	rod-out		rod-in	
	SI-method	CG-method	SI-method	CG-method
K-eff	0.976825	0.976805	0.961896	0.961899
No. of outer iterations	14	14	14	14
Convergence Criterion ε_K (for K)	10^{-5}	10^{-5}	10^{-5}	10^{-5}
Convergence Criterion ε (for Flux)	10^{-10}	10^{-4}	10^{-10}	10^{-4}
CPU (sec)	2170	204	2137	218

3.2 FBR Benchmark

This is a 3-D, 4-group FBR test case [5]. there are 5 regions: core, axial blanket, radial blanket and control rod (in/out). There are 14x14x30 uniform meshes in the $1/4^{th}$ core. The S_4 symmetric quadrature set was used. The results are given in Table-II.

Table II. Results of FBR benchmark

Case	rod-out		rod-in	
	SI-method	CG-method	SI-method	CG-method
K-eff	0.972929	0.973047	0.958739	0.958959
No. of outer iterations	18	18	18	18
Convergence Criterion εK (for K)	10^{-5}	10^{-5}	10^{-5}	10^{-5}
Convergence Criterion ε (for Flux)	10^{-8}	10^{-5}	10^{-8}	10^{-5}
CPU (sec)	1833	202	2002	261

3. CONCLUSIONS

The CG-method is seen to provide a speed-up of about 10 times over the simple SI-method for the 3-D whole core problems considered. The speed-up is expected to be even more for the heavy water reactors because SI-method convergence is slower due to less absorption. The method would be valuable for criticality calculations with many more energy groups which take significant computational efforts. It is expected to be useful for kinetics problems also where one has to solve a source problem in multiplicative medium for each time-step. The method is being tested for a large variety of problems.

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