Research on an efficient preconditioner using GMRES method for the MOC

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1. Introduction

The modeling accuracy of reactor analysis techniques has improved considerably with the progressive improvements in computational capabilities. The method of characteristics (MOC) solves the neutron transport equation using tracking lines which simulates the neutron paths. The MOC is an accurate calculation method and is becoming a major solver because of the rapid advancement of the computer. In this methodology, the transport equation is discretized into many spatial meshes and energy wise groups. And the discretization generates a large system which needs a lot of computational costs.

To reduce computational costs of MOC calculation, we investigate the Generalized Minimal RESidual (GMRES) method as an accelerator and developed an efficient preconditioner for the MOC calculation. The preconditioner we developed was made by simplifying rigorous preconditioner. And the efficiency was verified by comparing the number of iterations which is calculated by one dimensional MOC code.

2. Methods

2.1 Discretization of one dimensional MOC

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The multigroup transport equation to obtain the flux from an isotropic source, within a region i and energy group g, is

$$\frac{d}{ds}\varphi_g^i + \Sigma_{t,g}^i \varphi_g^i = Q_g^i, \tag{1}$$

where φ_g^i is the neutron angular flux in group g; $\Sigma_{t,g}^i$ is the total cross section in group g; s stands for the variable along the tracking line. The total source in Eq.(1) is composed of two terms: the within group source and outgroup source:

$$Q_g^i = W_g^i + S_g^i, \tag{2}$$

where

$$W_g^i = \sum_{s,g \to g}^i \phi_g^i,$$

$$S_g^i = \sum_{g',g' \neq g}^i \sum_{s,g' \to g}^i \phi_{g'}^i + \sum_{g'} \upsilon \Sigma_{f,g'}^i \phi_{g'}^i / K_{eff},$$

where ϕ_g^i is the neutron scalar flux in group $g; \Sigma_{s,A \to B}^i$ is the scattering cross section from group A to B. For a fixed direction, the equation is solved numerically:

$$\varphi_{n,g}^{i,out} = \varphi_{n,g}^{i,in} e^{-\Sigma_{t,g}^{i} \Delta s^{i}} + \frac{1 - e^{-\Sigma_{t,g}^{i} \Delta s^{i}}}{\Sigma_{t,g}^{i}} Q_{g}^{i}, \qquad (3)$$

where $\varphi_{n,g}^{i,out}$ and $\varphi_{n,g}^{i,in}$ are the incoming and the outgoing angular flux respectively. And n(=1...N) shows the number of direction of neutron travel. Discretized MOC system can be written in a form as

$$(\mathbb{I} - \mathbb{L}^{-1}\mathbb{W})\vec{\Phi} = \mathbb{L}^{-1}\mathbb{S},$$
(4)

where

- *Φ* : the vector which is composed of region scalar fluxes.
 I : identity matrix.
- \mathbb{L}^{-1} : sweeping matrix.
- W : within group scattering cross section matrix.
- S : out group source matrix.

2.2 GMRES method

The GMRES algorithm is commonly used to solve large nonsymmetric linear system of equationAx = b. This method makes an orthonormal basis $V = [v_1, v_2, ..., v_l]$ in Krylov subspace by using the Arnoldi process. A brief summary of the algorithm is given in Figure 1. In this paper, several preconditioners were investigated and the results were shown in the following section.

Calculate
$$\mathbf{r} = \mathbf{A}\mathbf{x} - \mathbf{b}, v_0 = r/||r_0||$$

Iterations: for $\mathbf{j}=\mathbf{1},...\mathbf{m}$
Arnoldi process

$$\begin{bmatrix} GMRES \\ \hat{v}_{j+1} = \mathbf{A}v_j \end{bmatrix} \text{ or } \begin{bmatrix} FGMRES \\ \omega_j = M^{-1}v_j \\ \hat{v}_{j+1} = \mathbf{A}v_j \end{bmatrix}$$

$$h_{j,k} = \langle \hat{v}_{j+1}, v_k \rangle \text{ for } \mathbf{k} \in \mathbf{c}_1, \mathbf{j} \end{bmatrix}$$

$$\hat{v}_{j+1} = \mathbf{A}v_j - \sum_{k=1}^{j} h_{j,k}v_k$$

$$h_{j+1,k} = || \hat{v}_{j+1} ||$$

$$v_{j+1} = \frac{\hat{v}_{j+1}}{h_{j+1,k}}$$
Updating the QR decomposition
Calculation of $|| r_j ||$
Convergence reached?

$$\bigvee \text{ yes}$$
End the iterative calculation
Update x

Figure 1 GMRES and FGMRES algorithm

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2.3 A preconditioner based on the diffusion theory.

GMRES algorithm can be accelerated by using proper preconditioning. One of the kinds of GMRES method is called FGMRES method which is shown in Figure 1. Acceleration techniques based on the diffusion theory has been investigated as a preconditioner of the system. In this paper, we verified the efficiency of inverse preconditioner ($\mathbb{I} + \mathbb{E}^{-1}\mathbb{W}$). where

$$\mathbb{E} = -\nabla \cdot D_g^i \nabla + \Sigma_{t,g}^i - \Sigma_{s,g \to g}^i, \tag{5}$$

2.4 A simplified preconditioner by the mean free path.

This preconditioner was made by simplifying rigorous preconditioner $(\mathbb{I} - \mathbb{L}^{-1}\mathbb{W})$. To reduce calculation time of making matrix elements and of inverse matrix, we ignored the linkage of regions which are optically far away from each other. The preconditioner M was simplified by the mean free path as an index as shown in Figure 2.





3. Results and Discussions

The numerical results are obtained for a 1200 meshes 1D problem. To evaluate the performance of acceleration techniques, two types of calculation which were different in cross section were performed. The results in Table 1 and Table 2 show the number of iterations and CPU time for different techniques. In table 1, we used MOX fuel and sodium cross sections. And in table 2, we used UO2 fuel and H2O cross sections.

Table 1 Number of iteratioins and CPU time: the MOX fuel

		FGMRES				
	GMRES	$\mathbb{I} + \mathbb{E}^{-1} \mathbb{W}$	simplified preconditioner			
			m=1	m=2	m=3	
Iterations	628	589	338	231	189	
CPU time(sec)	12.7	15.4	11.7	10.9	10.2	

All preconditioners succeed to reduce the number of

iterations in Table 1. And we obtained the best performance when m is 3. A preconditioner based on the diffusion theory does not reduce calculation time because the amount of production calculations between preconditioner and flux is relatively high.

Table 2							
Number of i	teratioins	and	CPU	time:	the	UO2	fuel

		FGMRES				
	GMRES	$\mathbb{I} + \mathbb{E}^{-1} \mathbb{W}$	simplified preconditioner			
			m=1	m=2	m=3	
Iterations	542	510	385	248	254	
CPU time(sec)	11.1	12.4	11.5	9.8	10.2	

As in the case of Table 1, all preconditioners reduce the number of iterations. In this case, we got the best performance when m is 2. As the preconditioner becomes rigorous, the calculation of the matrix needs more time. So the case m=3 was worse than the case m =2.

4. Conclusions

The preconditioner based on the diffusion theory and the simplified preconditioner can reduce CPU time and the number of iteratioin in GMRES algorithm. The simplified preconditioner using the mean free path was found to be very efficient. And the numbers of iteration were reduced more than 50 % especially when m is 2 or 3.

However, simplified preconditioner need large capacity of storage to calculate large problems. And we expect that this technique will be overcome by using methods such as multigrid method.

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