A Krylov Subspace Method for Unstructured Mesh S_N Transport Computation

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1. Introduction

Hong, et al., have developed a computer code MUST (***M**ulti-group **U**nstructured geometry **S**$_N$ **T**ransport*) for the neutral particle transport calculations in three-dimensional unstructured geometry [1]. In this code, the discrete ordinates transport equation is solved by using the discontinuous finite element method (DFEM) or the subcell balance methods with linear discontinuous expansion [2]. In this paper, the conventional source iteration in the MUST code is replaced by the Krylov subspace method to reduce computing time and the numerical test results are given.

2. Basic Concepts of Krylov Subspace Method

To solve 3-D particle transport equation by a deterministic method, the problem domain is divided in to small pieces and then governing equation is applied to each of them. In this way, a matrix equation is set up and it is solved in various ways. A preferred way of solving it is through sweeping process because in this way, it is not needed to make exact matrix form. Just sweeping through all elements and doing proper calculation for each cell is enough. Source iteration is simple and easy to use, but for some problem conditions it converges too slowly for practical use.

Krylov method basically solves the matrix equation, $Ax = b$. It seeks the solution in a special subspace called Krylov subspace, which is a spanned space of residual vectors [3].

$$K_l(A, r_0) = span\left\{r_0, Ar_0, A^2 r_0, \cdots\cdots, A^{l-1} r_0\right\}. \quad (1)$$

Looking for the solution in this subspace is a reasonable guess for nonsingular matrix A because there always exists a set of constants that satisfies

$$P_d(A,b) = I + a_1 A^1 + a_2 A^2 + \cdots + a_d A^d = 0\,. \quad (2)$$

By simply moving first term in Eq. (2), we obtain

$$\begin{aligned} I &= -[a_1 I + a_1 A^1 + \cdots + a_d A^{d-1}]A, \\ A^{-1} &= -[a_1 I + a_1 A^1 + \cdots + a_d A^{d-1}]. \end{aligned} \quad (3)$$

The solution that we are looking for exists in the Krylov subspace, where $r_0 = b$.

3. Implementation of Krylov Subspace Method

In Krylov subspace method, we need to generate Krylov subspace by multiplying matrix A to the residual vector. In source iteration for solving particle transport equation, solution is converged by iterative procedure [3, 4]:

$$\phi^{l+1} = \mathrm{D\,L^{-1}\,MS}\phi^{l} + \mathrm{D\,L^{-1}}\,q. \quad (4)$$

After one sweeping calculation, from the initial guess or previous step solution, ϕ^l, next step solution vector, ϕ^{l+1}, is obtained. This calculation is done iteratively until the solution converges, which means $\phi^{l+1} = \phi^l$. Then the Eq. (4) can be rewritten as

$$(\mathrm{I} - \mathrm{D\,L^{-1}\,MS})\phi = \mathrm{D\,L^{-1}}\,q. \quad (5)$$

This is a matrix equation of the form $Ax = b$ where $A = (\mathrm{I} - \mathrm{D\,L^{-1}\,MS})$, $b = \mathrm{D\,L^{-1}}\,q$. The action of the matrix A is not much different from that of transport sweeping. Therefore, whenever we need matrix action on some vector during Krylov subspace method, simply doing transport sweep is enough and this is already available in existing codes.

4. Test Problem and Numerical Results

We tested the Krylov subspace method on a simple test problem. The problem consists of two regions with different materials in each region. The source exists in inner small cube and is surrounded by moderator as shown in Figure 1. The problem domain is divided into 97980 elements of tetrahedron. The material properties are listed in Table I.

Table I. Material Properties of Test Problem

Source region	Moderator region
$\sigma_t = 1.0[cm^{-1}]$	$\sigma_t = 0.7\ [cm^{-1}]$
$\sigma_s = 0.7[cm^{-1}]$	$\sigma_s = 0.6[cm^{-1}]$
$\sigma_a = 0.3[cm^{-1}]$	$\sigma_a = 0.1[cm^{-1}]$
$q = 2.0[\#/cm^3]$	$q = 0.0[\#/cm^3]$

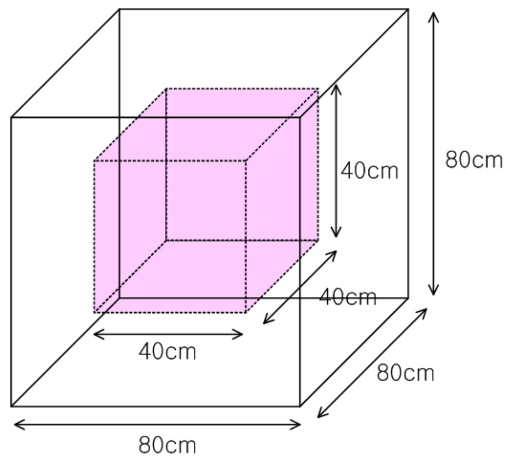

Fig. 1 Test Problem Description

A comparison between the results of conventional source iteration and Krylov subspace method is shown in Table II. It is clear that Krylov subspace method is efficient in the number of iterations and also in the computing time.

Table II. Comparisons of the Source Iteration and Krylov Subspace Method

	No. of iterations	CPU time [a]
Source Iteration	145	4097(sec)
Krylov Subspace Method	20	1811(sec)

[a]Intel Xeon 3.06GHz

It is well known that convergence rate becomes very slow as the scattering ratio gets closer to unity. However it seems that scattering ratio does not affect the convergence rate of the Krylov subspace method as much as it does for source iteration. For varying values of scattering ratio, source iteration and Krylov subspace method are compared in Table III.

Table III. Comparisons of the Source Iteration and Krylov Subspace Method for Various Scattering Ratio (c)

c		No. of iterations	CPU time
0.5	Source Iteration	39	1744
	Krylov Subspace Method	9	1310
0.6	Source Iteration	52	2028
	Krylov Subspace Method	15	1574
0.7	Source Iteration	74	2511
	Krylov Subspace Method	15	1576
0.8	Source Iteration	117	3470
	Krylov Subspace Method	17	1670
0.9	Source Iteration	244	6269
	Krylov Subspace Method	24	1980
0.95	Source Iteration	489	11593
	Krylov Subspace Method	38	2604

5. Conclusions and Further Study

Krylov subspace method can substitute the source iteration for the 3-D DFEM code MUST. Krylov subspace method itself is more efficient than conventional source iteration in number of iterations and computing time. It appears that the Krylov method is less sensitive to scattering ratio than source iteration. Furthermore, Krylov subspace method can easily adopt conventional acceleration methods in itself without painstaking work for modifying existing codes. Also the deficiencies of those methods lessen when they are used with Krylov subspace method. Implementing various acceleration methods such as CMR, CMFD and p-CMFD as preconditioners for “kryloved” MUST is in progress.

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