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Track truncation method for improving the computational efficiency of 2D matrix MOC

Yong Zheng, Minjun Peng *

Fundamental Science on Nuclear Safety and Simulation Technology Laboratory, Harbin Engineering University, Harbin 150001, China
College of Nuclear Science and Technology, Harbin Engineering University, Harbin 150001, China

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ABSTRACT

The method of characteristics (MOC) with matrix form has more favorable performance compared with its standard application. However, it is observed that the advantage decreases when the physical problem size becomes larger. The spatial domain decomposition method (DDM) is a better remedy to reduce computation burden for large scale problem, but increasing the outer iterations due to the decoupling between flat source regions. To overcome this drawback, the straightforward multi-domain coupling technique is studied and utilized in the current study based on a track truncation method (TTM). The resulting linear system is solved using preconditioned generalized minimal residual (PGMRES) method, a variant of Krylov subspace method. Numerical results for benchmark problems demonstrate the proposed acceleration technique is efficient in terms of memory usage and computation time without compromising accuracy for both hexagonal and rectangular geometries. For the large scale problem, it shows an ideal linear relationship between the memory/time required and the physical problem size rather than quadratic growth as before.

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1. Introduction

The method of characteristics (MOC, Askew, 1972) has become the most popular candidate to solve the neutron transport equation due to its excellent geometrical flexibility and natural parallelism. At present, the latest developed codes and the upgraded versions of previous software have introduced the MOC computation module to handle the arbitrary geometry for two dimension or three dimension neutron transport problem, such as DeCART (Joo et al., 2004), CRX (Hong and Cho, 1998), Chaplet (Kosaka and Saji, 2000), DRAGON (Marleau et al., 2011), CASMO-4 (Smith and Rhodes, 2002), nTRACER (Jung et al., 2009), MPACT (Kochunas et al., 2013; MPACT-Team, 2015), OpenMOC (Boyd et al., 2014) and so on. However, like other transport methods, the MOC method has the disadvantage of slow convergence, therefore an active area of research about MOC is to develop efficient acceleration techniques, such as the method of coarse mesh finite difference (CMFD, see Cho et al., 2008; Tang and Zhang, 2009), or other generalized diffusion acceleration techniques (Yamamoto, 2005; Cai et al., 2010; Zhu et al., 2016).

Derived from the recurrent characteristic sweeping operations, the method of characteristics with matrix form (MMOC, Zhang et al., 2011a, 2013; Wu et al., 2014) has potentially more favorable performance compared with its traditional implementation. In this method, the neutron scalar fluxes and boundary angular fluxes are involved explicitly in the linear system which is determined by the ray tracing information and cross section library. Consequently, the characteristic sweeping operations and inner iterations have been converted to solving the resulting linear algebraic equations. The method of characteristic direction probabilities (CDP, Hong and Cho, 1999; Liu et al., 2015a,b) also replaces the segment-wise sweeping operations using a series of linear algebraic expressions, however it keeps the inner iterations to converge the scalar flux in each energy group, and there is no linear system to be solved. Since these equations' coefficient matrices are unsymmetric and sparse in the MMOC method, the generalized minimal residual (GMRES, Saad and Shultz, 1986) method is chosen to handle this type of problem. Actually, the restart version of GMRES has been already used widely to solve the neutron transport problems (Turcksin et al., 2012; Zhang et al., 2011a). Although the algorithm has excellent performance, the benefit of the matrix form of MOC would be weakened significantly for the large scale problems. These difficulties arise from two aspects, namely, the storage space and computation time.

* Corresponding author at: Fundamental Science on Nuclear Safety and Simulation Technology Laboratory, Harbin Engineering University, Harbin 150001, China.
E-mail address: heupmj@163.com (M. Peng).

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To compensate the mentioned defects, the spatial domain decomposition method (DDM) and the Multitask-parallel mechanism have been adopted in the MMOC program-AutoMOC (Zhang et al., 2011a). In DDM, the entire geometry has been divided into several subdomains, the linear algebraic system was generated for each subdomain and solved on individual threads. These subdomains were coupled by the subdomain interface angular fluxes obtained from each thread. This technique could reduce computation time when there were not too many subdomains generated. However, it is hard to identify that the benefits are from the DDM or the parallelization, and there is a limitation of the number of subdomains since the outer iterations would increase with the increase of subdomains.

In the current paper, we analysed the temporal and spatial properties of MOC based on the preconditioned Krylov subspace technique, subsequently a track truncated method(TTM) was proposed and verified using the benchmark problems with hexagonal complicated geometry, i.e. HTTR benchmark problem (Zhang et al., 2011b) and rectangular geometry, i.e. OECD/NEA C5G7 MOX benchmark problem (Smith et al., 2003). The proposed method truncates the long characteristic line to several shorter "subtracks", which are coupled through the neutron angular flux continuity condition. In the conventional DDM, the subdomains' coupling was achieved by the information exchange among the activated threads, in the proposed method the coupling relationship of the subtracks is handled implicitly by the coefficient matrix for each energy group. The execution mode is unchanged from the previous code, namely, there is no additional modification to the previous procedures except for the inexpensive computation and post-processing for the track tracing.

The remainder of this paper is organized as follows: Section 2 describes the methodologies of this work, including the details about other essential techniques implemented in the current study, Section 3 displays the numerical experiments for the verification and evaluation of the proposed method, Section 4 makes the conclusions for the present work.

2. Theoretical model

2.1. Matrix characteristics method

The MOC method solves the characteristic form of the transport equation by following the straight neutron paths of the neutral particle:

$$\frac{d\psi(s)}{ds}+\Sigma_t(s)\psi(s)=q(s) \tag{1}$$

where ψ is the neutron angular flux; s is the local coordinate along the track. If the cross-section Σ_t and neutron source q are both assumed to be constants in a fine region i, the track's outgoing angular flux can be expressed as a source term and incident angular flux for the flat source region i:

$$\psi_{i,k}^{out}=\psi_{i,k}^{in}\exp(-\Sigma_{t,i}s_i)+\frac{q_i}{\Sigma_{t,i}}[1-\exp(-\Sigma_{t,i}s_i)] \tag{2}$$

where $\psi_{i,k}^{in}$ and $\psi_{i,k}^{out}$ are the incident and outgoing angular fluxes of track k on the region i, respectively; s is the segment length.

It is natural to obtain the outgoing flux with a known incident flux ψ_k^{in} on the boundary by using Eq. (2) recursively:

$$\psi_{I,k}^{out}=\psi_k^{in}e_{0,I}+\sum_{j=0}^{I}\frac{q_j}{\Sigma_{t,j}}\left[1-\exp\left(-\Sigma_{t,j}s_j\right)\right]e_{j+1,I} \tag{3}$$

where 0 and I denote the ID numbers of the first flat source region (FSR) and the last FSR traversed by track k; s is the segment length; q_j represents the neutron source in region j crossed by this track; $e_{j,I}$ represents the exponential attenuation coefficient from region j to I along the track k. They can be obtained by Eq. (4):

$$\begin{cases} q_j^g=\sum_{g'=1}^{G}\Sigma_{j,s,g'g}\phi_{j,g'}+\frac{\chi_{j,g}}{k_{eff}}\sum_{g'=1}^{G}(\nu\Sigma)_{j,f,g'}\phi_{j,g'} \\ e_{j,I}=\exp\left(-\Sigma_{t,j}s_j-\Sigma_{t,j+1}s_{j+1}\ldots-\Sigma_{t,I-1}s_{I-1}\right) \end{cases} \tag{4}$$

If the $\psi_{I,k}^{out}$ in Eq. (3) is the outgoing flux on the boundary, the K linear equations can be obtained through applying the boundary condition to all tracks (assuming K tracks in total). It should be noted that only the vacuum and albedo boundary conditions are considered in the current work. Transforming the K equations into operator form, one can obtain:

$$S_1\Phi+(E+S_1')\Psi=-S_1''Q \tag{5}$$

where Φ,Ψ and Q are the vectors of scalar fluxes, incident fluxes on the boundaries and sources(including the scattering source from other energy groups and the fission source), respectively; S_1,S_1' and S_1'' are the sweeping matrices of dimension $K\times L,K\times K$ and $K\times L$, respectively; L,K are the numbers of regions and tracks, respectively; E stands for the diagonal matrix which indicates the mapping relationship between tracks on the outer boundaries.

The segment average angular flux can be computed from the incident flux and the region's source term, further, the region average angular flux can be calculated in terms of the "width" of the segments and their average angular fluxes. After computing the weighted sum of the whole region average angular fluxes located in region i, the scalar flux of region i can be generated:

$$\phi_i=f_1(q_i)+\sum_{k\in i}\left[f_2(\psi_k^{in})+\sum_{j\in up(i)}f_3(q_j)\right] \tag{6}$$

where f_1,f_2 and f_3 represent the response functions; $k\in i$ refers to the tracks traversing the region i; and $j\in up(i)$ refers to the regions in the up-streaming direction of region i.

After leaving only the source term on the right hand side and rearranging Eq. (6), by taking all the flat source regions into account, another L linear equations with operator form can be obtained:

$$(S_2+D_2)\Phi+S_2'\Psi=-S_2''Q \tag{7}$$

where S_2 denotes the $L\times L$ sweeping matrix for the scalar flux contribution between fine regions; S_2' represents the $L\times K$ sweeping matrix involving the incident angular flux contribution; S_2'' is the $L\times L$ sweeping matrix for the source contribution between fine regions; D_2 is a $L\times L$ diagonal matrix whose elements are the differences between the transport and self-scattering cross sections. The Eqs. (5) and (7) can make up the closed linear algebraic system Eq. (8), which is the typical operator form of MMOC (Zheng et al., 2017) and is the resulting system to be solved iteratively using a preconditioned Krylov subspace technique:

$$\begin{bmatrix} S_2+D_2 & S_2' \\ S_1 & S_1'+E \end{bmatrix}\begin{bmatrix}\Phi\\ \Psi\end{bmatrix}=-\begin{bmatrix}S_2''\\ S_1''\end{bmatrix}Q \tag{8}$$

2.2. Computation complexity

Based on the aforementioned method, the coefficient matrix composed of S_1,S_2,S_1',S_2',E and D_2 would be sparse and irregular undoubtedly. In order to take advantage of the large number of zero elements, the compressed sparse row format (CSR, see Saad, 2003) was chosen as the storage scheme. In this scheme, the matrix construction involves three steps: building the matrix

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