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An acceleration technique for 2D MOC based on Krylov subspace and domain decomposition methods

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ABSTRACT

The method of characteristics (MOC) has great geometrical flexibility but poor computational efficiency in neutron transport calculations. The generalized minimal residual (GMRES) method, a type of Krylov subspace method, is utilized to accelerate a 2D generalized geometry characteristics solver AutoMOC. In this technique, a form of linear algebraic equation system for angular flux moments and boundary fluxes is derived to replace the conventional characteristics sweep (i.e. inner iteration) scheme, and then the GMRES method is implemented as an efficient linear system solver. This acceleration method is proved to be reliable in theory and simple for implementation. Furthermore, as introducing no restriction in geometry treatment, it is suitable for acceleration of an arbitrary geometry MOC solver. However, it is observed that the speedup decreases when the matrix becomes larger. The spatial domain decomposition method and multiprocessing parallel technology are then employed to overcome the problem. The calculation domain is partitioned into several sub-domains. For each of them, a smaller matrix is established and solved by GMRES; and the adjacent sub-domains are coupled by "inner-edges", where the trajectory mismatches are considered adequately. Moreover, a matched ray tracing system is developed on the basis of AutoCAD, which allows a user to define the sub-domains on demand conveniently. Numerical results demonstrate that the acceleration techniques are efficient without loss of accuracy, even in the case of large-scale and strong scattering problems in complex geometries.

1. Introduction

In the process of reactor physical analysis, neutron transport equation often has to be solved accurately in very complicated geometries. Among various deterministic methods for neutron transport calculation, the method of characteristics (MOC) is the best candidate to treat strong geometrical heterogeneities (Askew, 1972). In this algorithm, sets of trajectories crossing the computational domain are generated in each of the discretized directions and intersect numerous arbitrary-shaped spatial meshes with flat or linear source approximations. Then the neutron transport equation is solved by sweeping the trajectories repeatedly to obtain the angular fluxes and mean scalar flux in every mesh.

Owing to the great geometrical flexibility by nature, MOC has been included as an important neutron transport solving module by many reactor analyzing softwares in recent years (Sanchez et al., 1988; Knott et al., 1995; Halsall, 1998). AutoMOC is one of the MOC programs (Chen et al., 2008). Its novelty consists in the use of the powerful functionality on engineering graphics and customizations offered by the computer aided design software AutoCAD in geometry processing and ray tracing. Distinguished from some other MOC solvers which utilize modular ray tracing technique (Halsall, 1980; Cho et al., 2008; Tang and Zhang, 2009), AutoMOC is based on the long characteristics technique. It generates characteristics rays in the entire problem domain and hardly imposes limitation on geometry.

However, AutoMOC encounters computational efficiency problems just like other MOC solvers do; hence an effective and geometry-flexible acceleration technique is urgently needed. The well-known acceleration technique coarse-mesh finite difference (CMFD) method has been applied to MOC solvers for large-scale calculations in reactors (Joo et al., 2002; Cho et al., 2008; Tang and Zhang, 2009) and favorable effects were gained. However, the method which is based on the finite difference format has the inherent drawback of geometrical applicability. The difficulty is overcome by the generalized coarse-mesh rebalance (GCMR) (Yamamoto, 2005) and the generalized coarse-mesh finite difference (GCMFD) method (Chai et al., 2010). Unfortunately, a factor which determines the convergence property cannot be given as *a priori*, which is a flaw in theory though it could be handled numerically as an expedient. Some other techniques such as the multigrid method (Grassi, 2007) have been proposed to accelerate MOC in

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generalized geometry. However, sometimes the acceleration effects may be weakened by the time-consuming solution of acceleration equations.

In this study, an acceleration technique based on the Krylov subspace methods for linear algebraic equation systems is conducted. It requires no additional acceleration step and avoids redundant computational effort. A form of linear system is constructed to replace the conventional characteristics sweep (i.e. inner iteration) scheme in MOC. The angular flux moments and boundary angular fluxes are involved in the linear systems instead of the scalar fluxes and boundary currents respectively (Dahmani et al., 2005), which makes the description of transport problems more precisely. Then the equation systems are solved by the generalized minimal residual (GMRES) method, which is a widely-used Krylov subspace method for solving systems with non-symmetric coefficient matrices efficiently. Comparing with another Krylov subspace method Lanczos algorithm (Santandrea and Sanchez, 2002), the GMRES method skips the symmetrization process and permits the potential use of several preconditioners. The geometry flexibility of this technique is perfect due to the theoretical equivalence between the original MOC and the accelerated one. Moreover, it is reliable in theory and simple for implementation.

However, it is observed that the speedup decreases when the matrix becomes larger in the Krylov subspace acceleration method. The main reason is that the time spent on both the construction and solution of the matrix increases sharply as the matrix grows large. This problem causes the inability of the Krylov subspace acceleration method in dealing with multi-assembly-level or core-level computations.

The domain decomposition (DD) method is a powerful tool for large-scale scientific computations. Its principle is "divide-and-conquer". In this algorithm, the total computational domain is divided into several overlapping or non-overlapping sub-domains, each of which is coupled with its own adjacent sub-domains. Calculations are carried out separately in each sub-domain and then communications occur between adjacent ones. It has been proved that the above iteration process will finally converge to the true solution of the original problem if only the coupling conditions are appropriate (Saad, 1996). As a result, a large-scale problem is successfully converted into several smaller ones by the DD method. In addition, calculations in sub-domains are independent to some degree; hence multiprocessing parallel technology could be utilized to improve the computational efficiency.

The DD method has been applied to some famous MOC solvers as a parallel computing scheme. An angular DD method is invoked in CRX (Lee et al., 2000) and GALAXY (Yamaji et al., 2010), and laudable parallel efficiency is obtained though it is not so economical on treatments of the white boundary condition. A spatial DD method is utilized in CHAPLET (Kosaka and Saji, 2000), which is an assembly modular ray tracing MOC solver instead of a 2D generalized geometry one. In our study, a spatial non-overlapping domain decomposition method, which is based on the 2D generalized geometry Krylov-accelerated MOC solver AutoMOC, is proposed to solve the aforementioned problem that the Krylov subspace acceleration method is incapable of large-scale computations. By partitioning the space domain into sub-domains, a burdensome matrix is converted into smaller ones, which are much easier to be constructed and solved. Adjacent sub-domains are coupled by "inner-edges", where the trajectory mismatches between adjacent sub-domains are considered adequately. Multiprocessing parallel technology is utilized after an adjustment on the conventional computation flow. Moreover, a matched ray tracing tool is developed on the basis of the original AutoMOC ray tracing system, which allows the user to define the sub-domains on demand conveniently.

The remainder of this paper is organized as follows. Section 2 exhibits the methodology of this work, including the mathematical derivation and details in implementation. Section 3 is dedicated to some numerical results which demonstrate the relative efficiency and accuracy compared with the original program AutoMOC. Finally we draw some conclusions and make a few suggestions in Section 4.

2. Theoretical model

Two parts exist in this section. The first part is for the Krylov subspace acceleration method, including the derivation of the MOC linear system and implementation details. The second part is about the DD method, which is composed of the theoretics, the geometry processing technique and the parallelization technique.

2.1. The Krylov subspace acceleration method

2.1.1. Basic equations of MOC

In the MOC calculation, the computational domain is partitioned into a number of regions, in each of which the source and cross-section are both assumed to be constants. Hence the time-independent multigroup neutron transport equation can be written in region i on track line segment k by omitting the energy group superscripts g:

$$\frac{d\psi_{i,k}(s,\vec{\Omega})}{ds}+\Sigma_{t,i}\psi_{i,k}(s,\vec{\Omega})=Q_{i,k}(\vec{\Omega}) \tag{1}$$

where s is the local coordinate along the track line. Thus the angular flux distribution along the track line can be obtained by the analytical solution of Eq. (1):

$$\psi_{i,k}(s,\vec{\Omega})=\psi_{i,k}^{in}(\vec{\Omega})\exp(-\Sigma_{t,i}s)+\frac{Q_{i,k}(\vec{\Omega})}{\Sigma_{t,i}}\left[1-\exp(-\Sigma_{t,i}s)\right] \tag{2}$$

where $\psi_{i,k}^{in}(\vec{\Omega})$ is the incident angular flux to region i along line segment k in direction Ω. The mean angular flux in region i along direction Ω is considered as

$$\overline{\psi}_i(\vec{\Omega})=\frac{\sum_k \overline{\psi}_{i,k}(\vec{\Omega})s_{i,k}\delta A_k}{V_i} \tag{3}$$

here, $\overline{\psi}_{i,k}$ is the mean angular flux along segment k, which can be obtained by integrating Eq. (2) along k; and V_i is the volume of region i, which can be approximately represented as $V_i\approx\sum_k s_{i,k}\delta A_k$, where the sum is over all the segments in region i along direction Ω, involving the segment length $s_{i,k}$ and its width δA_k. Thus Eq. (3) has the following form:

$$\overline{\psi}_i(\vec{\Omega})=\frac{\sum_k \delta A_k\left[Q_i^{iso}s_{i,k}+Q_i^{aniso}(\vec{\Omega})s_{i,k}+\left(\psi_{i,k}^{in}((\vec{\Omega}))-\psi_{i,k}^{out}(\vec{\Omega})\right)\right]}{\Sigma_{t,i}V_i} \tag{4}$$

where $\psi_{i,k}^{out}$ is the exiting flux along k from region i; Q_i^{iso} and Q_i^{aniso} are respectively the isotropic and anisotropic source in region i. Hence the mean scalar flux in region i can be written after obtaining the mean angular flux in each discretized direction:

$$\phi_i=\int_{4\pi}\overline{\psi}_i(\vec{\Omega})d(\vec{\Omega})\approx\sum_{m=1}^{M}\omega_m\overline{\psi}_i(\vec{\Omega}) \tag{5}$$

where M is the total number of discretized directions; and ω_m is the weight of direction m.

On the treatment of reflective boundary conditions in complex geometry, mismatches between incoming and outgoing directions are often encountered due to the variety of outer boundary. As the illustration in Fig. 1, $\Omega_{m'}$ is the specular reflection direction of Ω_m.