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Synchronized forward-adjoint neutron transport using method of characteristics

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ABSTRACT

The method of characteristics has been widely used for neutron transport calculations in lattice physics computations. This method recently has attracted a lot of attention for whole core calculation because of its flexibility in geometry definition and to highly impose parallelization. One area of whole core calculation is perturbation calculation that needs forward-adjoint flux. The objective of the work presented in this paper is to develop a synchronized forward-adjoint neutron transport solver embedding in FAMOC code.

FAMOC is a new neutron transport code based on method of characteristics that is currently under development at Shahid Beheshti University (SBU). It is capable of simulating 2D models based on combinatorial geometry with first or second-order surfaces, and a multilevel lattice-universe base geometry model to rectangularly simulate. In this code, the same tracking data is used to compute forward and adjoint average flux. The forward and adjoint effective multiplication factor, and flux obtained by FAMOC code for 2D benchmark of C5G7 were found to be in good agreement with references.

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1. Introduction

The forward-adjoint flux is widely used in static perturbation theory including sensitivity coefficients, uncertainty analysis, and estimation of keff variations due to small changes in reactor core compositions. Since an advanced nuclear reactor core consists of a complicated pattern of fuel assemblies with fuel rods, it needs a flexible method to appropriately compute the forward-adjoint flux in the heterogeneous geometry. Most deterministic methods are based on discretization of the space variables (unlike Monte Carlo methods) and to impose some approximations in geometry. The method of characteristics (MOC) using a geometry approach similar to Monte Carlo method does impose no limitation on geometry ([Zangian et al., 2015\)](#page--1-0).

The MOC in neutron transport was first proposed by Askew in 1972 [\(Askew, 1972](#page--1-0)), and has been widely applied to various multigroup lattice transport codes including: CACTUS module in WIMS ([Halsall, 1980](#page--1-0)), CASMO-4 ([Edenius et al., 1995\)](#page--1-0), DRAGON ([Marleau](#page--1-0) [et al., 1994](#page--1-0)) and APOLLO2 ([Sanchez et al., 1988](#page--1-0)). The method gives accurate results even in complex geometries, strong absorber problems, strong anisotropic problems and so on, while its calculation preserves the simplicity of the SN method and can be highly parallelized and vectorized due to its nested loop structure. Hence some codes, such as ANEMONA ([Jevremovic et al., 2001](#page--1-0)), AutoMOC ([Chen et al., 2008](#page--1-0)), AGENT [\(Jevremovic et al., 2004](#page--1-0)), CRX [\(Hong and](#page--1-0) [Cho, 1998](#page--1-0)), CHAPLET ([Kosaka and Saji, 2000\)](#page--1-0), OpenMOC ([Boyd](#page--1-0) [et al., 2014\)](#page--1-0), and DeCART ([Cho et al., 2002](#page--1-0)) developed not only for lattice calculations but also for whole core calculations without homogenization.

Because of the computational complexity, the MOC based adjoint flux has been scarcely used in conventional codes and other methods used for this purpose. In this paper, we proposed an algorithm for synchronized solving of forward-adjoint neutron transport equation using MOC method. Benefitting a similar definition of forward and adjoint average flux, the same tracking data is used for this solver. Based on this solver, a new neutron transport code named FAMOC (forward-adjoint Method of Characteristics) was produced, which is specifically intended for reactor physics calculations. The code is being developed in the Department of Nuclear Engineering at Shahid Beheshti University (SBU). FAMOC was written in Fortran 90 programming language and it performs criticality calculation using multi-group isotropic cross sections. Eventually, the geometry and the physics models implemented in Corresponding author. Tel.: +98 21 29902546.
FAMOC, forward and adjoint flux and multiplication factor

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corresponding to the 2D benchmark of the C5G7 were verified ([Smith and Palmiotti, 2005](#page--1-0)).

2. Method of characteristics

Method of characteristics (or the Lagrange–Galerkin methods) is typically used to reduce first-order partial differential equations to ordinary differential equations, which are easier to solve. The principle idea of this method is to rewrite the governing equations by following Lagrange coordinates defined by specific trajectories, i.e. characteristics associated with the problem under consideration.

Recently, the method of characteristics has been widely used for neutron transport calculations in lattice physics computations so that the neutron transport equation is solved along characteristics, as they move across the complete domain.

The steady-state form of neutron transport equation is ([Cacuci,](#page--1-0) [2010](#page--1-0)):

$$
\overrightarrow{\Omega} \cdot \overrightarrow{\nabla} \Psi \left(\overrightarrow{r}, E, \overrightarrow{\Omega} \right) + \Sigma_t \left(\overrightarrow{r}, E \right) \Psi \left(\overrightarrow{r}, E, \overrightarrow{\Omega} \right) = Q \left(\overrightarrow{r}, E, \overrightarrow{\Omega} \right), \tag{1}
$$

where $\overrightarrow{\mathrm{r}}$ is the spatial position vector, E is the neutron energy, $\overrightarrow{\Omega}$ is the angular direction vector, $\Psi\Big(\overrightarrow{r},E,\overrightarrow{\Omega}\Big)$ is the angular flux, $\Sigma_{\rm t}\big(\stackrel{\rightharpoonup}{\rm r}, \texttt{E}\big)$ is the total cross-section and $\mathrm{Q}\Big(\stackrel{\rightharpoonup}{\rm r}, \texttt{E}, \overrightarrow{\Omega}\Big)$ is the source term. Using Lagrange coordinates defined by neutral particle trajectories, i.e. characteristics, $\vec{r} = \vec{r}_0 + s\vec{Q}$, the streaming term reduces to below simplified form:

$$
\overrightarrow{\Omega} \cdot \overrightarrow{\nabla} \Psi \left(\overrightarrow{r}, E, \overrightarrow{\Omega} \right) = \frac{d}{ds} \Psi \left(s, E, \overrightarrow{\Omega} \right), \tag{2}
$$

Along characteristics the differential operator of the neutron transport equation, undergoing coordinate change, transforms to a total derivative.

Substituting the above expression into Eq. (1) , we get,

$$
\frac{d}{ds}\Psi\left(s,E,\overrightarrow{\mathcal{Q}}\right)+\Sigma_{t}(s,E)\Psi\left(s,E,\overrightarrow{\mathcal{Q}}\right)=Q\left(s,E,\overrightarrow{\mathcal{Q}}\right)
$$
\n(3)

2.1. Forward neutron transport equation

The characteristic form of the multi-group, steady-state and isotropic neutron transport equation is given by the following:

$$
\frac{d\Psi_{(k,g)}(s)}{ds} + \Sigma_{t,g}\Psi_{(k,g)}(s) = Q_g(s),\tag{4}
$$

where k is index of track and the source term is further expressed in terms of scattering source and fission source,

$$
Q_g(s) = \sum_{g'} \Sigma_{s,g' \to g}(s) \phi_{g'}(s) + \frac{\chi_g(s)}{k_{\text{eff}}} \sum_{g'} \nu \Sigma_{f,g'}(s) \phi_{g'}(s), \tag{5}
$$

Eq. (4) using proper integration factor is changeable to total derivative

$$
\frac{d}{ds}\left(\Psi_{(k,g)}(s)e^{\Sigma_{t,g}s}\right) = Q_g(s)e^{\Sigma_{t,g}s}.
$$
\n(6)

Assuming spatial domain made of regions with piecewise-

uniform nuclear properties i.e. flat source region (FSR), the equation can be deduced as,

$$
\frac{d}{ds}\left(\Psi_{k,i,g}(s)e^{\Sigma_{tg} s}\right) = Q_{i,g}e^{\Sigma_{tg} s}.
$$
\n(7)

being index *i* representing track contribution in FSR_i.

Integrating Eq. (7) along the track segment $(s_{k,i})$, $\int_{s}^{s'}$ s' ds, and with the optical path length defined as $\tau_{k,i,g} = \Sigma_{t,g} (s'' - s')$, the outgoing angular flux $(\Psi_{k,i,g}(\mathbf{s}''))$ is:

$$
\Psi_{k,i,g}\left(s^{''}\right) = \Psi_{k,i,g}\left(s^{'}\right)e^{-\tau_{k,i,g}} + \frac{Q_{i,g}}{\Sigma_{t,g}}\left[1 - e^{-\tau_{k,i,g}}\right]
$$
\n⁽⁸⁾

Track averaged angular flux in group g, along the track segment is computed by integrating Eq. (8) over the track segment s_{ki} and dividing by the length of the segment $l_{k,i}$;

$$
\overline{\Psi}_{k,i,g}\left(s^{''}\right) = \frac{1}{l_{k,i}} \int_{s'}^{s''} \Psi_{k,i,g}(s)ds
$$
\n
$$
= \left[\frac{\Psi_{k,i,g}(s')}{\tau_{k,i,g}}\left(1 - e^{-\tau_{k,i,g}}\right) + \frac{Q_{i,g}}{\Sigma_{t,g}}\left(1 - \frac{\left(1 - e^{-\tau_{k,g}}\right)}{\tau_{k,i,g}}\right)\right]
$$
\n(9)

Using Eq. (8) , this equation can be introduce as below $(Boyd)$ $(Boyd)$ $(Boyd)$ [et al., 2014; Li, 2013](#page--1-0)):

$$
\overline{\Psi}_{k,i,g}\left(s^{''}\right) = \frac{Q_{i,g}}{\Sigma_{t,g}} + \frac{\Psi_{k,i,g}\left(s^{''}\right) - \Psi_{k,i,g}\left(s^{'}\right)}{\tau_{k,i,g}}
$$
(10)

Sub-cell averaged neutron angular flux is calculated via summation for all track averaged neutron angular flux in sub-cell i along direction k , and divide by volume of the sub-cell or FSR. This is done according to whatever the discrete ordinates approximation has dictated, determining how many track segments by which numbering of discrete azimuthal and polar angle there are in the sub-cell. Finally, the neutron scalar flux can be computed via summation over all directions in the quadrature set.

$$
\phi^{i,g} = \int\limits_{4\pi}^{\overline{W}} \overline{\Psi}_{i,g}(\Omega) d\Omega = 4\pi \sum\limits_{k}^{\overline{W}} \overline{\Psi}_{k,i,g} \omega_k \tag{11}
$$

It is the neutron scalar flux that is of primary interest to any steady state transport computation and additional information can be derived from this known steady state dependent variable ([Taylor, 2007](#page--1-0)).

2.2. Adjoint neutron transport equation

The multi-group, steady-state adjoint form of the neutron transport equation is:

$$
-\overrightarrow{\Omega}\cdot\overrightarrow{\nabla}\Psi_{g}^{\dagger}\left(\overrightarrow{r},\overrightarrow{\Omega}\right)+\Sigma_{t,g}\left(\overrightarrow{r}\right)\Psi_{g}^{\dagger}\left(\overrightarrow{r},\overrightarrow{\Omega}\right)=Q_{g}^{\dagger}\left(\overrightarrow{r}\right),\qquad(12)
$$

where the adjoint source term is further expressed in terms of scattering source and fission source,

$$
Q_{g}^{\dagger}(r) = \sum_{g'} \Sigma_{s,g \to g'}(r) \phi_{g'}^{\dagger}(r) + \frac{\nu \Sigma_{f,g}(r)}{k_{eff}^{\dagger}} \sum_{g'} \chi_{g'}(r) \phi_{g'}^{\dagger}(r) \tag{13}
$$

The characteristic form of this equation is given by the following:

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