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Solution of the neutron transport equation by the Method of Characteristics using a linear representation of the source within a mesh

Tanay Mazumdar [a,*], S.B. Degweker [b]

[a] Research Reactor Services Division, Bhabha Atomic Research Centre, Mumbai 400085, India
[b] Mathematical Physics and Reactor Theory Section, Bhabha Atomic Research Centre, Mumbai 400085, India

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ABSTRACT

A common assumption in the solution of the neutron transport equation by the Method of Characteristics (MOC) is that the source (or flux) is constant within a mesh. This assumption is adequate provided the meshes are small enough so that the spatial variation of flux within a mesh may be ignored. Whether a mesh is small enough or not depends upon the flux gradient across a mesh, which in turn depends on factors like the presence of strong absorbers, localized sources or vacuum boundaries. The flat flux assumption often requires a very large number of meshes for solving the neutron transport equation with acceptable accuracy as was observed in our earlier work on the subject. A significant reduction in the required number of meshes is attainable by using a higher order representation of the flux within a mesh. In this paper, we expand the source within a mesh up to first order (linear) terms, which permits the use of larger sized (and therefore fewer) meshes and thereby reduces the computation time without compromising the accuracy of calculation. Since the division of the geometry into meshes is through an automatic triangulation procedure using the Bowyer-Watson algorithm, representation of circular objects (cylindrical fuel rods) with coarse meshes is poorer and causes geometry related errors. A numerical recipe is presented to make a correction to the automatic triangulation process and thereby eliminate this source of error. A number of benchmark problems are analyzed to emphasize the advantage of the source expansion method and the need to correct the triangular representation of the geometry.

1. Introduction

A nuclear reactor is a heterogeneous assembly of its constituent materials such as fuel, moderator, structural material, control absorbers, reflector etc. Thus, in principle, the neutron transport equation should be solved for such a heterogeneous system to calculate multiplication factor, neutron flux, power distribution etc. Modern Monte Carlo codes routinely represent the heterogeneous geometry of a reactor exactly. Notwithstanding some attempts in recent times to carry out such an exact representation in deterministic codes, traditional deterministic reactor physics calculations follow a two step process, mainly because of limitations of computational resources. In the first step, called the lattice calculation, the neutron transport equation is solved using a large number of energy groups, in a small and representative region of the reactor [typically a fuel assembly], taking into account all details of the heterogeneous geometry. The detailed flux distribution thus obtained enables us to obtain few group homogenized cross sections of an equivalent material which replaces the actual materials in the representative region. In the second step, these homogenized cross sections are used to solve the three dimensional few group neutron diffusion equation for the entire core.

The integral transport theory methods and, more recently, the Method of Characteristics (MOC) are commonly used for lattice calculations (Askew, 1972; Hong and Cho, 1998; Chen et al., 2008; Yang and Satvat, 2012). The MOC offers several advantages over other commonly used methods in transport theory. Treatment of arbitrary geometry, anisotropic scattering and the ability to calculate detailed flux and power distribution over the region of interest are some of its advantages. A number of computer codes like DRAGON (Marleau et al., 2008), CASMO-4 (Smith and Rhodes, 2000), CASMO-5 (Rhodes et al., 2006), BOXER (Ray et al., 2016) and many more have already been developed based on MOC. With massive increase in computing power in recent times, it has become possible to solve the neutron transport equation directly for the entire reactor core without the need for homogenization (Sanchez, 2012), using the MOC. Three dimensional MOC codes require huge amounts of memory and computation time. Hence, hybrid methods, such as the 2D MOC (radial)/1D S_N (axial) fusion

* Corresponding author.
E-mail address: tanay_bwn@yahoo.co.in (T. Mazumdar).

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method (Lee and Cho, 2006), have been attempted. These methods take advantage of the core structure which is usually much simpler in the axial direction than in the radial direction.

One reason for the huge memory and time requirement using the MOC is the use of the flat flux (source) assumption within a mesh. The meshes must be rather small to obtain acceptable accuracy. This implies a large number of meshes and consequently high demands on computation time and memory. A possible way to reduce the computational resource requirement is to employ a higher order representation of the flux (source) within a mesh. In other words, the neutron flux or neutron source within a mesh is represented as a sum of polynomials in the spatial variables. This permits the use of a larger mesh size so that fewer of meshes are required. The polynomial expansion is generally restricted up to linear terms, which, according to literature (Masiello et al., 2009; Ferrer and Rhodes, 2016), provides a balanced optimization between speed and memory requirement as compared to higher-order expansions. In an earlier paper (Mazumdar and Degweker, 2015), we had described the development of a two dimensional assembly level code based on the MOC with the assumption of a constant or flat source within a mesh. The division of the geometry into meshes was through an automatic triangulation procedure using the Bowyer-Watson algorithm. As discussed above, such an approach requires a large number of meshes, and consequently huge computing resources. It becomes particularly difficult if it is to be extended in scope to core level calculations. Keeping this in mind, in the present paper, we describe an approach in which the source in a triangular mesh is expanded in polynomials, retaining up to the linear terms. The expansion coefficients are determined by setting up equations for the average source and its moments in a mesh. A major problem with this approach for geometries involving curved surfaces (e.g. cylindrical rods) is that a coarse mesh division by triangulation does not represent the circular boundary correctly. A method has been developed to use coarse meshes in circular geometry by modifying the shape of the meshes so that the geometry representation is exact.

The paper is organized as follows. In Section 2, the mathematical formulation of the linear representation of the source within a mesh is described. Section 3 describes the numerical scheme adopted to correct the shape of coarse meshes in the presence of cylindrical bodies. A number of benchmark problems are analyzed to emphasize the advantage of the source expansion method and the need to correct the triangular representation of the geometry. Results of flat as well as linear source methods for these problems are presented in Section 4. Finally in Section 5 we present our conclusions and discuss problems that need to be addressed in future.

2. Representation of source within coarse mesh in MOC

The steady state neutron transport equation, which describes the distribution of neutron angular flux (Ψ) as a function of space (r), direction (Ω) and energy group (g) in reactor core, is

$$\Omega \cdot \vec{\nabla} \Psi_g(\vec{r},\Omega) + \Sigma_g^t(\vec{r})\Psi_g(\vec{r},\Omega) = Q_g(\vec{r},\Omega) \tag{1}$$

where Σ_g^t is the total (absorption and scattering) macroscopic cross section in the g-th group and Q_g is the g-th group total neutron source (including fission source, scattering source and external source, if any). The source is related to the angular flux by the relation

$$Q_g(\vec{r},\Omega) = Q_g^{ext}(\vec{r},\Omega) + \sum_{g'=1}^{G}\int_{4\pi}(\chi_g \nu\Sigma_{fg'}(\vec{r}) + \Sigma_{sg'\to g}(\vec{r},\Omega' \cdot \Omega))\Psi_{g'}(\vec{r},\Omega')d\Omega' \tag{2a}$$

for the problem with an external source Q_g^{ext} and

$$Q_g(\vec{r},\Omega) = \sum_{g'=1}^{G}\int_{4\pi}\left(\frac{\chi_g \nu\Sigma_{fg'}(\vec{r})}{k} + \Sigma_{sg'\to g}(\vec{r},\Omega' \cdot \Omega)\right)\Psi_{g'}(\vec{r},\Omega')d\Omega' \tag{2b}$$

for the k eigenvalue problem.

Here $\Sigma_{sg' \to g}$ is the macroscopic scattering cross section from group g' to group g, χ_g is the g-th group fission spectrum, ν is the average number of neutrons released per fission and Σ_{fg} is the g-th group macroscopic fission cross section. Applying the Method of Characteristics (MOC), Eq. (1) can be converted into the following linear ordinary differential equation (ODE) (Bell and Glasstone, 1979) giving the variation of the angular flux along a straight line characteristic, $\vec{r} = \vec{r}_0 + s\Omega$, where s is the distance to the point (r) measured from an arbitrary starting point ($\vec{r}_0$) on the characteristic line.

$$\frac{d}{ds}\Psi_g(\vec{r}_0 + s\Omega,\Omega) + \Sigma_g^t(\vec{r}_0 + s\Omega)\Psi_g(\vec{r}_0 + s\Omega,\Omega) = Q_g(\vec{r}_0 + s\Omega,\Omega) \tag{3}$$

For obtaining the numerical solution of the equation, we divide the problem domain into a number of meshes such that each mesh has a uniform material composition. If we make the additional assumption of a flat source within a mesh, then it is straightforward to write down the following solution of the ODE [Eq. (3)] for a mesh i and direction j

$$\Psi_{i,j,g}^{out} = \Psi_{i,j,g}^{in}e^{-\Sigma_{i,g}^t s_{i,j}} + \frac{Q_{i,g}}{\Sigma_{i,g}^t}\left(1 - e^{-\Sigma_{i,g}^t s_{i,j}}\right) \tag{4}$$

where $Q_{i,g}$ is the flat source in mesh i and group g and $s_{i,j}$ is the "chord length" in mesh i, i.e. the length of the segment along direction j, in mesh i as shown in Fig. 1. The above equation [Eq. (4)] gives us the outgoing angular flux i.e. the flux at the end of a segment intercepted by the mesh boundary.

But, if we divide the domain into coarser (large sized) meshes in order to reduce computation time, then the flat source assumption will not be valid as the variation of source within a mesh is too large. Hence the solution cannot be given by Eq. (4). For better representation of the spatial variation of the source within a mesh, we expand it in terms of some suitable basis functions. The polynomial functions are the simplest ones to choose in this regard. As a minimal improvement over the flat source assumption, we carry out an expansion up to the linear terms and write

$$Q_{i,j,g}(x,y) = a_0 + a_1 x + a_2 y \tag{5}$$

where a_0, a_1 and a_2 are the expansion coefficients. In mesh i, a local coordinate system, whose origin is set at the centroid (X_c, Y_c) of the mesh, is considered and x, y are the coordinates measured with respect to this local coordinate system. So, $x = X - X_c$ and $y = Y - Y_c$ where (X, Y) and (X_c, Y_c) are the coordinates measured with respect to a global coordinate system. From now onwards, lower case letters will be used for local coordinates and upper case for global coordinates.

Since the transport equation is solved along a straight line characteristic in the direction j, we can replace X and Y, mentioned above, with ($X_0 + \Omega_x s$) and ($Y_0 + \Omega_y s$) respectively. Here (X_0, Y_0) is the point at which the straight line enters the mesh, s is the chord length measured along the line between the points (X_0, Y_0) and (X, Y) and Ω_x, Ω_y are direction cosines mathematically expressed as $\Omega_x = sin\theta cos\varphi$ and $\Omega_y = sin\theta sin\varphi$ where θ and φ are the spherical polar angles in the X, Y, Z coordinate system (Fig. 2). After making these substitutions, the source can be written as follows

$$Q_{i,j,g}(s) = b_0 + b_1 s \tag{6}$$