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Solution of neutron transport equation by Method of Characteristics

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ABSTRACT

A computer code based on Method of Characteristics (MOC) is developed to solve neutron transport equation for mainly assembly level lattice calculation with reflective and periodic boundary conditions and to some extent core level calculation with vacuum boundary condition. The code is able to simulate square, circular and hexagonal geometries and their combinations. Delaunay triangulation together with the Bower–Watson algorithm is used to divide the problem geometry into triangular meshes. Ray tracing technique is developed to draw characteristics lines along different directions over the geometry and the transport equation is solved over these lines to obtain neutron flux distribution and multiplication factor for the geometry. A number of benchmark problems available in literature are analyzed to demonstrate the capability and validity of the code.

1. Introduction

The first step in traditional, deterministic reactor physics analysis of nuclear reactors is lattice calculation, in which the neutron transport equation is solved within a representative region of the reactor, called the lattice cell. This provides fine mesh and fine group flux distribution in the lattice cell, which is used to calculate few group homogenized cross sections for core calculations. In earlier days the representative region used to be a 'pin cell', consisting of a single fuel rod and associated moderator, with reflective boundary conditions. The outer boundary was often converted from square (or hexagonal) to circular, to further simplify the geometry to that of a one dimensional problem. Due to the presence of heterogeneities such as control rods, water gaps or water rods, the lattice is not exactly periodic. Various corrections such as the use of a 'white boundary' instead of reflective and the use of a 'supercell', which includes a homogenized mixture of fuel and moderator to represent the spectrum external to the lattice cell, had to be included to get satisfactory results. An intermediate assembly calculation based on diffusion theory, using the homogenized and group condensed cross sections, was performed to obtain the homogenized assembly cross sections for the fuel assembly. Examples of the use of such methods are MURLI (Huria, 1978, 1984), EXCEL (Thilagam et al., 2009) and the LEOPARD–PDQ combination (Fujita et al., 1978).

Since seventies and early eighties, computer codes were developed for doing lattice calculations at the fuel assembly level directly. The integral transport theory using either the collision probability, the interface current or a combination of these methods (Tsuchihashi, 1970; Fayers et al., 1972; Janssen and Caspers, 1973, Janssen et al., 1974; Degweker, 1985) was popular for treating the complex geometries involved. The method has the added advantage that it can be formulated in terms of only the scalar flux, since the scattering anisotropy plays only a minor role and can be corrected by the use of transport cross sections.

Due to the phenomenal increase in computing power in recent years, there have been attempts at developing computational methods for solving the transport equation directly in full reactor core i.e. without the need for a separate lattice calculation for obtaining homogenized cross sections. The Method of Characteristics, commonly abbreviated as MOC (Askew, 1972; Hong and Cho, 1998; Chen et al., 2008; Sanchez, 2012; Yang and Satvat, 2012), seems to offer such a possibility. Several lattice level codes have incorporated the MOC as a method of solving the multigroup transport equation examples being DRAGON (Marleau et al., 2008), CASMO-4 (Smith and Rhodes, 2000) and CASMO-5 (Rhodes et al., 2006). Its advantages over commonly used methods for transport theory are (i) the ability to treat complex geometries commonly encountered in reactor cores, (ii) the ability to produce detailed flux and power distribution over the region of solution, (iii) the ability to handle anisotropic scattering and (iv) the ability to obtain solution in neutronically large sized domains. Commonly used methods viz. the collision probability method, the DSn method

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and the Monte Carlo method suffer from one or more of the above problems ((i) for DSn, (ii) for Monte Carlo, (iii) and (iv) for Collision probability). For these reasons the MOC is gaining popularity for not only lattice calculations but also for whole core calculations without homogenization.

A prerequisite for solving the transport equation by the MOC is the division of the problem domain into small meshes. Another prerequisite is the construction of a sufficiently large number of characteristic lines or rays, along which the transport equation is solved. The traditional way to divide the geometry into meshes is to divide the assembly into square or hexagonal cells of the lattice structure and to carry out further sub division of the cells into radial and azimuthal zones. This is the approach followed in Degweker (1985) and Ray and Degweker (2013). While it gives the user the freedom to choose the manner of division, it makes the preparation of the input more cumbersome.

In the present paper, we describe the development of the first phase of a code based on the MOC using an automatic procedure for mesh division based on the Delaunay triangulation technique along with the Bowyer–Watson algorithm. Presently the solution domain can be typical square or hexagonal fuel assemblies of PWRs, BWRs or VVERs. The ray tracing is carried out with the help of elementary coordinate geometry. The paper is organized as follows: The Method of Characteristics for solving the transport equation is described in Section 2. The mesh generation and ray tracing procedures are described in Section 3. In Section 4, we present the results of our calculations for a number of benchmark problems. Finally we present our conclusions.

2. Solution of neutron transport equation by MOC

The neutron transport equation is an integro-differential equation which describes the distribution of neutron angular flux (Ψ) as a function of space (r), angle (Ω), energy (E) and time (t) in reactor core. Since our interest is in steady state (mostly "k" eigenvalue) problems, for the present purpose, the steady state neutron transport equation is written below:

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

g is energy group corresponding to energy E, Σ_g^t is g-th group total (absorption and scattering) macroscopic cross section and Q_g is 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 relations:

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

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

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

for the k eigenvalue problem.

where $\Sigma_{sg'\to g}$ is macroscopic scattering cross section from group g' to group g, χ_g is g-th group fission spectrum, ν is average number of neutrons released per fission and Σ_{fg} is g-th group macroscopic fission cross section. Applying the Method of Characteristics (MOC), Eq. (1) is converted into a linear ordinary differential equation (Bell and Glasstone, 1979).

$$\frac{d}{ds}\Psi_g\left(\vec{r_0}+s\hat{\Omega},\hat{\Omega}\right)+\Sigma_g^t\left(\vec{r_0}+s\hat{\Omega}\right)\Psi_g\left(\vec{r_0}+s\hat{\Omega},\hat{\Omega}\right)=Q_g\left(\vec{r_0}+s\hat{\Omega},\hat{\Omega}\right) \tag{3}$$

The characteristics in this case are straight lines – essentially the collision free flight paths of the neutrons – whose equations are given by $\vec{r}=\vec{r_0}+s\hat{\Omega}$ where s is distance measured along $\hat{\Omega}$ direction from $\vec{r_0}$ which is an arbitrary starting point on the characteristic line. By varying the coordinates of $\vec{r_0}$ a set of lines parallel to the direction vector $\hat{\Omega}$ (in 3-dimensional space) is obtained. Changing $\hat{\Omega}$ gives another set of parallel lines with a different orientation. Eq. (3) can be solved along any of these lines, provided an initial value of the angular flux and the source distribution are known. The problem domain is divided into meshes having uniform material composition within each mesh. If we further assume that the flux variation within a mesh is small, we can take the source to be uniformly distributed (flat) within a mesh. It is then easy to write the following solution of Eq. (3) for a mesh i and direction j:

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

where $Q_{i,g}$ is the flat source in mesh i and group g. This gives us the following equation for the outgoing angular flux i.e. the flux at the end of a segment intercepted by the mesh boundary.

$$\Psi_{i,j,g}^{out}=\Psi_{i,j,g}^{in}e^{-\Sigma_{i,g}\Delta t}+\frac{Q_{i,g}}{\Sigma_{i,g}}\left(1-e^{-\Sigma_{i,g}\Delta t}\right) \tag{5}$$

Δt is length of the segment along direction j, in mesh i as shown in Fig. 1. The average angular flux for the given characteristic in mesh i for the direction j is:

$$\overline{\Psi}_{i,j,g}=\frac{Q_{i,g}}{\Sigma_{i,g}}+\frac{\Psi_{i,j,g}^{in}-\Psi_{i,j,g}^{out}}{\Sigma_{i,g}\Delta t} \tag{6}$$

What is required for calculating the source $Q_{i,g}$ (as well as the reaction rates) are the scalar flux and (in case of anisotropic scattering) other moments of the angular flux. This is obtained by first averaging the above expression over all characteristics parallel to the direction $\hat{\Omega}$ and passing through the mesh i. This is the average angular flux for direction j and mesh i. This must be then integrated over all directions to get the scalar flux.

In practice, we can obtain numerical values of the average angular flux only over a finite number of suitably chosen directions and over a finite number of characteristic lines in a given direction. The choice may be dictated by several considerations. For example one may choose the directions from the well known fully symmetric quadrature set used in the Sn method or some other set. Since our geometry is two dimensional, being uniform and infinite in the z direction, we choose a plane perpendicular to the z direction on which the lines are drawn. These lines are projections of the actual (3-D) characteristics. The orientation (θ_k, φ_j) of the characteristics is defined by a finite set of polar angles θ_k and azimuthal angles φ_j which is closed under reflection. The former are chosen such that $\mu_k=\cos\theta_k$ are points of a Gaussian quadrature set while the latter are uniformly distributed in the interval $[0,2\pi]$. For a given φ_j, (all the projections corresponding to different θ_k are common) in a plane we use a set of equally spaced lines which form the projections of the characteristics. The intercepts are calculated for the projected lines on the plane. Then they are converted into actual intercepts of the characteristics by dividing by $\sin\theta_k$.

If n is index number of the parallel lines passing through i-th mesh along direction (j,k), then an angular flux, averaged over all those lines with a weighting factor equals to the product of chord lengths (Δt) and separation between two consecutive parallel lines (Δw), can be defined as below: