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Enhanced finite difference scheme for the neutron diffusion equation using the importance function

Mehran Vagheian [a], Naser Vosoughi [b,*], Morteza Gharib [a]

[a] Amirkabir University of Technology (Tehran Polytechnic), Department of Energy Engineering & Physics, Hafez Avenue, Tehran, Iran
[b] Sharif University of Technology, Department of Energy Engineering, Azadi Street, Tehran, Iran

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ABSTRACT

Mesh point positions in Finite Difference Method (FDM) of discretization for the neutron diffusion equation can remarkably affect the averaged neutron fluxes as well as the effective multiplication factor. In this study, by aid of improving the mesh point positions, an enhanced finite difference scheme for the neutron diffusion equation is proposed based on the neutron importance function.

In order to determine the neutron importance function, the adjoint (backward) neutron diffusion calculations are performed in the same procedure as for the forward calculations. Considering the neutron importance function, the mesh points can be improved through the entire reactor core. Accordingly, in regions with greater neutron importance, density of mesh elements is higher than that in regions with less importance. The forward calculations are then performed for both of the uniform and improved non-uniform mesh point distributions and the results (the neutron fluxes along with the corresponding eigenvalues) for the two cases are compared with each other. The results are benchmarked against the reference values (with fine meshes) for Kang and Rod Bundle BWR benchmark problems. These benchmark cases revealed that the improved non-uniform mesh point distribution is highly efficient.

1. Introduction

The adjoint equation has been widely used in sensitivity analysis and uncertainty propagation in the field of reactor core calculations. One of the important applications of the adjoint equation is in the neutron importance determination (Bell and Glasstone, 1970; Duderstadt and Hamilton, 1991).

Adjoint-based methods have a rich history in Monte-Carlo (MC) variance reduction technique. The excessively long runtime calculations and slow convergence of the fission source of the MC method led to develop some variance reduction techniques including adjoint-based methods. In this connection, recently it has been shown that the runtime MC calculations can be significantly speeded up by considering the Russian roulette technique and a weight window map to bias MC particles based on the adjoint information (Zhang and Abdel-Khalik, 2014).

Determination of the forward/adjoint effective multiplication factor (k_{eff} and $k^{\dagger}_{eff}$, respectively), in core neutronic calculations is of great importance. The effective multiplication factor is usually determined using the power iteration method. The neutron diffusion equation can be solved by various numerical methods such as Box Scheme Finite Difference Method (Malmir et al., 2010, 2011), Direct Discrete Method (Ayyoubzadeh et al., 2012), Finite Element Method (Hosseini and Vosoughi, 2013), Nodal Expansion Method (Poursalehi et al., 2013). Among these, the Finite Difference Method (FDM) has priority on account of its simplicity. However, this method definitely is not more accurate than nodal or FEM methods.

The Box-Scheme Finite Difference Method (BSFDM) has been recently used for the forward/adjoint calculations owing to its efficiency (Malmir et al., 2010, 2011). This method is based on the neutron leakage calculation from each side of a mesh box.

To date various methods have been developed and introduced to use the adjoint-based mesh adaptivity methods in the case of posteriori error measurements (Ragusa and Wang, 2010; Lathouwers, 2011a; Wang and Ragusa, 2011). These error measures can be employed to determine the effective multiplication factor of the neutron transport equation efficiently (Lathouwers, 2011b). In the light of the fact that, mesh element positions have a great importance in the accuracy of the neutron diffusion calculations, the adjoint-based goal-oriented mesh adaptivity methods can be employed to optimize density of mesh elements through

* Corresponding author.
E-mail address: nvosoughi@sharif.edu (N. Vosoughi).

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the entire reactor core, though, at the cost of computing an adjoint solution (Ayyoubzadeh and Vosoughi, 2011).

The main aim of this study is to compare the results of the uniform and improved non-uniform mesh distribution for the steady state neutron diffusion calculations. Hence, two different benchmark problems, namely Kang (Kang and Hansen, 1971) and Rod Bundle BWR (Argonne Code Center, 1977), have been considered for this comparative study. The improved non-uniform mesh distribution is determined by a novel algorithm based on the well-known neutron importance function in each region and group. At first, it is necessary to perform the adjoint calculations for the aforementioned benchmark cases. Accordingly, the rectangular form of the Box-Scheme Finite Difference Method is applied to the matrix form of the forward/adjoint neutron diffusion equation. Then, using the power iteration method, the adjoint calculations are performed to determine the neutron importance function for the entire reactor core. For facilitating comparison, the forward calculations are performed numerically for both the uniform and improved non-uniform coarse mesh point distributions. Finally, all the results are benchmarked against the fine uniform mesh point distribution.

In the following and in Section 2, the matrix form of the BSFDM for the forward as well as the backward neutron diffusion equation is presented. The improved mesh point algorithm is explained in detail in Section 3. Section 4 contains the results of this method for two different benchmark problems. Finally, in Section 5, the conclusion of this study is presented.

2. Mathematical formulation

2.1. Discretization of the forward neutron diffusion equation

The two-group forward neutron diffusion equations are described in matrix form as follows (Malmir et al., 2011):

$$\begin{bmatrix} -\nabla\cdot D_1(r)\nabla+\Sigma_{a1}(r)+\Sigma_{s,1\to2}(r) & 0 \\ -\Sigma_{s,1\to2}(r) & -\nabla\cdot D_2(r)\nabla+\Sigma_{a2}(r) \end{bmatrix}\begin{bmatrix}\phi_1(r)\\ \phi_2(r)\end{bmatrix} = \frac{1}{k_{eff}}\begin{bmatrix} \nu_1\Sigma_{f1}(r) & \nu_2\Sigma_{f2}(r) \\ 0 & 0 \end{bmatrix}\begin{bmatrix}\phi_1(r)\\ \phi_2(r)\end{bmatrix}, \tag{1}$$

where subscripts 1 and 2 denote the fast and thermal neutron energy groups, respectively, and all the other parameters have their usual meaning.

Using the Box-Scheme Finite Difference Method one can discretize Eq. (1) for different geometries. The Box-Scheme Finite Difference Method was first developed for rectangular geometries (Nakamura, 1977). Then, Malmir et al. (2011) applied this method for triangular and hexagonal geometries. Fig. 1 properly shows the mesh box properties for the rectangular geometry.

Using the Box-Scheme Finite Difference Method one can consider Eq. (1) in 2-D 2-group as follows:

$$\begin{bmatrix} \sum_{j=1}^{4}\frac{2\times D_1^i\times D_1^j}{D_1^i\times\Delta^j+D_1^j\times\Delta^i}+\left(\Sigma_{a1}^i+\Sigma_{s,1\to2}^i\right)\Delta^i & 0 \\ -\Sigma_{s,1\to2}^i\Delta^i & \sum_{j=1}^{4}\frac{2\times D_2^i\times D_2^j}{D_2^i\times\Delta^j+D_2^j\times\Delta^i}+\Sigma_{a2}^i\Delta^i \end{bmatrix}\times\begin{bmatrix}\phi_1^i\\ \phi_2^i\end{bmatrix} + \sum_{j=1}^{4}\begin{bmatrix} -\frac{2\times D_1^i\times D_1^j}{D_1^i\times\Delta^j+D_1^j\times\Delta^i} & 0 \\ 0 & -\frac{2\times D_2^i\times D_2^j}{D_2^i\times\Delta^j+D_2^j\times\Delta^i}\end{bmatrix}\times\begin{bmatrix}\phi_1^j\\ \phi_2^j\end{bmatrix} = \frac{1}{k_{eff}}\begin{bmatrix} \nu_1\Sigma_{f1}^i\Delta^i & \nu_2\Sigma_{f2}^i\Delta^i \\ 0 & 0\end{bmatrix}\times\begin{bmatrix}\phi_1^i\\ \phi_2^i\end{bmatrix}, \tag{2}$$

where the mesh boxes (j), $[j=1,\ldots,4]$, represent the adjacent neighbors of the mesh box (i) and Δ is the size of one side of each mesh box as is depicted in Fig. 1.

2.2. Discretization of the adjoint neutron diffusion equation

To solve the adjoint neutron diffusion equation, firstly one can consider Eq. (2) as follows:

$$L\phi=\frac{1}{k_{eff}}F\phi \tag{3}$$

where L and F are called the loss and fission operators, respectively. Then, the transposition of Eq. (3) gives:

$$L^{\dagger}\psi=\frac{1}{k_{eff}}F^{\dagger}\psi, \tag{4}$$

in which $L^{\dagger}$ and $F^{\dagger}$ are the transposes of L and F, respectively. In addition, ψ refers to the neutron importance function (or the adjoint flux) (Bell and Glasstone, 1970; Lamarsh, 1965). Thus, considering Eqs. (2) and (4), the matrix form of the adjoint neutron diffusion equation can be written as follows:

$$\begin{bmatrix} \sum_{j=1}^{4}\frac{2\times D_1^i\times D_1^j}{D_1^i\times\Delta^j+D_1^j\times\Delta^i}+\left(\Sigma_{a1}^i+\Sigma_{s,1\to2}^i\right)\Delta^i & -\Sigma_{s,1\to2}^i\Delta^i \\ 0 & \sum_{j=1}^{4}\frac{2\times D_2^i\times D_2^j}{D_2^i\times\Delta^j+D_2^j\times\Delta^i}+\Sigma_{a2}^i\Delta^i \end{bmatrix}\times\begin{bmatrix}\psi_1^i\\ \psi_2^i\end{bmatrix} + \sum_{j=1}^{4}\begin{bmatrix} -\frac{2\times D_1^i\times D_1^j}{D_1^i\times\Delta^j+D_1^j\times\Delta^i} & 0 \\ 0 & -\frac{2\times D_2^i\times D_2^j}{D_2^i\times\Delta^j+D_2^j\times\Delta^i}\end{bmatrix}\times\begin{bmatrix}\psi_1^j\\ \psi_2^j\end{bmatrix} = \frac{1}{k_{eff}}\begin{bmatrix} \nu_1\Sigma_{f1}^i\Delta^i & 0 \\ \nu_2\Sigma_{f2}^i\Delta^i & 0\end{bmatrix}\times\begin{bmatrix}\psi_1^i\\ \psi_2^i\end{bmatrix}, \tag{5}$$

where ψ^i and ψ^j denote the neutron importance function for the mesh boxes (i) and (j), respectively. It should be noted that Eq. (5) can be obtained directly by the transposition of Eq. (2).

3. Methodology

To improve the mesh point positions based on the neutron importance function in the entire reactor geometry, firstly it is necessary to perform adjoint neutron diffusion calculations. These calculations are performed using the power iteration method. It should be noted that the convergence criteria, for the neutron flux and eigenvalue variations in the inner and outer iterations, can be chosen based on the reported benchmark values.

The main idea of the mesh improvement is that, in regions with higher neutron importance, higher density of mesh elements should be used than that in regions with lower importance. This can be expressed as follows:

Step 1. Determination of the fast and the thermal neutron importance functions using the power iteration method.
This step should be performed to obtain the neutron importance value for each mesh of the entire reactor geometry.

Step 2. Calculation of the average neutron importance function in all mesh points over the group energies, as follows:

$$\psi_{average}^{i,j}=\frac{\psi_1^{i,j}+\psi_2^{i,j}}{2} \tag{6}$$