On the Effect of the Diffusion Coefficient Treatment in Finite Difference Schemes of Diffusion Equation

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INTRODUCTION

Ongoing research has focused on the development of more accurate numerical approximations of the neutron transport equation to predict the behavior of neutrons in nuclear reactors without overwhelming current computational resources [1]. The diffusion equation greatly simplifies the neutron transport equation without sacrificing too much predictive accuracy. This allows for scientific research and practical application to proceed without prohibitive computational costs [2]. This paper specifically intends to explore various numerical treatments of the diffusion coefficient in the finite difference schemes for solving the neutron diffusion equation, with the aim of determining the best candidate to be implemented in the finite difference method (FDM) based diffusion code to minimizes numerical convergence error [3].

In FDM, the spatial domain of study is divided into intervals or meshes. The flux is averaged over each mesh to allow for computational simplicity in this area of the diffusion equation, thereby limiting the number of unknowns and increasing the simplicity of the equation. For this reason, FDM produces a relatively simple formulation to the diffusion equation that does not overly-tax limited computational resources [4].

In this paper, we present four different ways to approximate the diffusion coefficient as it appears in the finite difference scheme of the diffusion equation. Numerical solutions based on these approximations are produced respectively. The relative accuracy of each solution is revealed by comparison to the analytic solution of the specified one-dimensional (1D) example problem. The best numerical treatment of the diffusion coefficient is determined based on the error analysis of the one-dimensional cases. These research efforts, however, will be extended to a multi-dimensional problem using the results obtained in this paper.

THEORY

Considering one energy group and using standard notations, the 1D diffusion equation can be described as

$$-\frac{d}{dx}\left(D(x)\frac{d\phi}{dx}\right)+\Sigma_a(x)\phi(x)=S(x). \qquad (1)$$

The two corresponding boundary conditions (B.C.) on the left and right side the problem can be described by general forms as follows:

$$\alpha_L\phi_L+\beta_L J_L=g_L, \quad \alpha_R\phi_R+\beta_R J_R=g_R, \qquad (2)$$

where the subscript L and R represent the left and right boundary, respectively. α_L, β_L, g_L, α_R, β_R, and g_R are known constants. ϕ and J stand for flux and current at the boundary. If we label the discretization meshes for the 1D problem as the one shown in Fig. 1, we have

$$\phi_L=\phi_{\frac{1}{2}},\ J_L=J_{\frac{1}{2}};\ \phi_R=\phi_{N+\frac{1}{2}},\ J_R=J_{N+\frac{1}{2}}. \qquad (3)$$

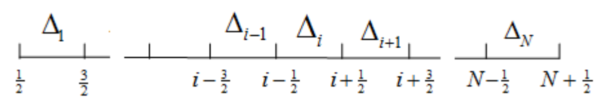

Fig. 1. The one-dimensional discretization mesh.

To derive the FDM scheme for the diffusion equation, we first integrated Eq.(1) over the mesh i, that is

$$\int_{x_{i+\frac{1}{2}}}^{x_{i+\frac{1}{2}}} dx\left[-\frac{d}{dx}\left(D(x)\frac{d\phi}{dx}\right)+\Sigma_a(x)\phi(x)\right]=\int_{x_{i+\frac{1}{2}}}^{x_{i+\frac{1}{2}}} dxS(x) \qquad (4)$$

Defining the mesh-averaged flux and source as follows

$$\phi_i=\frac{1}{\Delta x_i}\int_{x_{i+\frac{1}{2}}}^{x_{i+\frac{1}{2}}}\phi(x)dx,\ \ S_i=\frac{1}{\Delta x_i}\int_{x_{i+\frac{1}{2}}}^{x_{i+\frac{1}{2}}}S(x)dx, \qquad (5)$$

and assuming constant material properties within the mesh, Eq.(4) becomes

$$\int_{x_{i+\frac{1}{2}}}^{x_{i+\frac{1}{2}}} dx\left[-\frac{d}{dx}\left(D(x)\frac{d\phi}{dx}\right)\right]+\Sigma_{a,i}\phi_i\Delta x_i=S_i\Delta x_i. \qquad (6)$$

The second order derivative term (the diffusion term) in the equation can be processed as follows:

$$\begin{aligned}\int_{x_{i+\frac{1}{2}}}^{x_{i+\frac{1}{2}}} dx\left[-\frac{d}{dx}\left(D(x)\frac{d\phi}{dx}\right)\right]&=-\left(D(x)\frac{d\phi}{dx}\bigg|_{x_{i+\frac{1}{2}}}-D(x)\frac{d\phi}{dx}\bigg|_{x_{i-\frac{1}{2}}}\right)\\&\approx-\left(D_{i+\frac{1}{2}}\frac{\phi_{i+1}-\phi_i}{\Delta x_{i+\frac{1}{2}}}-D_{i-\frac{1}{2}}\frac{\phi_i-\phi_{i-1}}{\Delta x_{i-\frac{1}{2}}}\right)\end{aligned} \qquad (7)$$

Here we used the center-difference scheme to handle the derivatives at the mesh boundaries, and notate

$$\Delta x_{i+\frac{1}{2}} = \frac{1}{2}\left(\Delta x_i + \Delta x_{i+1}\right), \quad \Delta x_{i-\frac{1}{2}} = \frac{1}{2}\left(\Delta x_{i-1} + \Delta x_i\right) \tag{8}$$

Thus, the diffusion equation can be written as

$$-\left(D_{i+\frac{1}{2}} \frac{\phi_{i+1} - \phi_i}{\Delta x_{i+\frac{1}{2}}} - D_{i-\frac{1}{2}} \frac{\phi_i - \phi_{i-1}}{\Delta x_{i-\frac{1}{2}}} \right) + \Sigma_{a,i}\phi_i \Delta x_i = S_i \Delta x_i \tag{9}$$

Eq.(9) is the finite difference scheme obtained generally applied to the internal meshes in the domain. For the boundary meshes, slightly different treatment has to be employed to incorporate the boundary conditions provided in Eq.(2). For the leftmost mesh ($i = 1$), the diffusion term in the diffusion equation can be evaluated as follows:

$$\begin{aligned} -\int_{x_{\frac{3}{2}}}^{x_{\frac{1}{2}}} dx \frac{d}{dx}\left(D(x)\frac{d\phi}{dx} \right) &= -\left(D(x)\frac{d\phi}{dx}\bigg|_{x_{\frac{3}{2}}} - D(x)\frac{d\phi}{dx}\bigg|_{x_{\frac{1}{2}}} \right) \\ &\approx -\left(D_{\frac{3}{2}} \frac{\phi_2 - \phi_1}{\Delta x_{\frac{3}{2}}} + \frac{g_L - \alpha_L \phi_{\frac{1}{2}}}{\beta_L} \right) \end{aligned} \tag{10}$$

Here we used the following result derived from the boundary conditions [see Eq.(2)] to express the current at the left boundary ($x = x_{\frac{1}{2}}$)

$$J_{\frac{1}{2}} == -D(x)\frac{d\phi}{dx}\bigg|_{x_{\frac{1}{2}}} = \frac{g_L - \alpha_L \phi_{\frac{1}{2}}}{\beta_L}. \tag{11}$$

With Eq.(10), the finite difference scheme of the diffusion equation at the leftmost mesh can be written as

$$-\left(D_{\frac{3}{2}} \frac{\phi_2 - \phi_1}{\Delta x_{\frac{3}{2}}} + \frac{g_L - \alpha_L \phi_{\frac{1}{2}}}{\beta_L} \right) + \Sigma_{a,1}\phi_1 \Delta x_1 = S_1 \Delta x_1 \tag{12}$$

To further reduce the redundancy of the unknowns in the system of equations, we may assume that the flux at the left boundary is equal to the average flux of the leftmost mesh

$$\phi_{\frac{1}{2}} \approx \phi_1. \tag{13}$$

With this approximation, the FDM scheme for the leftmost cell becomes

$$-\left(D_{\frac{3}{2}} \frac{\phi_2 - \phi_1}{\Delta x_{\frac{3}{2}}} + \frac{g_L - \alpha_L \phi_1}{\beta_L} \right) + \Sigma_{a,1}\phi_1 \Delta x_1 = S_1 \Delta x_1 . \tag{14}$$

The same procedure can be applied to the rightmost mesh, producing the following FDM scheme for this mesh ($i = N$)

$$\left(\frac{g_R - \alpha_R \phi_N}{\beta_R} + D_{N-\frac{1}{2}} \frac{\phi_N - \phi_{N-1}}{\Delta x_{N-\frac{1}{2}}} \right) + \Sigma_{a,N}\phi_N \Delta x_N = S_N \Delta x_N \tag{15}$$

Eq.(9), (14), and (15) construct a complete system of equations that can be used to uniquely determine the solution of the diffusion equation. However, there is one parameter in these equations not been clearly defined yet, the diffusion coefficients at the mesh interfaces. This is the part that we attempt to address in this paper.

In this paper, we will apply four different approximations to the diffusion coefficients at the interfaces of the meshes and analyze the influence of these approximations to the accuracy of the diffusion solutions, particularly in the problems with heterogeneous materials configured. The four different approximations are summarized as follows:

a) Form of an arithmetic mean of neighboring meshes

$$D_{i+\frac{1}{2}} = \frac{D_{i+1} + D_i}{2} \tag{16}$$

b) Form of an arithmetic mean of neighboring meshes with mesh size weighted

$$D_{i+\frac{1}{2}} = \frac{D_{i+1}\Delta x_{i+1} + D_i \Delta x_i}{\Delta x_{i+1} + \Delta x_i} \tag{17}$$

c) Form of a harmonic mean of neighboring meshes

$$D_{i+\frac{1}{2}} = \left(\frac{\frac{1}{D_i} + \frac{1}{D_{i+1}}}{2} \right)^{-1} \tag{18}$$

d) Form of a harmonic mean of neighboring meshes with mesh size weighted

$$D_{i+\frac{1}{2}} = \left(\frac{\frac{\Delta x_i}{D_i} + \frac{\Delta x_{i+1}}{D_{i+1}}}{\Delta x_{i+1} + \Delta x_i} \right)^{-1} \tag{19}$$

These results will then be compared to the analytic solution to the one-dimensional neutron transport theory in an effort to determine which solution presents the most accurate reflection of reactor conditions.

RESULTS

1. Example One:

This is a one-region (one material) problem. It is imposed with reflective boundary condition (BC) on the left side, and vacuum BC on the right side. Constant external neutron source is provided everywhere in the problem. The analytic solution (exact solution) to this simple problem is easily obtained. The deviations between the numerical solutions from the above four different implementation of diffusion coefficients and the exact solution is shown in Fig. 2 below.

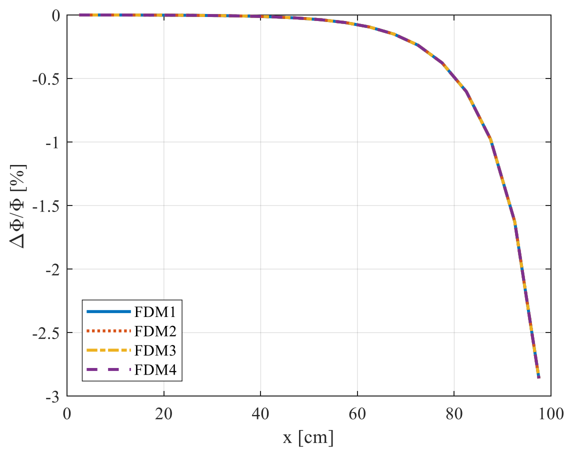

Figure 2. Flux deviations from the exact solution.

As seen in Fig. 2, the relative errors increased as it neared the vacuum boundary on the right side. This is mainly due to the approximation made for boundary flux [see Eq.(13)]. Since all errors nearly overlap each other, this example did not yield conclusive judgment about which treatment of the diffusion coefficient best matches analytic results and minimizes error. Due to the nature of the one-region problem that has same diffusion coefficient everywhere, this is not a surprising result.

2. Example Two:

This is a two-region (two materials) problem with vacuum BC imposed on the left side, and reflective BC on the right side. The constant fixed source is only provided in the left region. For this simple configuration, the analytic solution still can be obtained using characteristic functions of the diffusion equation. The similar error analysis is performed as the first example, and the deviations of four different realizations are shown in Fig. 3.

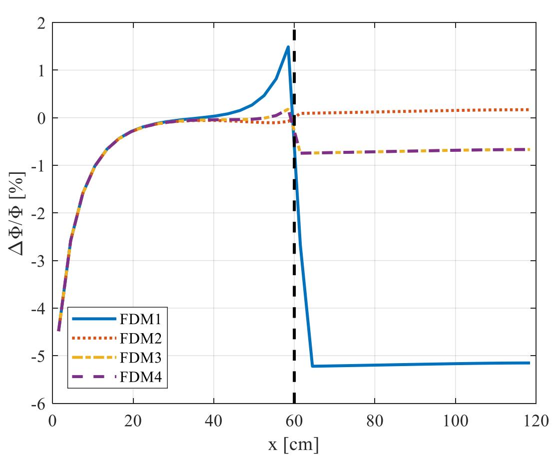

Figure 3. Flux deviations from the exact solution.

By contrast, a two-region problem yielded clear results about which treatment of the diffusion coefficient produced the most accurate results when compared with an analytical solution. The simple error analysis on the two-region problem informs the FDM2—arithmetic mean with weighted mesh sizing—obtains the best solution for this problem. A more sophisticated multi-region problem can be exercised in the similar manner to check the accuracy of different FDM methods.

CONCLUSION

This exploration of the effect of different treatments of the diffusion coefficient produced an unsurprising and inconclusive result when applied to a one-region problem, due to the unvarying nature of the diffusion coefficient in one-region simulations. By contrast, in applying various treatments of the diffusion coefficient to a two-region problem, clear results emerged that the arithmetic mean of neighboring meshes with weighted mesh size produced the smallest deviation from the analytic solution. Therefore, this study suggests that arithmetic mean with weighted mesh sizing is the most accurate of the four methods tested when considering the diffusion coefficient in finite difference method. However, this preliminary result is not entirely conclusive. More research using more complex conditions is needed in order to confirm these suggestions.

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