Finite Difference Scheme for the 1D One-Group Steady State Neutron Diffusion Equation

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This document summarizes the implementation of the finite difference scheme for solving the fixed source problem for the 1D one-group steady state neutron diffusion equation. This equation is given in Eq. (1):

$$-\frac{d}{dx}D(x)\,\frac{d}{dx}\phi(x)+\Sigma_a(x)\,\phi(x)=\frac{1}{k_{\mathit{eff}}}\nu\Sigma_f(x)\,\phi(x) \tag{1}$$

The fixed source problem is usually solved during power iterations. It assumes a known source flux, which results in a known source $S(x)$. This converts Eq. (1) as follows:

$$-\frac{d}{dx}D(x)\,\frac{d}{dx}\phi(x)+\Sigma_a(x)\,\phi(x)=S(x)\,. \tag{2}$$

The NDE is based on approximating the net current density $J(x)$ using Fick's law:

$$J(x)=-D(x)\,\frac{d}{dx}\phi(x)\,. \tag{3}$$

Two forms of finite difference discretization will be shown — a strict finite difference-based one, and the more practical finite volume-like one.

1 Strict Finite Difference Discretization

The strict "finite difference" approximation consists of simply evaluating all values at specified mesh points $\{x_i\}$, and approximating the streaming term as follows (for an equally spaced mesh with interval Δx):

$$-\frac{d}{dx}D(x)\,\frac{d}{dx}\phi(x)\bigg|_{x=x_i}\cong\left(-\frac{D_i-D_i^*}{\Delta x^2}\right)\phi_{i-1}+\left(\frac{2D_i}{\Delta x^2}\right)\phi_i+\left(-\frac{D_i+D_i^*}{\Delta x^2}\right)\phi_{i+1}, \tag{4}$$

in which D_i^* is given by:

$$D_i^*=\frac{\Delta x}{2}\left(\frac{dD}{dx}\right)_i. \tag{5}$$

Here the subscript i indicates evaluation at $x = x_i$. The resulting discretized NDE is therefore:

$$\left(-\frac{D_i - D_i^*}{\Delta x^2}\right)\phi_{i-1} + \left(\frac{2D_i}{\Delta x^2} + \Sigma_{ai}\right)\phi_i + \left(-\frac{D_i + D_i^*}{\Delta x^2}\right)\phi_{i+1} = S_i. \tag{6}$$

The issue with this scheme is that, like any true finite difference scheme, it cannot enforce conservation of integral quantities — in this case, it cannot conserve neutrons. For this reason, true finite difference schemes like this are almost never used. The finite volume-like finite difference discretization, which does conserve neutrons, is presented in the next section.

2 Finite Volume-Like Discretization

The finite volume discretization begins by dividing the spatial domain into mesh cells, indexed as shown in Figure 1.

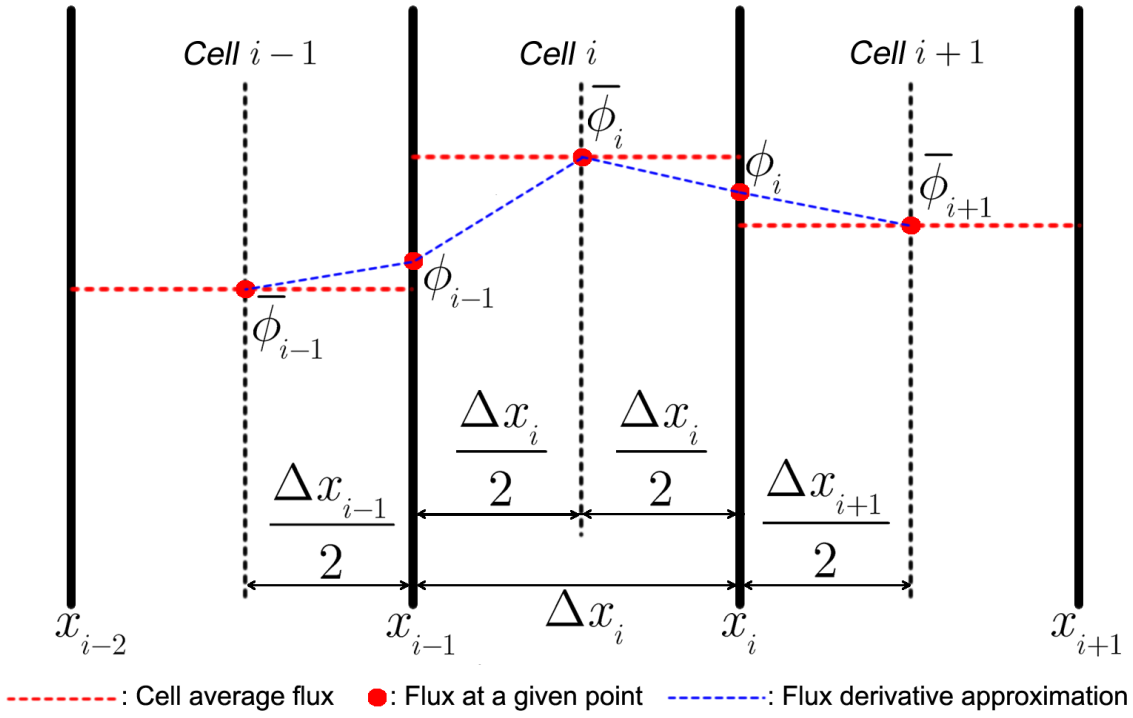

Figure 1: Mesh Cell Notation

The following notation will be used: $\bar{\phi}_i$ is the cell i average flux, Δx_i is the width of cell i, x_i is the right boundary of cell i and ϕ_i is the flux at $x = x_i$. It is assumed that material properties and source densities are uniform within a cell, which means that an interface should occur at a cell boundary, and never within a cell. The assumption about source densities is good, because since the cell-average fluxes $\{\phi_i\}$ are being solved for, and the product cross sections are assumed constant, the source densities are constant as well.

We will discretize the equation for the interior cell i first, by integrating Eq. (2) over $x \in [x_{i-1}, x_i]$. The streaming term becomes:

$$\begin{aligned}\int_{x_{i-1}}^{x_i} dx - \frac{d}{dx} D(x) \frac{d}{dx}\phi(x) &= \left(-D(x)\frac{d}{dx}\phi(x)\right)_i - \left(-D(x)\frac{d}{dx}\phi(x)\right)_{i-1} = \\ &= -D_i\left(\frac{d\phi}{dx}\right)_i + D_{i-1}\left(\frac{d\phi}{dx}\right)_{i-1},\end{aligned} \tag{7}$$

which, by Eq. (3), is also given by:

$$-D_i\left(\frac{d\phi}{dx}\right)_i + D_{i-1}\left(\frac{d\phi}{dx}\right)_{i-1} = -J_{i-1} + J_i. \tag{8}$$

The cell-average fluxes are the unknowns in this scheme, and are given by:

$$\overline{\phi}_i = \frac{1}{\Delta x_i}\int_{x_{i-1}}^{x_i} dx\phi(x)\,. \tag{9}$$

Because the other terms are assumed constant within each cell, they integrate trivially, which yields the following discretized equation:

$$-J_{i-1} + J_i + \Delta x_i \Sigma_{ai}\overline{\phi}_i = \Delta x_i S_i, \tag{10}$$

in which S_i is given by:

$$S_i = \frac{1}{k_{eff}}\nu\Sigma_{fi}\overline{\phi}_i. \tag{11}$$

Next, we need to express J_i in terms of the cell-average fluxes. The best way to do so also conserves the net current densities through each cell boundary; that is, the neutron current density (in cross sectional area) leaving the cell i through its right boundary must be the same net current density that enters the left boundary of cell $i+1$. To do so, we express J_{i^-} and J_{i^+}, the net current densities immediate to the left and to the right of x_i, respectively. To do so, we make the key assumption (which ties this method back to finite difference): the flux at the center of cell i is assumed to be equal to the average flux in cell i. This is called a "cell-centered edge flux approximation" in finite volume method.

Note, that in most fields, such as heat transfer and fluid dynamics, "flux" through an edge refers to what is referred to as "net current density" in neutron transport. This is where the "edge flux" term comes from, and why it refers to the cell boundary net current densities in this case.

As shown in Figure 1 using the blue dashed lines, $\left(\frac{d\phi}{dx}\right)_{i^\pm}$ are approximated through two-point finite difference approximations:

$$\left(\frac{d\phi}{dx}\right)_{i^-} = \frac{\phi_i - \overline{\phi}_i}{\Delta x_i/2}, \tag{12a}$$

$$\left(\frac{d\phi}{dx}\right)_{i^+} = \frac{\overline{\phi}_{i+1} - \phi_i}{\Delta x_{i+1}/2}. \tag{12b}$$

The corresponding net current densities are approximated using Eqs. (12) in Fick's law:

$$J_{i^-} = -D_i \left(\frac{d\phi}{dx}\right)_{i^-} = -D_i \frac{\phi_i - \overline{\phi}_i}{\Delta x_i/2}, \tag{13a}$$

$$J_{i^+} = -D_{i+1} \left(\frac{d\phi}{dx}\right)_{i^+} = -D_{i+1} \frac{\overline{\phi}_{i+1} - \phi_i}{\Delta x_{i+1}/2}. \tag{13b}$$

These two quantities must be equal for current continuity, which yields:

$$J_i = -D_i \frac{\phi_i - \overline{\phi}_i}{\Delta x_i/2} = -D_{i+1} \frac{\overline{\phi}_{i+1} - \phi_i}{\Delta x_{i+1}/2}, \tag{14}$$

solving which for ϕ_i yields:

$$\phi_i = \left(\frac{\Delta x_{i+1} D_i}{\Delta x_{i+1} D_i + \Delta x_i D_{i+1}}\right) \overline{\phi}_i + \left(\frac{\Delta x_i D_{i+1}}{\Delta x_{i+1} D_i + \Delta x_i D_{i+1}}\right) \overline{\phi}_{i+1}. \tag{15}$$

Substituting Eq. (15) back into Eq. (13a) (could instead substitute it into Eq. (13b)) yields:

$$J_i = \left(\frac{2 D_i D_{i+1}}{\Delta x_{i+1} D_i + \Delta x_i D_{i+1}}\right) \overline{\phi}_i + \left(-\frac{2 D_i D_{i+1}}{\Delta x_{i+1} D_i + \Delta x_i D_{i+1}}\right) \overline{\phi}_{i+1}. \tag{16}$$

J_{i-1}, therefore, is given by:

$$J_{i-1} = \left(\frac{2 D_{i-1} D_i}{\Delta x_i D_{i-1} + \Delta x_{i-1} D_i}\right) \overline{\phi}_{i-1} + \left(-\frac{2 D_{i-1} D_i}{\Delta x_i D_{i-1} + \Delta x_{i-1} D_i}\right) \overline{\phi}_i. \tag{17}$$

Finally, substituting Eqs. (16) and (17) into Eq. (10) and rearranging yields the finite difference approximation to the interior cell i:

$$\begin{aligned} &\left[-\frac{2 D_{i-1} D_i}{\Delta x_i D_{i-1} + \Delta x_{i-1} D_i}\right] \overline{\phi}_{i-1} + \left[\Delta x_i \Sigma_{ai} + \frac{2 D_i D_{i-1}}{\Delta x_{i-1} D_i + \Delta x_i D_{i-1}} + \right. \\ &\left. + \frac{2 D_i D_{i+1}}{\Delta x_{i+1} D_i + \Delta x_i D_{i+1}}\right] \overline{\phi}_i + \left[-\frac{2 D_i D_{i+1}}{\Delta x_{i+1} D_i + \Delta x_i D_{i+1}}\right] \overline{\phi}_{i+1} = \Delta x_i S_i. \end{aligned} \tag{18}$$

Equation (18) can be simplified by defining a coefficient vector $\{c_i\}$ as follows:

$$c_i = -\frac{2 D_{i-1} D_i}{\Delta x_i D_{i-1} + \Delta x_{i-1} D_i}, \tag{19}$$

with Eq. (18) becoming:

$$c_i \overline{\phi}_{i-1} + \Big[\Delta x_i \Sigma_{ai} - c_i - c_{i+1}\Big] \overline{\phi}_i + c_{i+1} \overline{\phi}_{i+1} = \Delta x_i S_i. \tag{20}$$

Lastly, we need to approximate the reflective and vacuum boundary conditions (BCs). Let x_L and x_R be the locations of the left and right boundaries of the slab reactor, respectively.

Assuming N cells in the reactor, $x_L = x_0$ and $x_R = x_N$. The boundary cells' fluxes are $\overline{\phi}_1$ and $\overline{\phi}_N$, respectively. J_0 and J_N terms are affected by the left and right boundary conditions, respectively. The left boundary conditions' treatment will be discussed below.

The reflective boundary condition states the following:

$$J_0 = 0, \tag{21}$$

and while it is nonphysical for a full reactor, it can be used to represent a plane of symmetry (if one exists), therefore reducing the size of problem by a factor of 2. J_1 is unaffacted, so substituting J_0 and J_1 into Eq. (10) for $i = 1$ and rearranging then yields the finite difference approximation to boundary cell 1 with reflective BC:

$$\left[\Delta x_1 \Sigma_{a1} + \frac{2D_1 D_2}{\Delta x_2 D_1 + \Delta x_1 D_2}\right] \overline{\phi}_1 + \left[-\frac{2D_1 D_2}{\Delta x_2 D_1 + \Delta x_1 D_2}\right] \overline{\phi}_2 = \Delta x_1 S_1. \tag{22}$$

The vacuum boundary condition can be modeled in two different ways. A rough approximation simply states:

$$\phi_0 = 0, \tag{23}$$

which can be substituted into Eq. (13b) with $i = 0$ to yield J_0:

$$J_0 = \left[-\frac{2D_1}{\Delta x_1}\right] \overline{\phi}_1, \tag{24}$$

substituting which, together with (again unaffected) J_1, into Eq. (10) for $i = 1$ and rearranging then yields the finite difference approximation to boundary cell 1 with zero flux (rough approximation of vacuum) boundary condition:

$$\left[\Delta x_1 \Sigma_{a1} + \frac{2D_1}{\Delta x_1} + \frac{2D_1 D_2}{\Delta x_2 D_1 + \Delta x_1 D_2}\right] \overline{\phi}_1 + \left[-\frac{2D_1 D_2}{\Delta x_2 D_1 + \Delta x_1 D_2}\right] \overline{\phi}_2 = \Delta x_1 S_1. \tag{25}$$

Again, Eq. (23) is only a rough approximation of the vacuum BC. A more accurate approximation is to set the incoming (directed to the right) partial current J_0^+ to zero. Rightward partial current is given by (from the P_1 expansion that led to the one group 1D diffusion equation):

$$J^+(x) = \frac{1}{4}\phi(x) - \frac{1}{2}D(x)\,\frac{d}{dx}\phi(x)\,, \tag{26}$$

which with $x = x_0$ and $J_0^+ = 0$ and Eq. (3) yields:

$$0 = \frac{1}{4}\phi_0 + \frac{1}{2}J_0. \tag{27}$$

Solving Eq. (27) yields:

$$\phi_0 = -2J_0, \tag{28}$$

substituting which into Eq. (13b) with $i = 0$ yields:

$$J_0 = -D_1 \frac{\overline{\phi}_1 + 2J_0}{\Delta x_1/2}, \tag{29}$$

solving which for J_0 yields:

$$J_0 = \left(-\frac{2D_1}{\Delta x_1 + 4D_1} \right) \overline{\phi}_1. \tag{30}$$

Substituting J_0 and J_1 (again, unaffected) into Eq. (10) for $i = 1$ and rearranging then yields the finite difference approximation to boundary cell 1 with vacuum boundary condition:

$$\left[\Delta x_1 \Sigma_{a1} + \frac{2D_1}{\Delta x_1 + 4D_1} + \frac{2D_1 D_2}{\Delta x_2 D_1 + \Delta x_1 D_2} \right] \overline{\phi}_1 + \left[-\frac{2D_1 D_2}{\Delta x_2 D_1 + \Delta x_1 D_2} \right] \overline{\phi}_2 = \Delta x_1 S_1. \tag{31}$$

All of these boundary conditions can be constructed for cell N as well, although the current densities involved will now need to be J_N instead of J_0 and J_N^- instead of J_0^+. The right boundary condition will not be fully treated here, but the expression for $J^-(x)$ is provided for reference:

$$J^-(x) = \frac{1}{4}\phi(x) + \frac{1}{2}D(x)\,\frac{d}{dx}\phi(x)\,. \tag{32}$$