Nuclear Reactor Theory Project #2
Group #3

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I. Introduction & Background

Proving the capabilities and safety of a reactor design requires effective modeling of the neutron flux in the core (expressed in equation 1). For real cores, however, this is impossible, and must be first simplified, then discretized to provide the solution for a representative mesh. Certain simplifications can be applied to help make the problem easier to solve, since it allows the time dependent terms to be removed.

1) Isotropic assumption: ignoring the direction of the incoming neutron. This effectively drops all terms involving 2) Monoenergetic assumption: ignoring the energy variance of the neutrons. This means that a single set of cross sections can be used and allows us to ignore neutrons scattering into and out of the domain of interest 3) Homogeneity assumption: assuming that all core materials are evenly mixed throughout the volume of interest. This allows us to ignore discrete boundaries between materials 4) Steady-state assumption: assuming that the system has been in this state for a long period and that no transients occur.

For this project we have analyzed a simplified, monoenergetic, source through a homogeneous multiplying medium in one dimension. These assumptions simplify the transport equation to that presented in equation 2.

In the following sections, we will first describe the terms in equation 2, then provide an analytical solution. We will also provide an analysis of the accuracy of the analysis as a function of the number of nodes. Finally, we will analzye the solution for different coordinate systems to equation 2. Cartesian , cylindrical and spherical are the systems of interest.

$$\frac{\partial n}{\partial t} + v\hat{\Omega}\cdot\nabla n + v\Sigma_t n\left(\mathbf{r}, E', \hat{\Omega}, t\right) = \int_{4\pi} d\hat{\Omega}' \int_0^\infty dE' v'\Sigma_s\left(E' \to E, \hat{\Omega}' \to \hat{\Omega}\right) n\left(\mathbf{r}, E', \hat{\Omega}', t\right) + s\left(\mathbf{r}, E, \hat{\Omega}, t\right) \quad (1)$$

$$-D_m \frac{\mathrm{d}^2\phi}{\mathrm{d}x^2} + \Sigma_a^m \phi = \frac{1}{k}\nu\Sigma_f^m \phi \quad (2)$$

The following eigenvector problem must be solved:

$$\mathbf{A}\vec{b} = \mathbf{F}\vec{b} \quad (3)$$

II. Methodology

Equation 2 is a simplified description of neutron diffusion through a finite medium, similar to a point source travelling through a shielding material to a detector. The flux, therefore, depends on the transport cross section. This is accounted for in the term D_m, which is related to the transport coefficient by $D_m = 3\Sigma_{tr}^{-1}$. Values for Σ_{tr} for typical reactor materials are found in table I.

A. Numerical Approximation

It is rare to be faced with a design that allows for an analytical solution. Fortunately, numerical analysis methods exist that allow for approximation of the analytical solution. By dividing our hypothetical medium into discrete sections with nodes at the boundaries between these sections, it is possible to express the flux vector with equation 4:

$$\mathbf{A}\vec{\phi} = \mathbf{F}\vec{\phi} \quad (4)$$

Material	$\Sigma_{tr}(\mathrm{cm}^{-1})$	$\Sigma_a(\mathrm{cm}^{-1})$	$\nu\Sigma_f(\mathrm{cm}^{-1})$	*Relative Absorption*
H	1.79×10^{-2}	8.08×10^{-3}	0	0.053
O	7.16×10^{-3}	4.90×10^{-6}	0	0
Zr	2.91×10^{-3}	7.01×10^{-4}	0	0.005
Fe	9.46×10^{-4}	3.99×10^{-3}	0	0.026
^{235}U	3.08×10^{-4}	9.24×10^{-2}	0.145	0.602
^{238}U	6.95×10^{-3}	1.39×10^{-2}	1.20×10^{-2}	0.091
^{10}B	8.77×10^{-6}	3.41×10^{-2}	0	0.223
	3.62×10^{-2}	0.1532	0.1570	1.000

TABLE I
Macroscopic Cross Sections

where $\vec{\phi}$ is the flux at each node. The operator $\mathbf{F}$ describes the source of the multiplying medium. Initial guesses of 1 were used forThe operator $\mathbf{A}$ can be derived using the two-node approximation of the second derivative formula:

$$\left.\frac{\partial^2\phi}{\partial x^2}\right|_i \approx \frac{\phi_{i-1} - 2\phi_i + \phi_{i+1}}{\Delta x^2}$$

For non-edge nodes and the far right node, the derivation can be performed as follows:

$$\begin{aligned}
-D_m \frac{\mathrm{d}^2\phi}{\mathrm{d}x^2} + \Sigma_a\phi &= \frac{1}{k}\nu\Sigma_f^m\phi \\
-D_m \int_{x_i-\frac{\Delta x}{2}}^{x_i+\frac{\Delta x}{2}} \frac{\mathrm{d}^2\phi}{\mathrm{d}x^2}\,\mathrm{d}x + \int_{x_i-\frac{\Delta x}{2}}^{x_i+\frac{\Delta x}{2}} \Sigma_a\phi\,\mathrm{d}x &= \int_{x_i-\frac{\Delta x}{2}}^{x_i+\frac{\Delta x}{2}} \frac{1}{k}\nu\Sigma_f^m\phi_i\,\mathrm{d}x \\
-D_m \left.\frac{\mathrm{d}\phi}{\mathrm{d}x}\right|_{x_i-\frac{\Delta x}{2}}^{x_i+\frac{\Delta x}{2}} + \int_{x_i-\frac{\Delta x}{2}}^{x_i+\frac{\Delta x}{2}} \Sigma_a\phi dx &= \frac{1}{k}\nu\Sigma_f^m\phi_i \int_{x_i-\frac{\Delta x}{2}}^{x_i+\frac{\Delta x}{2}} \mathrm{d}x \\
-D_m \left(\frac{\phi_{i+1}-\phi_i}{\Delta x} - \frac{\phi_i-\phi_{i-1}}{\Delta x}\right) + \int_{x_i-\frac{\Delta x}{2}}^{x_i+\frac{\Delta x}{2}} \Sigma_a\phi dx &= \frac{1}{k}\nu\Sigma_f^m\phi_i \left[\left(x_i+\frac{\Delta x}{2}\right) - \left(x_i-\frac{\Delta x}{2}\right)\right] \\
-D_m \left(\frac{\phi_{i+1}-\phi_i}{\Delta x} - \frac{\phi_i-\phi_{i-1}}{\Delta x}\right) + \Sigma_a\phi_i\Delta x &= \frac{1}{k}\nu\Sigma_f^m\phi_i\Delta x
\end{aligned}$$

Dividing each term by Δx gives:

$$\left(\frac{-D_m}{\Delta x^2}\right)\phi_{i-1} + \left(\frac{2D_m}{\Delta x^2} + \Sigma_a\right)\phi_i + \left(\frac{-D_m}{\Delta x^2}\right)\phi_{i+1} = \frac{1}{k}\nu\Sigma_f^m\phi_i$$

From this we see that our operator $\mathbf{A}$ will have non-corner terms and right bottom corner terms: **

$$\begin{bmatrix}
\cdots & \cdots & \cdots & \cdots & \cdots \\
\frac{-D_m}{\Delta x^2} & \frac{2D_m}{\Delta x^2} + \Sigma_a & \frac{-D_m}{\Delta x^2} & 0 & \cdots \\
0 & \frac{-D_m}{\Delta x^2} & \frac{2D_m}{\Delta x^2} + \Sigma_a & \frac{-D_m}{\Delta x^2} & \cdots \\
 & & \ddots & & \\
\cdots & 0 & \frac{-D_m}{\Delta x^2} & \frac{2D_m}{\Delta x^2} + \Sigma_a & \frac{-D_m}{\Delta x^2}
\end{bmatrix}$$

$$\vec{J}(0) = -D_m \left.\frac{\mathrm{d}\phi}{\mathrm{d}x}\right|_0 \tag{5}$$

** We then solve for our top row using the boundary condition in equation 5:

$$\begin{aligned}
-D_m \frac{\phi_1-\phi_0}{\Delta x} + D_m \left.\frac{\mathrm{d}\phi}{\mathrm{d}x}\right|_0 + \int_0^{\Delta x/2} \Sigma_a\phi dx &= \frac{1}{k}\nu\Sigma_f^m\phi \\
-D_m \frac{\phi_1-\phi_0}{\Delta x} + \int_0^{\Delta x/2} \Sigma_a\phi dx &= \int_0^{\Delta x/2} \frac{1}{k}\nu\Sigma_f^m\phi dx \\
-D_m \frac{\phi_1-\phi_0}{\Delta x} + \Sigma_a\phi_0 \int_0^{\Delta x/2} dx &= \frac{1}{k}\nu\Sigma_f^m\phi 0i \int_0^{\Delta x/2} dx \\
-D_m \frac{\phi_1-\phi_0}{\Delta x} + \Sigma_a\phi_0\frac{\Delta x}{2} &= \frac{1}{k}\nu\Sigma_f^m\phi_0\frac{\Delta x}{2}
\end{aligned}$$

Divide by Δx on both sides:

$$\begin{aligned}
-D_m \frac{\phi_1-\phi_0}{\Delta x^2} + \frac{1}{2}\Sigma_a\phi_0 &= \frac{1}{k}\nu\Sigma_f^m\phi_0\frac{1}{2} \\
\frac{-D_m}{\Delta x^2}\phi_1 + \left(\frac{D}{\Delta x^2} + \frac{1}{2}\Sigma_a\right)\phi_0 &= \frac{1}{2k}\nu\Sigma_f^m\phi_0
\end{aligned}$$

This gives a final matrix $\mathbf{A}$ (for N nodes):

$$\begin{bmatrix} \frac{D_m}{\Delta x^2}+\frac{1}{2}\Sigma_a & -\frac{-D_m}{\Delta x^2} & 0 & 0 & \dots & 0 \\ -\frac{-D_m}{\Delta x^2} & \frac{2D_m}{\Delta x^2}+\Sigma_a & -\frac{-D_m}{\Delta x^2} & 0 & \dots & 0 \\ 0 & -\frac{-D_m}{\Delta x^2} & \frac{2D_m}{\Delta x^2}+\Sigma_a & -\frac{-D_m}{\Delta x^2} & \dots & 0 \\ 0 & 0 & -\frac{-D_m}{\Delta x^2} & \frac{2D}{\Delta x^2}+\Sigma_a & \dots & 0 \\ \dots & \dots & \dots\dots & \frac{D_m}{\Delta x^2}+\frac{1}{2}\Sigma_a & -\frac{-D_m}{\Delta x^2} & \\ 0 & \dots & 0 & 0-\frac{-D_m}{\Delta x^2} & \frac{2D_m}{\Delta x^2}+\frac{1}{2}\Sigma_a & \end{bmatrix}$$

This gives a final matrix $\mathbf{F}$ (for N nodes):

$$\begin{bmatrix} \frac{1}{2k}\nu\Sigma_f\phi_0 \\ \frac{1}{k}\nu\Sigma_f\phi_1 \\ \frac{1}{k}\nu\Sigma_f\phi_2 \\ \frac{1}{k}\nu\Sigma_f\phi_3 \\ \dots \\ \frac{1}{k}\nu\Sigma_f\phi_{N-1} \end{bmatrix}$$

A similar method was used to find matrix $\mathbf{A}$ for cylindrical and spherical coordinates. However the center averaged method was used to maneuver ϕ.

For cylindrical coordinates, the following equation was used to derive $\mathbf{A}$:

$$-D_m\frac{d^2\phi}{dr^2}+\frac{1}{r}\frac{d\phi}{dx}+\Sigma_a\phi=\frac{1}{k}\nu\Sigma_f^m\phi$$

The resulting matrix $\mathbf{A}$ (for N nodes) is:

$$\begin{bmatrix} \frac{1}{2}\Sigma_a+\frac{D_m}{(2i-1)\Delta r^2}+\frac{D_m}{r^2} & -\frac{D_m}{(2i-1)\Delta r^2}-\frac{D_m}{r^2} & 0 & \dots & 0 \\ \frac{-D_m}{\Delta r^2}\left(1+\frac{1}{2i-1}\right) & \frac{2D_m}{\Delta r^2}+\Sigma_a & -\frac{-D_m}{\Delta r^2}\left(1-\frac{1}{2i-1}\right) & \dots & 0 \\ 0 & -\frac{-D_m}{\Delta r^2}\left(1-\frac{1}{2i-1}\right) & \frac{2D_m}{\Delta r^2}+\Sigma_a & \frac{-D_m}{\Delta r^2}\left(1-\frac{1}{2i-1}\right) & 0 \\ \dots & \dots\dots & \frac{2D_m}{\Delta r^2}+\Sigma_a & 0 & \\ 0 & 0 & 0 & -\frac{-D_m}{\Delta r^2}\left(1-\frac{1}{2i-1}\right) & \frac{2D_m}{\Delta r^2}+\Sigma_a \end{bmatrix}$$

For spherical coordinates, the following equation was used to derive $\mathbf{A}$:

$$-D_m\frac{d^2\phi}{dr^2}+\frac{2}{r}\frac{d\phi}{dx}+\Sigma_a\phi=\frac{1}{k}\nu\Sigma_f^m\phi$$

The resulting matrix $\mathbf{A}$ (for N nodes) is:

$$\begin{bmatrix} \frac{1}{2}\Sigma_a+\frac{2D_m}{(2i-1)\Delta r^2}+\frac{D_m}{r^2} & -\frac{D_m}{(2i-1)\Delta r^2}-\frac{2D_m}{r^2} & 0 & \dots & 0 \\ \frac{-D_m}{\Delta r^2}\left(1+\frac{2}{2i-1}\right) & \frac{2D_m}{\Delta r^2}+\Sigma_a & -\frac{-D_m}{\Delta r^2}\left(1-\frac{2}{2i-1}\right) & \dots & 0 \\ 0 & \frac{-D_m}{\Delta r^2}\left(1-\frac{2}{2i-1}\right) & \frac{2D_m}{\Delta r^2}+\Sigma_a & \frac{-D_m}{\Delta r^2}\left(1-\frac{2}{2i-1}\right) & 0 \\ \dots & \dots\dots & \frac{2D_m}{\Delta r^2}+\Sigma_a & 0 & \\ 0 & 0 & 0 & -\frac{-D_m}{\Delta r^2}\left(1-\frac{2}{2i-1}\right) & \frac{2D_m}{\Delta r^2}+\Sigma_a \end{bmatrix}$$

III. Results

A Fortran program was developed to implement the discrete solution to the transport equation. The source code is included as an attachment to this report. The code uses $\mathbf{A}\vec{b}=\mathbf{F}\vec{b}$ to converge to the solution. And initial guess value for b is assumed (we use $\vec{f}=1$ for all discrete points but any values could be used but convergence time will vary). Our b vector is then multiplied by the inverse (obtained using LU decomposition) of our A matrix describe in the Methodology section above. We

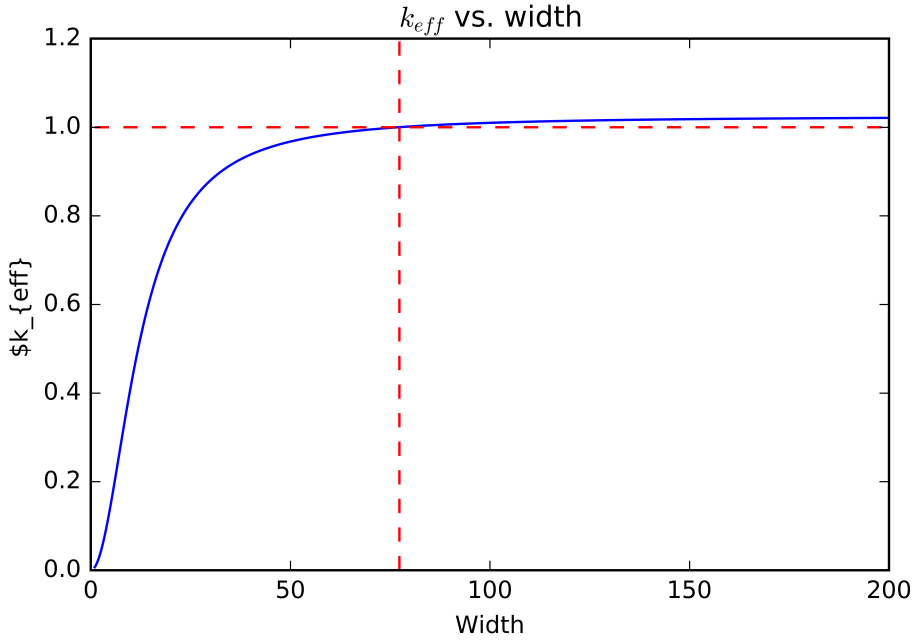

Fig. 1. k_eff vs. Width

then repeated the matrix multiplication with the newly obtained flux until the ch ange upon iteration in the eigenvalues and eigenvectors is lower than some minimum error specified.

The program allowed an analysis of a one-dimensional core filled with a multiplying medium. The flux distribution was solved for by iteratively seeking out eigenvalues of the material matrix.

In addition to finding the flux profile of the slab, the program also finds at what width the material with a specific Σ_f and Σ_a is critical. It achieves this by nesting the loop described above into an additional loop which tests if $k = 1 \pm errormargin$ and slightly changes the width accordingly until k converges to that value.

Our numerical calculation of the given parameters gave a critical width of $154.79\,\mathrm{cm}$. This was checked against a calculated value of width using the criticality condition $B_g^2 = B_m^2$:

$$\begin{aligned} B_g^2 &= B_m^2 \\ \left(\frac{\pi}{\tilde{a}}\right) &= \frac{\nu\Sigma_f - \Sigma_a}{D} \\ \tilde{a} &= \pi\sqrt{\frac{D}{\nu\Sigma_f - \Sigma_a}} \\ \tilde{a} &= 154.65\,\mathrm{cm} \end{aligned} \tag{6}$$

Substituting the values used to perform our numerical calculations, we arrive at a width of $w = 154.65\,\mathrm{cm}$, a very close match. A plot of k_{eff} vs. slab width can be seen in figure 1.

As with the previous project, it was worth noting how the values converged as the number of nodes was increased. As such, the program was run with different parameters to determine the convergence. The results of this can be seen in figure 2. From this, it is clear that this method converges by or before $N = 500$ nodes, since this appears very similar to $N = 10^3$ nodes (allowing for normalization of the flux).

IV. Conclusions

We provide an analysis of a simplified one-group, one-dimensional neutron diffusion in a multiplying medium. The various approaches to this problem produced similar but slightly different solutions, implying that careful choice of methodology is necessary in solving similar problems.

It is worth noting that the nature of numerical computation leaves even experienced programmers vulnerable to the idiosyncracies of computers and programming languages. Difficult-to-debug implicit casting of variables plagued the software used to perform the calculations, which were found only once the results were compared with a well-understood analytic

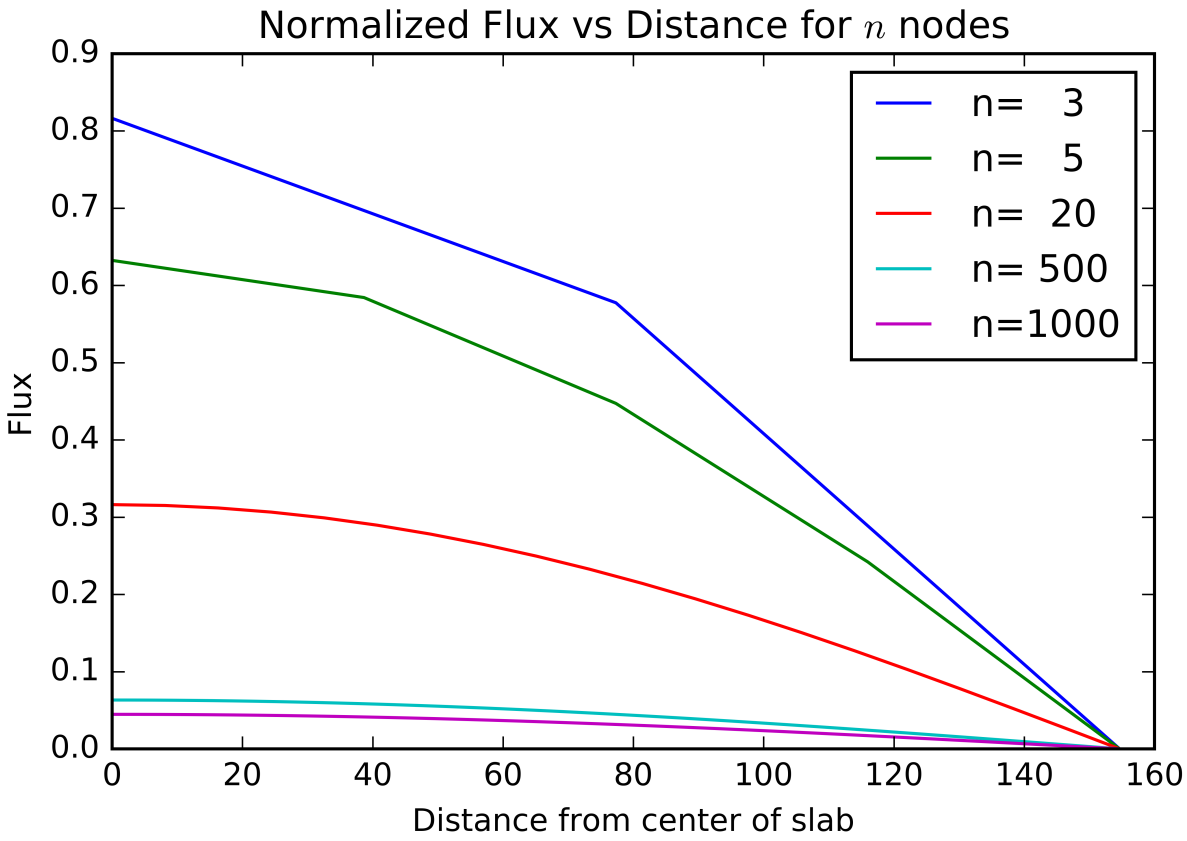

Fig. 2. Normalized Flux vs. Width as a function of the number of nodes

solution. New programs designed to simulate systems that resist such analytic analysis will not have such safeguards, necessitating additional care.

A. Group Member Responsibilities

Pseudocode: All Coding: Andrew and JR Derivations: Dory, Lee, Fan Report: Dory and JR