ABSTRACT

DAWN, WILLIAM C. Sodium Cooled Fast Reactor Simulations with the Finite Element Method. (Under the direction of Scott P. Palmtag and David J. Kropaczek.)

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Sodium Cooled Fast Reactor Simulations with the Finite Element Method

by
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DEDICATION

To the future of clean energy.

BIOGRAPHY

The author was born in a small town …

ACKNOWLEDGEMENTS

I would like to thank my advisor for his help.

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CHAPTER 1

INTRODUCTION

Let's start with a few paragraph basics, here is how to make **bold**, and *italics*, and *emphasized*. Let's say you need to cite something in your references, simply type `\cite{key}`, which produces [ER35]. Some other references are [GVL96] and [LK74]. Some LaTeX compilers require a second compilation for citations and references to be sorted and matched properly in the resulting document.

Here is a quotation:

> Alice, Bob and Carol are boring. Who would even want to know their secret?

Let's say we need to make a list, try this on for size

1. NCSU is great
2. I like NCSU
3. I really hope I can find a job when I graduate!

1.1 Math enviroments

1.1.1 Equations

There are many different ways to write equations, for example we could put $a^2 + b^2 = c^2$ directly into a sentence. Or we could use the equation enviroment and do

$$a^2 + b^2 = c^2. \tag{1.1}$$

And from here we can later reference it by simply doing typing `\ref{label}`, which gives 1.1. However, defining and using equation and figure reference macros will ensure that the equation references are consistent, instead of having Eq. (1), Equation 3, Eqn 4 scattered through the thesis. This template file defines `\eref` and `\fref` for this purpose. You can modify the macros to your liking in the `YourName-thesis.tex` file. For example, the command `\eref{label}` gives Eq. 1.1.

If you don't need to reference an equation you may simply do this

$$a^2 + b^2 = c^2.$$

For Greek letters you must go to the math enviroments, for example α, β, and γ. Let's look at equations that cover multiple lines, none of these equations may be true or mean anything, but so that the reader can get some ideas. In addition I will use some other useful notations like subscripts, superscripts, fractions, etc. One important item of note is that one uses the "ampersand" symbol to line up equations (also look at how I used quotations).

$$\begin{aligned} \gamma_1 &= \alpha^{\beta} + \psi_0 \frac{\psi_1}{\psi_2 + \psi_3} && (1.2) \\ &= \beta_1 + \beta_2 + \ldots + \beta_k \\ &\rightarrow E(\gamma_2) && (1.3) \end{aligned}$$

Alternatively, one can specify a slightly different enviroment if none of the equations need to be numbered. Remember that if you are planning on referring to them later on, you must use a "label" statement.

$$\begin{aligned} \gamma_1 &= n^{-1/2} \sum_{i=1}^{n} \left[h(X_i, \beta_0) - E\{h(X_i, \beta_0)\} \right] \\ &\rightarrow \hat{q} \pm \frac{\partial \gamma_2}{\partial \beta}. \end{aligned}$$

Lastly there may be times in which you want to use a non-italicized word your formula, such as an indicator function that may look like this $\mathrm{I}\{\mu_i(1,\beta) > \mu_i(0,\beta)\}$, if so just use the "mbox" statement.

You could use a multiline equation for long equations. The environment is `multline`. Insert `\\` for line breaks.

$$\dot{\cdot}\cdot\vec{\nabla}\psi(\vec{r},\dot{\cdot},E)+\Sigma_t(\vec{r},E)\psi(\vec{r},\dot{\cdot},E)=$$
$$\int_{4\pi}d\dot{\cdot}'\int_0^\infty dE'\,\Sigma_s(\vec{r},\dot{\cdot}'\rightarrow\dot{\cdot},E'\rightarrow E)\psi(\vec{r},\dot{\cdot}',E')+Q(\vec{r},\dot{\cdot},E),$$

we operate with $\int_0^\infty(\cdot)\,dE$ to obtain

$$\dot{\cdot}\cdot\vec{\nabla}\tilde{\psi}(\vec{r},\dot{\cdot})+\Sigma_t(\vec{r})\tilde{\psi}(\vec{r},\dot{\cdot})=$$
$$\int_{4\pi}d\dot{\cdot}'\int_0^\infty dE'\,\psi(\vec{r},\dot{\cdot}',E')\left[\int_0^\infty dE\,\Sigma_s(\vec{r},\dot{\cdot}'\rightarrow\dot{\cdot},E'\rightarrow E)\right]+\tilde{Q}(\vec{r},\dot{\cdot}),$$

CHAPTER 2

FINITE ELEMENT NEUTRON DIFFUSION

2.1 Introduction

For typical nuclear reactor applications, diffusion theory well approximates the neutron distribution within the reactor. The neutron diffusion equation is a second order partial differential equation in space and energy. In standard notation, the continuous neutron diffusion equation is presented as

$$-\nabla\cdot(D(\mathbf{r},E)\nabla\phi(\mathbf{r},E))+\Sigma_t(\mathbf{r},E)\phi(\mathbf{r},E)= \frac{\chi(\mathbf{r},E)}{k_{eff}}\int_0^\infty \nu_f(\mathbf{r},E')\Sigma_f(\mathbf{r},E')\phi(\mathbf{r},E')\,dE'+\int_0^\infty \Sigma_s(\mathbf{r},E'\rightarrow E)\phi(\mathbf{r},E')\,dE' \quad (2.1)$$

Where D is the diffusion constant, ϕ is the scalar neutron flux, Σ_t is the total cross section, χ is the fission neutron spectrum, k_{eff} is the effective neutron multiplication factor, Σ_f is the fission cross section, ν_f is the neutron yield per fission, and $\Sigma_s(\mathbf{r},E'\rightarrow E)$ is the scattering cross section for neutrons at position $\mathbf{r}$ scattering from energy E' to E.

The neutron diffusion equation must be discretized in space and energy to be solved numerically. Energy discretization is relatively straight-forward and is performed using the multigroup method. Spatial discretization requires more attention and will be done with the Finite Element Method (FEM). This method is selected for several reasons. It allows for easily increasing the order of the method by increasing the order of the elements with no changing of the mesh required. Coordinates of nodes can be easily updated to reflect physical phenomena such as thermal expansion (Chapter

4). Additionally, material properties are calculated on an element basis allowing for fine detail updates to the material properties during the calculation.

For energy discretization, An energy structure is described as $\{E_g\}$ for $g = 1,2,\ldots,G$ and by convention

$$E_G > E_{G-1} > \ldots > E_2 > E_1$$

Then, multigroup constants can be calculated based on the energy group structure and the known cross sections. Multigroup constants are calculated to preserve the number of neutrons produced or destroyed. That is, the calculation preserves reaction rates where the reaction rate for reaction x is defined as $R_x = \Sigma_x \phi$. Multigroup constants are then calculated. A formal derivation is given in [DH76] and the results are presented below.

$$D_g(\mathbf{r}) = \frac{\int_{E_g}^{E_{g-1}} D(\mathbf{r},E')\nabla\phi(\mathbf{r},E)\,dE}{\int_{E_g}^{E_{g-1}} \nabla\phi(\mathbf{r},E)\,dE} \tag{2.2}$$

$$\Sigma_{t,g}(\mathbf{r}) = \frac{\int_{E_g}^{E_{g-1}} \Sigma_t(\mathbf{r},E)\phi(\mathbf{r},E)\,dE}{\int_{E_g}^{E_{g-1}} \phi(\mathbf{r},E)\,dE} \tag{2.3}$$

$$\nu\Sigma_{f,g}(\mathbf{r}) = \frac{\int_{E_g}^{E_{g-1}} \nu_f(\mathbf{r},E)\Sigma_f(\mathbf{r},E)\phi(\mathbf{r},E)\,dE}{\int_{E_g}^{E_{g-1}} \phi(\mathbf{r},E)\,dE} \tag{2.4}$$

$$\Sigma_{s,g\to g'}(\mathbf{r}) = \frac{\int_{E_g'}^{E_{g'-1}} \int_{E_g}^{E_{g-1}} \Sigma_s(\mathbf{r},E'\to E)\phi(\mathbf{r},E')\,dE\,dE'}{\int_{E_g}^{E_{g-1}} \phi(\mathbf{r},E)\,dE} \tag{2.5}$$

$$\chi_g(\mathbf{r}) = \int_{E_g}^{E_{g-1}} \chi(\mathbf{r},E)\,dE \tag{2.6}$$

$$\phi_g(\mathbf{r}) = \int_{E_g}^{E_{g-1}} \phi(\mathbf{r},E)\,dE \tag{2.7}$$

Note that cross sections $\nu_f(\mathbf{r},E)$ and $\Sigma_f(\mathbf{r},E)$ have been combined. This is necessary and a mathematical result of the group collapse. Then, Eq. 2.1 can be discretized in energy as

$$-\nabla\cdot(D_g(\mathbf{r})\nabla\phi_g(\mathbf{r})) + \Sigma_{t,g}(\mathbf{r})\phi_g(\mathbf{r}) = \frac{\chi_g(\mathbf{r})}{k_{eff}} \sum_{g'=1}^{G} \nu\Sigma_{f,g'}(\mathbf{r})\phi_{g'}(\mathbf{r}) + \sum_{g'=1}^{G} \Sigma_{s,g'\to g}(\mathbf{r})\phi_{g'}(\mathbf{r}) \tag{2.8}$$

The neutron diffusion equation has now been discretized in energy. Spatial dicretization will be based on the Finite Element Method (FEM) and will be discussed in Sec. 2.2.1.

The total neutron cross section includes the contribution due to self-scattering. That is, due to $\Sigma_{s,g\to g}$. This can be removed from Eq. 2.8 for simplicity.

$$-\nabla\cdot(D_g(\mathbf{r})\nabla\phi_g(\mathbf{r}))+\Sigma_{r,g}(\mathbf{r})\phi_g(\mathbf{r})=\frac{\chi_g(\mathbf{r})}{k_{eff}}\sum_{g'=1}^{G}\nu\Sigma_{f,g'}(\mathbf{r})\phi_{g'}(\mathbf{r})+\sum_{g'=1,g'\neq g}^{G}\Sigma_{s,g'\to g}(\mathbf{r})\phi_{g'}(\mathbf{r}) \tag{2.9}$$

Where $\Sigma_{r,g}$ is the removal cross section and $\Sigma_{r,g}(\mathbf{r})=\Sigma_{t,g}(\mathbf{r})-\Sigma_{s,g\to g}(\mathbf{r})$. For simplicity, the neutron sources in Eq. 2.9 can be combined into a single term.

$$-\nabla\cdot(D_g(\mathbf{r})\nabla\phi_g(\mathbf{r}))+\Sigma_{r,g}(\mathbf{r})\phi_g(\mathbf{r})=q_g(\mathbf{r}) \tag{2.10}$$

Where $q_g(\mathbf{r})$ is the combined neutron source at position $\mathbf{r}$. q can then be further divided into contributions due to fission (q_{fiss}), up- scattering (q_{up}) when a neutron increases in energy, and down-scattering when a neutron decreases in energy (q_{down}).

$$q_g(\mathbf{r})=q_{fiss,g}(\mathbf{r})+q_{up,g}(\mathbf{r})+q_{down,g}(\mathbf{r}) \tag{2.11}$$

$$q_{fiss,g}(\mathbf{r})=\frac{\chi_g(\mathbf{r})}{k_{eff}}\sum_{g'=1}^{G}\nu\Sigma_{f,g'}(\mathbf{r})\phi_{g'}(\mathbf{r}) \tag{2.12}$$

$$q_{up,g}(\mathbf{r})=\sum_{g'=g+1}^{G}\Sigma_{s,g'\to g}(\mathbf{r})\phi_{g'}(\mathbf{r}) \tag{2.13}$$

$$q_{down,g}(\mathbf{r})=\sum_{g'=1}^{g}\Sigma_{s,g'\to g}(\mathbf{r})\phi_{g'}(\mathbf{r}) \tag{2.14}$$

Where the difference between q_{up} and q_{down} are the limits of the summation. This form allows for operator splitting of the neutron source term. In an iterative scheme, it will be necessary for fission and up-scatter sources to use a different flux iterate than down-scatter so this division will prove useful.

2.2 Formulation

2.2.1 Derivation

The only remaining continuous variable in the problem is the spatial variable $\mathbf{r}$. This will be discretized according to the Finite Element Method (FEM). The form of the diffusion equation to be discretized is Eq. 2.10. The problem is solved in a finite domain $\mathbf{r}\in\Omega$ where $\partial\Omega$ represents the boundary of the domain where some boundary condition is specified. Boundary condition options

provided include

1. Mirror. $\nabla\phi_g(\mathbf{r}) = 0$ for $\mathbf{r} \in \partial\Omega$.
2. Albedo. $D_g(\mathbf{r})\nabla\phi_g(\mathbf{r}) + \aleph\phi_g(\mathbf{r}) = 0$ for $\mathbf{r} \in \partial\Omega$ where $\aleph$ is a real constant specified by the user. For vacuum conditions, $\alpha = \frac{1}{2}$.
3. Zero Flux. $\phi_g(\mathbf{r}) = 0$ for $\mathbf{r} \in \partial\Omega$.

(Note: the order of the above list corresponds to the order of boundary condition precedent in code with the greater the integer, the greater the precedent.)

Finite Element derivation begins with Eq. 2.10. The equation is multiplied by a testing function $v(\mathbf{r}) \in H_1(\Omega)$ Where H is the Sobolev Space. Then, the equation is integrated over the problem domain. This yields the Weak Form or Variational Form of the problem.

$$-\nabla\cdot(D_g(\mathbf{r})\nabla\phi_g(\mathbf{r})) + \Sigma_{r,g}(\mathbf{r})\phi_g(\mathbf{r}) = q_g(\mathbf{r}) \tag{2.15}$$

$$-\nabla\cdot(D_g(\mathbf{r})\nabla\phi_g(\mathbf{r}))v(\mathbf{r}) + \Sigma_{r,g}(\mathbf{r})\phi_g(\mathbf{r})v(\mathbf{r}) = q_g(\mathbf{r}) \tag{2.16}$$

$$-\int_\Omega \nabla\cdot(D_g(\mathbf{r})\nabla\phi_g(\mathbf{r}))v(\mathbf{r})\,d\Omega \int_\Omega \Sigma_{r,g}(\mathbf{r})\phi_g(\mathbf{r})v(\mathbf{r})\,d\Omega = \int_\Omega q_g(\mathbf{r})v(\mathbf{r})\,d\Omega \tag{2.17}$$

For the purposes of this application, material cross sections and the neutron source are assumed to be constant within an element. Then, the integral can be partitioned into a sum of integrals over the elements in the domain assuming the set of elements $\{\Omega_e\} = \Omega$ for $e = 1, 2, \ldots, E$ where E is the total number of elements.

$$-\sum_{e=1}^{E} D_{g,e}\int_{\Omega_e}\nabla\cdot\nabla\phi_g(\mathbf{r})v(\mathbf{r})\,d\Omega_e + \sum_{e=1}^{E}\Sigma_{r,g,e}\int_{\Omega_e}\phi_g(\mathbf{r})v(\mathbf{r})\,d\Omega_e = \sum_{e=1}^{E} q_{g,e}\int_{\Omega_e} v(\mathbf{r})\,d\Omega_e \tag{2.18}$$

The Second Green's Theorem is used to simplify the integral in the first term. A proof can be found in [Li18] in Theorem 9.2.

$$-\int_{\Omega_e}\nabla\cdot\nabla\phi_g(\mathbf{r})v(\mathbf{r})\,d\Omega_e = -\int_{\partial\Omega_e}\frac{\partial\phi_g(\mathbf{r})}{\partial\mathbf{n}}v(\mathbf{r})\,ds + \int_{\Omega_e}\nabla\phi_g(\mathbf{r})\cdot\nabla v(\mathbf{r})\,d\Omega_e \tag{2.19}$$

Where $\frac{\partial\phi_g(\mathbf{r})}{\partial\mathbf{n}}$ is the outward normal derivative and the integral ds is a line integral in two dimensions or a surface integral in three dimensions. Recognizing that this quantity will only be relevant on the boundary of the problem, the value of the outward normal derivative may be specified in a boundary condition. Specifically, the Albedo boundary condition which has the following form for

$\mathbf{r} \in \partial\Omega$.

$$D_g(\mathbf{r})\nabla\phi_g(\mathbf{r}) + \aleph\phi_g(\mathbf{r}) = 0 \tag{2.20}$$

$$\nabla\phi_g(\mathbf{r}) = \frac{-\aleph\phi_g(\mathbf{r})}{D_g} \tag{2.21}$$

Substituting Eq. 2.19 into Eq. 2.18 and assuming the outward normal derivative is specified in the form of an Albedo boundary condition.

$$-\sum_{e=1}^{E} D_{g,e} \int_{\partial\Omega_e} v(\mathbf{r}) \frac{\partial\phi_g(\mathbf{r})}{\partial\mathbf{n}}\, ds + \sum_{e=1}^{E} D_{g,e} \int_{\Omega_e} \nabla\phi_g(\mathbf{r}) \cdot \nabla v(\mathbf{r})\, d\Omega_e + \sum_{e=1}^{E} \Sigma_{r,g,e} \int_{\Omega_e} \phi_g(\mathbf{r}) v(\mathbf{r})\, d\Omega_e = \sum_{e=1}^{E} q_{g,e} \int_{\Omega_e} v(\mathbf{r})\, d\Omega_e \tag{2.22}$$

$$\sum_{e=1}^{E} \aleph \int_{\partial\Omega_e} v(\mathbf{r})\phi_g(\mathbf{r})\, ds + \sum_{e=1}^{E} D_{g,e} \int_{\Omega_e} \nabla\phi_g(\mathbf{r}) \cdot \nabla v(\mathbf{r})\, d\Omega_e + \sum_{e=1}^{E} \Sigma_{r,g,e} \int_{\Omega_e} \phi_g(\mathbf{r}) v(\mathbf{r})\, d\Omega_e = \sum_{e=1}^{E} q_{g,e} \int_{\Omega_e} v(\mathbf{r})\, d\Omega_e \tag{2.23}$$

Now the function of interest $\phi_g(\mathbf{r})$ is assumed to be a linear combination of chosen basis functions $\{N_i\}$.

$$\phi_g(\mathbf{r}) = \sum_{i=1}^{N} \alpha_{g,i} N_i(\mathbf{r}) \tag{2.24}$$

Where coefficients $\{\alpha_i\}$ are unknown and will be determined. Typically, these basis functions have unit magnitude and are centered at the node points so the coefficients α_i are the approximated solution at the nodes. Basis functions are typically polynomials of arbitrary magnitude. Linear and quadratic polynomials are common but for the application presented here, only linear basis functions are explored. The test function $v(\mathbf{r})$ is also chosen as a linear combination of the basis functions.

$$v(\mathbf{r}) = \sum_{j=1}^{N} N_j(\mathbf{r}) \tag{2.25}$$

The testing function is arbitrary so the magnitude is fixed to the magnitude of the basis function.

Eq. 2.24 and Eq. 2.25 are plugged into Eq. 2.23. This yields a linear system of equations.

$$\sum_{e=1}^{E} \aleph \sum_{i=1}^{N} \alpha_{i,g} \int_{\partial\Omega_e} N_i(\mathbf{r}) N_j(\mathbf{r})\, ds + \sum_{e=1}^{E} D_{g,e} \sum_{i=1}^{N} \alpha_{i,g} \int_{\Omega_e} \nabla N_i(\mathbf{r}) \cdot \nabla N_i(\mathbf{r})\, d\Omega_e + \sum_{e=1}^{E} \Sigma_{r,g,e} \sum_{i=1}^{N} \alpha_{i,g} \int_{\Omega_e} N_i(\mathbf{r}) N_i(\mathbf{r})\, d\Omega_e = \sum_{e=1}^{E} q_{g,e} \sum_{i=1}^{N} \int_{\Omega_e} N_i(\mathbf{r})\, d\Omega_e \quad (2.26)$$

$$\sum_{i=1}^{N} \alpha_{i,g} \sum_{j=1}^{N} \left(\sum_{e=1}^{E} \aleph \int_{\partial\Omega_e} N_i(\mathbf{r}) N_j(\mathbf{r})\, ds + \sum_{e=1}^{E} D_{g,e} \int_{\Omega_e} \nabla N_i(\mathbf{r}) \cdot \nabla N_j(\mathbf{r})\, d\Omega_e + \sum_{e=1}^{E} \Sigma_{r,g,e} \int_{\Omega_e} N_i(\mathbf{r}) N_j(\mathbf{r})\, d\Omega_e \right) = \sum_{i=1}^{N} \left(\sum_{e=1}^{E} q_{g,e} \int_{\Omega_e} N_i(\mathbf{r})\, d\Omega_e \right) \quad (2.27)$$

$$a(N_i, N_j) = f(N_i) \quad (2.28)$$

$$\mathbf{Au} = \mathbf{f} \quad (2.29)$$

$a(N_i, N_j)$ is the bilinear form and $f(N_i)$ is the linear form of the finite element system. In matrix notation, $\mathbf{A}$ is described by the integral quantities (more to follow), $\mathbf{u} = \{\alpha_i\}$, and $\mathbf{f}$ is described by the source integral quantity.

Inspecting the matrix $\mathbf{A}$ and the vector $\mathbf{f}$ reveals the following.

$$A_{i,j,g,e} = \aleph \int_{\partial\Omega_e} N_i(\mathbf{r}) N_j(\mathbf{r})\, ds + D_{g,e} \int_{\Omega_e} \nabla N_i(\mathbf{r}) \cdot \nabla N_j(\mathbf{r})\, d\Omega_e + \Sigma_{r,g,e} \int_{\Omega_e} N_i(\mathbf{r}) N_j(\mathbf{r})\, d\Omega_e \quad (2.30)$$

$$f_{i,g,e} = q_{g,e} \int_{\Omega_e} N_i(\mathbf{r})\, d\Omega_e \quad (2.31)$$

Then,

$$A_{i,j,g} = \sum_{e=1}^{E} A_{i,j,g,e} \quad (2.32)$$

$$f_{i,g} = \sum_{e=1}^{E} f_{i,g,e} \quad (2.33)$$

which leads to the natural population of the matrix $\mathbf{A}$ on an element-by-element basis. That is, the matrix $\mathbf{A}$ is assembled by looping through all of the elements and summing their contribution to the

matrix. Note that the contribution due to the surface integral will be zero in elements not on the boundary and may also be zero for problems with select boundary conditions. The population of the vector **f** is done similarly. Then, the matrix **A** and the vector **f** are known for each energy group. The equations are solved on group at a time and ϕ_g is calculated and stored.

Though the notation may be obtuse, the above reduces to a linear system of equations. These equations are constructed from the integral quantities specified by the FEM and the coefficients given by the cross sections and fixed source regions. The integral quantities themselves are expressed explicitly in the next section.

2.2.2 Matrix Quantities

For certain simple elements, the integral quantities described in Eq. 2.30 and Eq. 2.31 have exact analytic forms. The for this application, linear triangles and linear wedges are investigated and many of the integrals have exact expressions. If these quantities cannot be expressed exactly or doing so would be computationally difficult, quadratures can be used and for certain problems, these quadratures can express the integrals exactly. This will be discussed in Sec. 2.2.3.

2.2.2.1 Linear Triangles

Linear triangles are common to two dimensional finite element methods and have been investigated in many applications [Hos17] [HV13] [HSD15]. This is a triangle defined by three corner coordinates with basis functions located on each corner [Sch06].

Originally proposed in [Whi85], there are simple expressions for the quantities. The expression for the line integral is found in [Eng05]. For a triangle with corners $\{x_i, y_i\}$.

$$\int_{\Omega_e} \nabla N_i(\mathbf{r}) \cdot \nabla N_j(\mathbf{r})\, d\Omega_e = \frac{1}{4A_e}((x_{i+1}-x_{i+2})(x_{j+1}-x_{j+2})+(y_{i+1}-y_{i+2})(y_{j+1}-y_{j+2})) \tag{2.34}$$

$$\int_{\Omega_e} N_i(\mathbf{r}) N_j(\mathbf{r})\, d\Omega_e = \frac{A_e}{12}(1+\delta_{ij}) \tag{2.35}$$

$$\int_{\Omega_e} N_i(\mathbf{r})\, d\Omega_e = \frac{A_e}{3} \tag{2.36}$$

$$\int_{\partial\Omega_e} N_i(\mathbf{r}) N_j(\mathbf{r})\, ds = \frac{L_e}{6}(1+\delta_{ij}) \tag{2.37}$$

$$\tag{2.38}$$

Where A_e is the area of the triangular element L_e is the length of the edge between node i and

node j, and δ_{ij} is the Kronecker delta such that

$$\delta_{ij} = \begin{cases} 0 & \text{if } i \neq j \\ 1 & \text{if } i = j \end{cases} \tag{2.39}$$

For higher order triangular elements, it will be necessary to employ a quadrature.

2.2.2.2 Linear Wedges

Wedge elements have not reached the same commonality as triangular elements but are extruded triangles. Geometrically, the shape is a pentahedron or a triangular prism. However, their exact geometric relation is not fixed and the nodes are free to expand. These shapes are unique because three of the faces are quadrilateral and two of the faces are triangular. The values presented herein are not yet found in literature and are calculated by there author and published here for the first time.

$$\int_{\Omega_e} N_i(\mathbf{r}) N_j(\mathbf{r})\, d\Omega_e = \frac{V_e}{2} \begin{pmatrix} \frac{1}{18} & \frac{1}{36} & \frac{1}{36} & \frac{1}{36} & \frac{1}{72} & \frac{1}{72} \\ \frac{1}{36} & \frac{1}{18} & \frac{1}{36} & \frac{1}{72} & \frac{1}{36} & \frac{1}{72} \\ \frac{1}{36} & \frac{1}{36} & \frac{1}{18} & \frac{1}{72} & \frac{1}{72} & \frac{1}{36} \\ \frac{1}{36} & \frac{1}{72} & \frac{1}{72} & \frac{1}{18} & \frac{1}{36} & \frac{1}{36} \\ \frac{1}{72} & \frac{1}{36} & \frac{1}{72} & \frac{1}{36} & \frac{1}{18} & \frac{1}{36} \\ \frac{1}{72} & \frac{1}{72} & \frac{1}{36} & \frac{1}{36} & \frac{1}{36} & \frac{1}{18} \end{pmatrix} \tag{2.40}$$

$$\int_{\Omega_e} N_i(\mathbf{r})\, d\Omega_e = \frac{V_e}{12} \tag{2.41}$$

$$\int_{\partial\Omega_e} N_i(\mathbf{r}) N_j(\mathbf{r})\, d\partial\Omega_e = \begin{cases} \frac{A_\triangle}{12}(1+\delta_{ij}) & \text{if triangle} \\ \frac{A_\square}{36}(1+\delta_{ij})(1-\frac{1}{2}\delta_{i,(5-j)}) & \text{if quadrilateral} \end{cases} \tag{2.42}$$

Where V_e is the volume of the element. This matrix is indexed A_{ij} and is presented as a matrix because of its irregular form. Notice the integral containing the gradient operator has been omitted because if it could be computed analytically, it would be less computationally efficient than using a quadrature.

2.2.3 Quadratures

Quadratures are sets of coordinates and weights which allow for the exact integration of polynomials of given order. For a given set of weights $\{w_i\}$ and a set of coordinates $\{\mathbf{x}\}$, the quadrature can be

expressed as follows.

$$\int_{\Omega} f(\mathbf{x})\, d\Omega \approx \sum_{i=1}^{N} w_i f(\mathbf{x}_i) \tag{2.43}$$

where Ω is an arbitrary domain described by $\{\mathbf{x}_i\}$. The above quadrature will exactly integrate a polynomial of the order of the quadrature. It is not necessarily true that N be the order of the quadrature.

For one dimensional integrals, the Gaussian quadrature is common and the most compact quadrature. The Gaussian quadrature exactly integrates a polynomial of order n using exactly n points. Weights and coordinates for this quadrature set are presented in [Kam11]. For this quadrature, $n = N$.

Two dimensional and three dimensional quadratures are necessary for the solution of this problem. Triangular quadratures are not as simply derived as line quadratures and the number of points need not equal the order of the polynomial integrated. The triangular quadrature as implemented here is symmetric and open. That is, there are no points on the boundary of the triangle. The structure for this triangular quadrature is found in [Den10].

Quadrilateral quadrature sets are simply tensor products of two line Gaussian quadratures. For an order N polynomial, now n^2 points are required.

Wedge quadrature sets are simply tensor products of a line Gaussian quadrature and a triangular quadrature.

All of the quadratures described here are tabulated for a reference element be it a line, a triangle, a quadrilateral, or a wedge. Integration in the FEM is performed on an arbitrary element in space. Therefore, it is necessary to perform a coordinate transform when using a quadrature set.

$$\int_{\Omega} f(\mathbf{x})\, d\Omega = \int_{\Omega_{ref}} f(\mathbf{x})|\mathbf{J}|\, d\Omega \approx \sum_{i=1}^{N} w_i f(\mathbf{x}_i)|\mathbf{J}_i| \tag{2.44}$$

where $\mathbf{J}$ is the Jacobian matrix, $\mathbf{J}_i$ is the Jacobian matrix at quadrature coordinate $\mathbf{x}_i$, and $|\cdot|$ represents the matrix determinant. Notationally, $J = |\mathbf{J}|$ and is termed the Jacobi.

For simple elements, the Jacobi is constant over the element and can be precalculated to save from allocating, populating, and taking the determinant of a matrix for each integration point. For the elements of concern, these values are presented below as found in [Fel04].

Table 2.1 Jacobian Determinants

Element	Jacobi	J
Triangle	$J = \frac{1}{2}\|\mathbf{J}\|$	A_e
Quadrilateral	$J = \|\mathbf{J}\|$	$\frac{1}{4}A_e$
Wedge	$J = \frac{1}{2}\|\mathbf{J}\|$	$\frac{1}{2}V_e$

2.3 Implementation

2.3.1 Algorithm

Algorithm 1 General Iteration Scheme

Initialize $\phi^{(0)}$
Order the nodes of the problem into RCM order.
Calculate Σ_s, Σ_t, and $\nu\Sigma_f$ for each element
Calculate Stiffness Matrix A for each group. Store this.
while Power Iteration **do**
    $s = s + 1$
    Update q_{fiss} and q_{up} from previous data $\phi^{(s-1)}$
    Update χ in each element using previous data
    for $g = 1, G$ **do**
        Update q_{down} from current data $\phi^{(s)}$
        Calculate total effective source in each element
        Update Load Vector with new source
        Solve $\mathbf{Au} = \mathbf{f}$ using an iterative technique
        Parse $\mathbf{u}$ for ϕ nodal solution
        Calculate element-average $\bar{\phi}$
    end for
    Update k_{eff}
    Check convergence
end while

2.3.2 Memory and Storage

The Finite Element matrix **A** is large and sparse so a sparse storage implementation is required.

2.3.3 Linear System Solution

2.4 Reference Results

2.4.1 Triangular Element Manufactured Solutions

2.4.1.1 One Dimension, One-Group, Fixed Source

2.4.1.2 One Dimension, One-Group, Criticality

2.4.1.3 One Dimension, Two-Group, Criticality

2.4.1.4 One Dimension, One-Group, Two-Region, Criticality

2.4.1.5 Two Dimension, One-Group, Criticality

2.4.2 Two Dimension Reactors

2.4.2.1 VVER440

2.4.2.2 SNR

2.4.2.3 HWR

2.4.2.4 IAEA

2.4.3 Wedge Element Manufactured Solution Finite Cylinder

2.4.4 Three Dimension Reactors

2.4.4.1 MONJU

2.4.4.2 KNK

CHAPTER 3

THERMAL HYDRAULICS

3.1 Axial Convection Model

3.2 Radial Conduction Model

3.2.1 Derivation

3.2.2 Relations

3.3 Cross Section Treatment

3.4 Results

CHAPTER 4

THERMAL EXPANSION

4.1 Necessity of Modeling

4.2 Model Details

4.3 Implementation

4.4 Results

CHAPTER 5

CONCLUSIONS

5.1 Results Discussion

5.2 Code Enhancements

5.3 Further Investigations

BIBLIOGRAPHY

[Den10] Deng, S. *Quadrature Formulas in Two Dimensions*. 2010.

[DH76] Duderstadt, J. J. & Hamilton, L. J. *Nuclear Reactor Analysis*. New York: Wiley, 1976.

[ER35] Einstein, A. & Rosen, N. "The particle problem in the general theory of relativity". *Physical Review* **48**.1 (1935), pp. 73–77.

[Eng05] Engblom, S. *The Finite Element Method*. 2005.

[Fel04] Felippa, C. A. *Advanced Finite Element Methods*. Boulder, CO: University of Colorado at Boulder, 2004.

[GVL96] Golub, G. & Van Loan, C. *Matrix computations*. Johns Hopkins Univ Pr, 1996.

[Hos17] Hosseini, S. A. "Sensitivity Analysis of the Galerkin Finite Element Method Neutron Diffusion Solver to the Shape of the Elements". *Nuclear Engineering and Technology* **49**.1 (2017), pp. 29–42.

[HSD15] Hosseini, S. A. & Saadatian-Derakhshandeh, F. "Galerkin and Generalized Least Squares finite element: A comparative study for multi-group diffusion solvers". *Progress in Nuclear Energy* **85** (2015), pp. 473–490.

[HV13] Hosseini, S. A. & Vosoughi, N. "Development of two-dimensional, multigroup neutron diffusion computer code based on GFEM with unstructured triangle elements". *Annals of Nuclear Energy* **51** (2013), pp. 213–226.

[Kam11] Kamermans, M. "Gaussian Quadrature Weights and Abscissae" (2011).

[LK74] Larsen, E. & Keller, J. "Asymptotic solution of neutron transport problems for small mean free paths". *Journal of Mathematical Physics* **15** (1974), p. 75.

[Li18] Li, Z. et al. *Numerical Solution of Differential Equations*. Cambridge: Cambridge, 2018.

[Sch06] Schroeder, W. et al. *The Visualization Toolkit*. 4th ed. Kitware, 2006.

[Whi85] White, R. E. *An Introduction ot the Finite Element Method with Applications to Nonlinear Problems*. New York: Wiley, 1985.

APPENDIX

APPENDIX A

LOREM IPSUM

A.1 A First Section

A.1.0.0.1 Filler Text

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Table A.1 A table in the appendix.

System	Author
TEX	Donald Knuth
LATEX	Leslie Lamport

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A.2 A Second Section

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