Verification of "Discontinuous Finite Element Formulations for Neutron Transport in Spherical-Geometry"

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February 17, 2016

Contents

1 Derivation of spherical-geometry transport equations

1.1 Finite element in space, S_N in angle

This derivation follows the derivation by Mercimek and Özgener [3] in methodology, but defines the integration constants differently. The conservative form of the spherical geometry transport equation is

$$\mu \frac{\partial}{\partial r}\left(r^2 \psi\right) + r \frac{\partial\left[\left(1-\mu^2\right)\psi\right]}{d\mu} + r^2 \sigma\left(r\right)\psi\left(r,\mu\right) = r^2 q\left(r,\mu\right), \tag{1}$$

with the variables as described in Table 1.

Variable	Units	Description
r	cm	Distance from the center of the sphere
μ	-	Cosine of the polar angle
$\psi\left(r,\mu\right)$	$\mathrm{cm}^{-2}\cdot\mathrm{s}^{-1}$	Angular flux
$\sigma\left(r,\mu\right)$	cm^{-1}	Total macroscopic cross section
$q\left(r,\mu\right)$	$\mathrm{cm}^{-3}\cdot\mathrm{s}^{-1}$	Internal source, scattering and fission

Table 1: Variables in spherical-geometry transport equation

Use discrete ordinates μ_m with corresponding weights w_m to simplify the solution,

$$\int_{-1}^{1} \psi\left(r,\mu\right) d\mu \approx \sum_{m=1}^{M} w_m \psi_m\left(r\right), \tag{2}$$

using the angular differencing scheme from Lewis and Miller [2],

$$\mu_m \frac{\partial}{\partial r}\left(r^2 \psi_m\left(r\right)\right) + \frac{r}{w_m}\left[\alpha_{m+1/2}\psi_{m+1/2}\left(r\right) - \alpha_{m-1/2}\psi_{m-1/2}\left(r\right)\right] + r^2\sigma\left(r\right)\psi_m\left(r\right) = r^2 q_m\left(r\right), \tag{3}$$

with the following definitions of the half-ordinate quantities:

$$\alpha_m = \alpha_{m+1/2} + \alpha_{m-1/2}, \tag{4a}$$

$$\psi_m = \frac{\psi_{m+1/2} + \psi_{m-1/2}}{2}, \tag{4b}$$

$$\alpha_{1/2} = \alpha_{M+1/2} = 0, \tag{4c}$$

$$\alpha_{m+1/2} = \alpha_{m-1/2} - \mu_m w_m. \tag{4d}$$

From these, each $\psi_{m+1/2}$ can be calculated, given that ψ_m and $\psi_{m-1/2}$ have already been calculated. This is made possible by defining a special direction for $\mu_{1/2} = -1$,

$$-\frac{\partial}{\partial r}\left(\psi_{1/2}\left(r\right)\right) + \sigma\left(r\right)\psi_{1/2}\left(r\right) = q_{1/2}\left(r\right), \tag{5}$$

which is not dependent on its neighboring half-ordinate quantities. Once $\psi_{1/2}\left(r\right)$ is calculated, $\psi_1, \psi_{3/2}, \ldots, \psi_{M-1/2} \ldots \psi_M$ can be calculated in that order. To continue the derivation, change these equations into local variables $r \in (0,R) \to \xi \in (-1,1)$:

$$\frac{2\mu_m}{\Delta r_i}\frac{\partial}{\partial \xi}\left(r^2\left(\xi\right)\psi_m\left(\xi\right)\right) + \frac{2r\left(\xi\right)}{w_m}\left[2\alpha_{m+1/2}\psi_m\left(\xi\right) - \left(\alpha_{m-1/2}+\alpha_{m-1/2}\right)\psi_{m-1/2}\left(\xi\right)\right] + r^2\left(\xi\right)\sigma_i\psi_m\left(\xi\right) = r^2\left(\xi\right)q_m\left(\xi\right). \tag{6}$$

Use equal weight and basis functions (the Garlerkin formulation) defined as

$$w_\alpha(\xi) = b_\alpha(\xi) = \frac{1}{2}(1 + \xi_\alpha \xi), \tag{7}$$

with $\xi_\alpha = \{-1, 1\}$. Note that this α subscript is different from the α differencing coefficients. Use the following notation for integration over the variable ξ inside of a cell:

$$\langle\cdot\rangle_\xi = \int_{-1}^{1} (\cdot)\, d\xi. \tag{8}$$

Multiply the transport equation by weight functions $w_\beta(\xi)$ and integrate over a single spatial cell:

$$\frac{2\mu_m}{\Delta r_i}\left\langle w_\beta(\xi)\frac{\partial}{\partial\xi}\left(r^2(\xi)\psi_m(\xi)\right)\right\rangle_\xi + \frac{2r(\xi)}{w_m}\left\langle w_\beta(\xi)\left[2\alpha_{m+1/2}\psi_m(\xi) - \left(\alpha_{m-1/2} + \alpha_{m-1/2}\right)\psi_{m-1/2}(\xi)\right]\right\rangle_\xi \\ + \left\langle w_\beta(\xi)\, r^2(\xi)\,\sigma_i\psi_m(\xi)\right\rangle_\xi = \left\langle w_\beta(\xi)\, r^2(\xi)\, q_m(\xi)\right\rangle_\xi. \tag{9}$$

Integrate the first term by parts,

$$\frac{2\mu_m}{\Delta r_i}\left[r^2(\xi)\psi_m(\xi)w_\beta(\xi)\right]_{\xi=-1}^{1} - \frac{2\mu_m}{\Delta r_i}\left\langle r^2(\xi)\psi_m(\xi)\frac{d}{d\xi}w_\beta(\xi)\right\rangle_\xi \\ + \frac{2}{w_m}\left[2\alpha_{m+1/2}\left\langle r(\xi)\psi_m(\xi)w_\beta(\xi)\right\rangle_\xi - \alpha_m\left\langle r(\xi)\psi_{m-1/2}(\xi)w_\beta(\xi)\right\rangle_\xi\right] \\ + \sigma_i\left\langle r^2(\xi)\psi_m(\xi)w_\beta(\xi)\right\rangle_\xi = \left\langle r^2(\xi)q_m(\xi)w_\beta(\xi)\right\rangle_\xi, \tag{10}$$

and expand ψ_m in terms of its basis functions,

$$\psi_m = \sum_{\alpha=1}^{A} b_\alpha(\xi)\psi_m^\alpha, \tag{11}$$

to get (with an implied sum over ψ_m^α):

$$\overbrace{2\mu_m\left[r^2(\xi)b_\alpha(\xi)w_\beta(\xi)\right]_{\xi=-1}^{1}}^{j_{\alpha,\beta}^{r,l}}\psi_m^\alpha - \overbrace{2\mu_m\left\langle r^2(\xi)b_\alpha(\xi)\frac{d}{d\xi}w_\beta(\xi)\right\rangle_\xi}^{k_{\alpha,\beta}}\psi_m^\alpha \\ + \frac{2\Delta r_i}{w_m}\left[\overbrace{2\alpha_{m+1/2}\left\langle r(\xi)b_\alpha(\xi)w_\beta(\xi)\right\rangle_\xi}^{k_{\alpha,\beta}}\psi_m^\alpha - \overbrace{\alpha_m\left\langle r(\xi)b_\alpha(\xi)w_\beta(\xi)\right\rangle_\xi}^{\ell_{\alpha,\beta}}\psi_{m-1/2}^\alpha\right] \\ + \overbrace{\Delta r_i\left\langle r^2(\xi)b_\alpha(\xi)w_\beta(\xi)\right\rangle_\xi}^{m_{\alpha,\beta}}\sigma_i\psi_m^\alpha = \overbrace{\Delta r_i\left\langle r^2(\xi)b_\alpha(\xi)w_\beta(\xi)\right\rangle_\xi}^{m_{\alpha,\beta}}q_m^\alpha, \tag{12}$$

Define the constants

$$
\begin{aligned}
j^{r}_{\alpha,\beta,m} &= 2\mu_m \left[r^2(\xi)\, b_\alpha(\xi)\, w_\beta(\xi)\right]_{\xi=1} \\
&= \frac{1}{8}\mu_m \left(\Delta r_i + 2\bar{r}_i\right)^2 \left(1+\xi_\alpha\right)\left(1+\xi_\beta\right) && \text{(13a)} \\
j^{\ell}_{\alpha,\beta,m} &= -2\mu_m \left[r^2(\xi)\, b_\alpha(\xi)\, w_\beta(\xi)\right]_{\xi=-1} \\
&= -\frac{1}{8}\mu_m \left(\Delta r_i - 2\bar{r}_i\right)^2 \left(-1+\xi_\alpha\right)\left(-1+\xi_\beta\right) && \text{(13b)} \\
k_{\alpha,\beta,m} &= 2\mu_m \left\langle r^2(\xi)\, b_\alpha(\xi)\, \frac{d}{d\xi} w_\beta(\xi)\right\rangle_\xi + \frac{4\Delta r_i \alpha_{m+1/2}}{w_m} \left\langle r(\xi)\, b_\alpha(\xi)\, w_\beta(\xi)\right\rangle_\xi \\
&= \frac{1}{12 w_m}\left[\mu_m w_m \left(\Delta r_i^2 + 12\bar{r}_i^2 + 4\Delta r_i \bar{r}_i \xi_\alpha\right)\xi_\beta + 4\alpha_{m-1/2}\Delta r_i \left(\Delta r_i\left(\xi_\alpha+\xi_\beta\right) + 2\bar{r}_i\left(3+\xi_\alpha\xi_\beta\right)\right)\right] && \text{(13c)} \\
\ell_{\alpha,\beta,m} &= -\frac{2\Delta r_i \alpha_m}{w_m}\left\langle r(\xi)\, b_\alpha(\xi)\, w_\beta(\xi)\right\rangle_\xi \\
&= -\frac{\alpha_m \Delta r_i}{6 w_m}\left[\Delta r_i\left(\xi_\alpha+\xi_\beta\right) + 2\bar{r}_i\left(3+\xi_\alpha\xi_\beta\right)\right] && \text{(13d)} \\
m_{\alpha,\beta} &= \Delta r_i \left\langle r^2(\xi)\, b_\alpha(\xi)\, w_\beta(\xi)\right\rangle_\xi \\
&= \frac{\Delta r_i}{120}\left[20\Delta r_i \bar{r}_i\left(\xi_\alpha+\xi_\beta\right) + 20\bar{r}_i^2\left(3+\xi_\alpha\xi_\beta\right) + \Delta r_i^2\left(5+3\xi_\alpha\xi_\beta\right)\right] && \text{(13e)}
\end{aligned}
$$

and the equation becomes

$$
\left(f^{r}_{\alpha,\beta,m} + f^{\ell}_{\alpha,\beta,m} + k_{\alpha,\beta,m} + m_{\alpha,\beta}\sigma_i\right)\psi^\alpha_m + \ell_{\alpha,\beta,m}\psi^\alpha_{m-1/2} = m_{\alpha,\beta}\psi^\alpha_m \tag{14}
$$

Take the same steps for the special direction, first changing variables to ξ,

$$
-\frac{2}{\Delta r_i}\frac{\partial}{\partial \xi}\left(\psi_{1/2}(\xi)\right) + \sigma(\xi)\,\psi_{1/2}(\xi) = q_{1/2}(\xi), \tag{15}
$$

integrating over a spatial cell,

$$
-\frac{2}{\Delta r_i}\left\langle w_\beta(\xi)\frac{\partial}{\partial \xi}\left(\psi_{1/2}(\xi)\right)\right\rangle_\xi + \sigma_i \left\langle w_\beta(\xi)\,\psi_{1/2}(\xi)\right\rangle_\xi = \left\langle w_\beta(\xi)\, q_{1/2}(\xi)\right\rangle_\xi, \tag{16}
$$

using integration by parts to get the boundary terms,

$$
\frac{2}{\Delta r_i}\left[\psi_{1/2}(\xi)\, w_\beta(\xi)\right]^1_{\xi=-1} + \frac{2}{\Delta r_i}\left\langle \psi_{1/2}(\xi)\frac{\partial}{\partial \xi} w_\beta(\xi)\right\rangle_\xi + \sigma_i\left\langle \psi_{1/2}(\xi)\, w_\beta(\xi)\right\rangle_\xi = \left\langle q_{1/2}(\xi)\, w_\beta(\xi)\right\rangle_\xi, \tag{17}
$$

inserting the expansions for ψ and q,

$$
\begin{aligned}
&\overbrace{2\left[b_\alpha(\xi)\, w_\beta(\xi)\right]^1_{\xi=-1}}^{j^{r,\ell}_{\alpha,\beta,}}\psi^\alpha_{1/2} + \overbrace{2\left\langle b_\alpha(\xi)\frac{\partial}{\partial \xi} w_\beta(\xi)\right\rangle_\xi}^{k_{\alpha,\beta}}\psi^\alpha_{1/2} + \overbrace{\Delta r_i\left\langle b_\alpha(\xi)\, w_\beta(\xi)\right\rangle_\xi}^{m_{\alpha,\beta}}\sigma_i\psi^\alpha_{1/2} \\
&\qquad = \overbrace{\Delta r_i\left\langle b_\alpha(\xi)\, w_\beta(\xi)\right\rangle_\xi}^{m_{\alpha,\beta}} q^\alpha_{1/2},
\end{aligned} \tag{18}
$$

and simplifying using the constants:

$$
\begin{aligned}
\tilde{j}^r_{\alpha,\beta} &= 2\left[b_\alpha\left(\xi\right)w_\beta\left(\xi\right)\right]_{\xi=1} \\
&= \frac{1}{2}\left(1+\xi_\alpha\right)\left(1+\xi_\beta\right), && \text{(19a)} \\
\tilde{j}^\ell_{\alpha,\beta} &= -2\left[b_\alpha\left(\xi\right)w_\beta\left(\xi\right)\right]_{\xi=-1} \\
&= -\frac{1}{2}\left(1-\xi_\alpha\right)\left(1-\xi_\beta\right), && \text{(19b)} \\
\tilde{k}_{\alpha,\beta} &= 2\left\langle b_\alpha\left(\xi\right)\frac{\partial}{\partial\xi}w_\beta\left(\xi\right)\right\rangle_\xi \\
&= \xi_\beta && \text{(19c)} \\
\tilde{m}_{\alpha,\beta} &= \Delta r_i\left\langle b_\alpha\left(\xi\right)w_\beta\left(\xi\right)\right\rangle_\xi \\
&= \frac{1}{6}\Delta r_i\left(3+\xi_\alpha\xi_\beta\right). && \text{(19d)}
\end{aligned}
$$

This gives the equation

$$
\left(\tilde{j}^r_{\alpha,\beta,-}+\tilde{j}^\ell_{\alpha,\beta}+\tilde{k}_{\alpha,\beta}+\tilde{m}_{\alpha,\beta}\sigma_i\right)\psi^\alpha_{1/2}=\tilde{m}_{\alpha,\beta}q^\alpha_{1/2},
$$

which can be solved independently of the half-ordinate terms.

1.2 Finite element in space and angle

NOTE: This derivation leads to equations that appear to be unstable and could be incorrectly formulated. It is included as a work in progress. Switching to numerical solution for the matrix coefficients could help.

Begin from the spherical-geometry transport equation (Eq. 1) as before. Make two changes of variables, first in the spatial variable from $r\in[0,R]\to\xi\in[-1,1]$ and second in the angular variable from $\mu\in[-1,0]\to\eta^-\in[-1,1]$ and $\mu\in[0,1]\to\eta^+\in[-1,1]$, with

$$
\begin{aligned}
r\left(\xi\right) &= \bar{r}_i+\frac{\Delta r_i}{2}\xi && \text{(20a)} \\
\xi\left(r\right) &= \frac{2}{\Delta r_i}\left(r-\bar{r}_i\right) && \text{(20b)} \\
\mu\left(\eta\right) &= \frac{1}{2}\left(\eta+\eta_\pm\right) && \text{(20c)} \\
\eta\left(\mu\right) &= 2\mu-\eta_\pm && \text{(20d)}
\end{aligned}
$$

to get

$$
\mu\left(\eta\right)\frac{d\xi}{dr}\frac{\partial}{\partial\xi}\left(r^2\left(\xi\right)\psi\left(\xi,\eta\right)\right)+r\left(\xi\right)\frac{d\eta}{d\mu}\frac{\partial\left[\left(1-\mu^2\left(\eta\right)\right)\psi\left(\xi,\eta\right)\right]}{\partial\eta}+r^2\left(\xi\right)\sigma\left(\xi\right)\psi\left(\xi,\eta\right)=r^2\left(\xi\right)q\left(\xi,\eta\right), \tag{21}
$$

or

$$
\left(\frac{2}{\Delta r_i}\right)\mu\left(\eta\right)\frac{\partial}{\partial\xi}\left(r^2\left(\xi\right)\psi\left(\xi,\eta\right)\right)+2r\left(\xi\right)\frac{\partial\left[\left(1-\mu^2\left(\eta\right)\right)\psi\left(\xi,\eta\right)\right]}{\partial\eta}+r^2\left(\xi\right)\sigma\left(\xi\right)\psi\left(\xi,\eta\right)=r^2\left(\xi\right)q\left(\xi,\eta\right). \tag{22}
$$

The basis and weight functions for this problem will be

$$w_\alpha(\xi,\eta) = b_\alpha(\xi,\eta) = \frac{1}{4}(1+\xi_\alpha\xi)(1+\eta_\alpha\eta) \tag{23}$$

with the constants as defined in Table2.

α	ξ_α	η_α
1	-1	-1
2	-1	1
3	1	-1
4	1	1

Table 2: DFEM constants

ψ and q will be expanded as

$$\psi(\xi,\eta) = \sum_\alpha b_\alpha(\xi,\eta)\psi_\alpha, \tag{24a}$$

$$q(\xi,\eta) = \sum_\alpha b_\alpha(\xi,\eta)q_\alpha. \tag{24b}$$

Operate on the equation by $\langle(\cdot)\,w_\beta(\xi,\eta)\rangle_{\xi,\eta} = \int_{-1}^{1}\int_{-1}^{1}(\cdot)\,w_\beta(\xi,\eta)\,d\xi d\eta$ and let $\sigma(\xi)=\sigma_i$ in each cell:

$$\left\langle \mu(\eta)\,w_\beta(\xi,\eta)\frac{\partial}{\partial\xi}\left\{r^2(\xi)\,\psi(\xi,\eta)\right\}\right\rangle_{\xi,\eta} + \Delta r_i\left\langle r(\xi)\,w_\beta(\xi,\eta)\frac{\partial}{\partial\eta}\left\{\left(1-\mu^2(\eta)\right)\psi(\xi,\eta)\right\}\right\rangle_{\xi,\eta} \\ + \left(\frac{\Delta r_i}{2}\right)\sigma_i\left\langle r^2(\xi)\,w_\beta(\xi,\eta)\,\psi(\xi,\eta)\right\rangle_{\xi,\eta} = \left(\frac{\Delta r_i}{2}\right)\left\langle r^2(\xi)\,w_\beta(\xi,\eta)\,q(\xi,\eta)\right\rangle_{\xi,\eta}. \tag{25}$$

Integrate by parts in the first two terms:

$$\left\langle \mu(\eta)\left[w_\beta(\xi,\eta)\,r^2(\xi)\,\psi(\xi,\eta)\right]_{\xi=-1}^{1}\right\rangle_\eta - \left\langle \mu(\eta)\,r^2(\xi)\,\psi(\xi,\eta)\frac{\partial}{\partial\xi}w_\beta(\xi,\eta)\right\rangle_{\xi,\eta} \\ + \Delta r_i\left(\left\langle r(\xi)\left[w_\beta(\xi,\eta)\left(1-\mu^2(\eta)\right)\psi(\xi,\eta)\right]_{\eta=-1}^{1}\right\rangle_\xi - \left\langle r(\xi)\left(1-\mu^2(\eta)\right)\psi(\xi,\eta)\frac{\partial}{\partial\eta}w_\beta(\xi,\eta)\right\rangle_{\xi,\eta}\right) \\ + \left(\frac{\Delta r_i}{2}\right)\sigma_i\left\langle r^2(\xi)\,w_\beta(\xi,\eta)\,\psi(\xi,\eta)\right\rangle_{\xi,\eta} = \left(\frac{\Delta r_i}{2}\right)\left\langle r^2(\xi)\,w_\beta(\xi,\eta)\,q(\xi,\eta)\right\rangle_{\xi,\eta}. \tag{26}$$

Use the basis functions to expand the equation:

$$\overbrace{\left\langle \mu(\eta)\left[w_\beta(\xi,\eta)\,r^2(\xi)\,b_\alpha(\xi,\eta)\right]_{\xi=-1}^{1}\right\rangle_\eta}^{j_{\alpha,\beta,\pm}^{r,\ell}}\psi_\alpha - \overbrace{\left\langle \mu(\eta)\,r^2(\xi)\,b_\alpha(\xi,\eta)\frac{\partial}{\partial\xi}w_\beta(\xi,\eta)\right\rangle_{\xi,\eta}}^{k_{\alpha,\beta,\pm}}\psi_\alpha \\ + \overbrace{\Delta r_i\left\langle r(\xi)\left[w_\beta(\xi,\eta)\left(1-\mu^2(\eta)\right)b_\alpha(\xi,\eta)\right]_{\eta=-1}^{1}\right\rangle_\xi}^{\ell_{\alpha,\beta,\pm}}\psi_\alpha - \overbrace{\Delta r_i\left\langle r(\xi)\left(1-\mu^2(\eta)\right)b_\alpha(\xi,\eta)\frac{\partial}{\partial\eta}w_\beta(\xi,\eta)\right\rangle_{\xi,\eta}}^{k_{\alpha,\beta,\pm}}\psi_\alpha \\ + \overbrace{\left(\frac{\Delta r_i}{2}\right)\sigma_i\left\langle r^2(\xi)\,w_\beta(\xi,\eta)\,b_\alpha(\xi,\eta)\right\rangle_{\xi,\eta}}^{m_{\alpha,\beta}}\psi_\alpha = \overbrace{\left(\frac{\Delta r_i}{2}\right)\left\langle r^2(\xi)\,w_\beta(\xi,\eta)\,b_\alpha(\xi,\eta)\right\rangle_{\xi,\eta}}^{m_{\alpha,\beta}}\psi_\alpha. \tag{27}$$

Let

$$
\begin{aligned}
j^{r}_{\alpha,\beta,\pm} &= \left\langle \mu\left(\eta\right)\left[w_{\beta}\left(\xi,\eta\right) r^{2}\left(\xi\right) b_{\alpha}\left(\xi,\eta\right)\right]_{\xi=1}\right\rangle_{\eta} \\
&= \frac{1}{192}\left[\left(\eta_{\alpha}+\eta_{\beta}+3\eta_{\pm}+\eta_{\alpha}\eta_{\beta}\eta_{\pm}\right)\left(\Delta r_{i}+2\bar{r}_{i}\right)^{2}\left(\xi_{\alpha}+1\right)\left(\xi_{\beta}+1\right)\right], &\text{(28a)}\\
j^{\ell}_{\alpha,\beta,\pm} &= \left\langle \mu\left(\eta\right)\left[w_{\beta}\left(\xi,\eta\right) r^{2}\left(\xi\right) b_{\alpha}\left(\xi,\eta\right)\right]_{\xi=-1}\right\rangle_{\eta} \\
&= -\frac{1}{192}\left[\left(\eta_{\alpha}+\eta_{\beta}+3\eta_{\pm}+\eta_{\alpha}\eta_{\beta}\eta_{\pm}\right)\left(\Delta r_{i}-2\bar{r}_{i}\right)^{2}\left(\xi_{\alpha}-1\right)\left(\xi_{\beta}-1\right)\right], &\text{(28b)}\\
k_{\alpha,\beta,\pm} &= -\left\langle \mu\left(\eta\right) r^{2}\left(\xi\right) b_{\alpha}\left(\xi,\eta\right)\frac{\partial}{\partial\xi} w_{\beta}\left(\xi,\eta\right)\right\rangle_{\xi,\eta} - \Delta r_{i}\left\langle r\left(\xi\right)\left(1-\mu^{2}\left(\eta\right)\right) b_{\alpha}\left(\xi,\eta\right)\frac{\partial}{\partial\eta} w_{\beta}\left(\xi,\eta\right)\right\rangle_{\xi,\eta} \\
&= -\frac{1}{288}\left(\eta_{\alpha}+\eta_{\beta}+3\eta_{\pm}+\eta_{\alpha}\eta_{\beta}\eta_{\pm}\right)\left(\Delta r_{i}^{2}+12\bar{r}_{i}^{2}+4\Delta r_{i}\bar{r}_{i}\xi_{\alpha}\right)\xi_{\beta} \\
&\quad+\frac{\Delta r_{i}}{288}\eta_{\beta}\left(-11+2\eta_{\alpha}\eta_{\pm}+3\eta_{\pm}^{2}\right)\left(\Delta r_{i}\left(\xi_{\alpha}+\xi_{\beta}\right)+2\bar{r}_{i}\left(3+\xi_{\alpha}\xi_{\beta}\right)\right) \\
&= -\frac{1}{288}\left(\eta_{\alpha}+\eta_{\beta}+3\eta_{\pm}+\eta_{\alpha}\eta_{\beta}\eta_{\pm}\right)\left(\Delta r_{i}^{2}+12\bar{r}_{i}^{2}+4\Delta r_{i}\bar{r}_{i}\xi_{\alpha}\right)\xi_{\beta} \\
&\quad+\frac{\Delta r_{i}}{288}\eta_{\beta}\left(-8+2\eta_{\alpha}\eta_{\pm}\right)\left(\Delta r_{i}\left(\xi_{\alpha}+\xi_{\beta}\right)+2\bar{r}_{i}\left(3+\xi_{\alpha}\xi_{\beta}\right)\right), &\text{(28c)}\\
\ell_{\alpha,\beta,\pm} &= \Delta r_{i}\left\langle r\left(\xi\right)\left[w_{\beta}\left(\xi,\eta\right)\left(1-\mu^{2}\left(\eta\right)\right) b_{\alpha}\left(\xi,\eta\right)\right]_{\eta=-1}^{1}\right\rangle_{\xi} \\
&= -\frac{\Delta r_{i}}{96}\left(2\eta_{\pm}+\eta_{\beta}\left(-3+\eta_{\pm}^{2}\right)+\eta_{\alpha}\left(-3+2\eta_{\beta}\eta_{\pm}+\eta_{\pm}^{2}\right)\right)\left(\Delta r_{i}\left(\xi_{\alpha}+\xi_{\beta}\right)+2\bar{r}_{i}\left(3+\xi_{\alpha}\xi_{\beta}\right)\right) \\
&= -\frac{\Delta r_{i}}{96}\left(2\eta_{\pm}-2\eta_{\beta}+2\eta_{\alpha}\left(-1+\eta_{\beta}\eta_{\pm}\right)\right)\left(\Delta r_{i}\left(\xi_{\alpha}+\xi_{\beta}\right)+2\bar{r}_{i}\left(3+\xi_{\alpha}\xi_{\beta}\right)\right) &\text{(28d)}\\
m_{\alpha,\beta} &= \left(\frac{\Delta r_{i}}{2}\right)\sigma_{i}\left\langle r^{2}\left(\xi\right) w_{\beta}\left(\xi,\eta\right) b_{\alpha}\left(\xi,\eta\right)\right\rangle_{\xi,\eta} \\
&= \frac{\Delta r_{i}}{1440}\left[\left(3+\eta_{\alpha}\eta_{\beta}\right)\left(20\Delta r_{i}\bar{r}_{i}\left(\xi_{\alpha}+\xi_{\beta}\right)+20\bar{r}_{i}^{2}\left(3+\xi_{\alpha}\xi_{\beta}\right)+\Delta r_{i}^{2}\left(5+3\xi_{\alpha}\xi_{\beta}\right)\right)\right], &\text{(28e)}
\end{aligned}
$$

to simplify the equation to

$$
\left(j^{r}_{\alpha,\beta,\pm}+j^{\ell}_{\alpha,\beta,\pm}+k_{\alpha,\beta,\pm}+\ell_{\alpha,\beta,\pm}+\sigma_{i} m_{\alpha,\beta}\right)\psi_{\alpha} = m_{\alpha,\beta} q_{\alpha}. \tag{29}
$$

The sweeps are then performed for $\mu \gtrless 0$ [4] with boundary values for $\mu = 0$ from the other direction to enforce relaxed continuity.

2 Results and Discussion

Three separate, critical configurations were examined, each of them a sphere with a vacuum boundary condition. The results of the linear discontinuous finite element solution with S_N discrete-ordinates are examined below. Included are the error in the solution from $k = 1$ and the wall time to run the simulations. These results are compared to those from identical simulations run by Mercimek and Özgener [3].The results for the k-eigenvalue were computed using the power iteration method, in which k is updated for power iteration $i + 1$ as

$$k_{i+1} = k_i \frac{\|\nu\Sigma_f \phi_{i+1}\|}{\|\nu\Sigma_f \phi_i\|}, \tag{30}$$

where $\|(\cdot)\|$ is the sum over all groups, cells and nodes. Then the fission source for power iteration i is scaled as

$$q_f = \frac{\chi}{k_i} \nu\Sigma_f \phi. \tag{31}$$

This process continues until the change in k from iteration to iteration is less than a defined tolerance $\epsilon = 10^{-10}$:

$$\frac{|k_{i+1} - k_i|}{k_{i+1}} < \epsilon. \tag{32}$$

The code was written in C++ using Trilinos libraries [1] for matrix solution. Results were calculated using linear finite elements for all combinations of

- Number of cells from 1 to 100
- Even number of Gauss-Legendre ordinates from 2 to 64.

The code used for the calculations and the full, tabulated results are available at https://github.com/brbass/manatee and https://github.com/brbass/NERS-561/tree/master/proj/code, respectively.

2.1 U-D_2O

The U-D_2O system is a simple, homogeneous bare sphere. Table 3 contains the cross section data for this problem.

The results from Figure 1 indicate that for any number of ordinates greater than two, the error in the calculations is around 10^{-4} or lower. For low numbers of ordinates, the results do not improve significantly when adding more cells, which also applies to low numbers of cells and variation in the number of ordinates. In this and subsequent problems, there's a nearly linear region in which the error is particularly low; this corresponds to approximately the point at which there are one or two ordinates for each cell (or around one ordinate per direction for each cell). Increasing the number of cells or ordinates independently past this point actually decreases the accuracy of the solution. This region is small for the low number of cells and ordinates but increases in size as the number of cells and ordinates hits about sixty.

The results showed agreement to six decimal places (as many as were available) with the results reported by Mercimek and Özgener in what they call the LD2 method (which is the method implemented in this code). For 5 elements and 32 ordinates, for instance, they reported a k_{eff} of 0.999932, which is identical to the result from this code.

The number of iterations to converge on the solution was 338-339 for all the cases above about ten cells and four ordinates. The solution time (Figure 2) increased approximately linearly for the number of cells and ordinates.

ν	σ_f	σ_s	σ_t	R
1.70	0.054628	0.464338	0.54628	22.017156

Table 3: U-D_2O, data

2.2 Uranium

The uranium system models a two-group, homogeneous bare sphere of 93% enriched uranium. See Table 4 for the cross section data for this problem.

When compared with the first problem, the solution to this problem took between 968-969 iterations, or about three times as many, to converge, which can be attributed to the coupling of the downscatter from the fast energy group (Group 1) to the thermal energy group (Group 2) and the fission source provided by the thermal group to the fast group. Following that same trend, the k-eigenvalue took more elements and more ordinates to converge to the same error as the previous problem (see Figure 3) and the calculations took longer to converge (see Figure 4).

Group	ν	σ_f	$\sigma_{s,g\to g}$	$\sigma_{s,g\to g'}$	σ_t	χ	R
1	2.50	0.0010484	0.62568	0.029227	0.65696	1.0	16.049836
2	2.50	0.050632	2.44383	-	2.52025	0	

Table 4: Uranium, data

2.3 U-235

The U-235 system is a two-region problem with a U-235 core and an outer reflector of H_2O, with the cross sections in Table 5.

This problem finished the quickest (see Figure 6) and with the fewest iterations (114 for all the problems). The data would suggest this, as the uranium in this case is highly absorbing compared to materials from the previous problems. The error in k was the largest for this case, with the number of ordinates as the factor whose increase would appear to benefit the problem the most, as can be seen from Figure 5. While the other problems were heterogeneous, this problem had a boundary at which the problem changed from strongly absorbing to strongly scattering, which could indicate that greater resolution is needed in the angular variable at material boundaries.

	ν	σ_f	σ_s	σ_t	R_{inner}	R_{outer}
U-235	2.679198	0.065280	0.248064	0.32640	0	6.12745
H_2O	0.0	0.0	0.293760	0.32640	6.12745	15.318626

Table 5: U-235, data

2.4 Figures

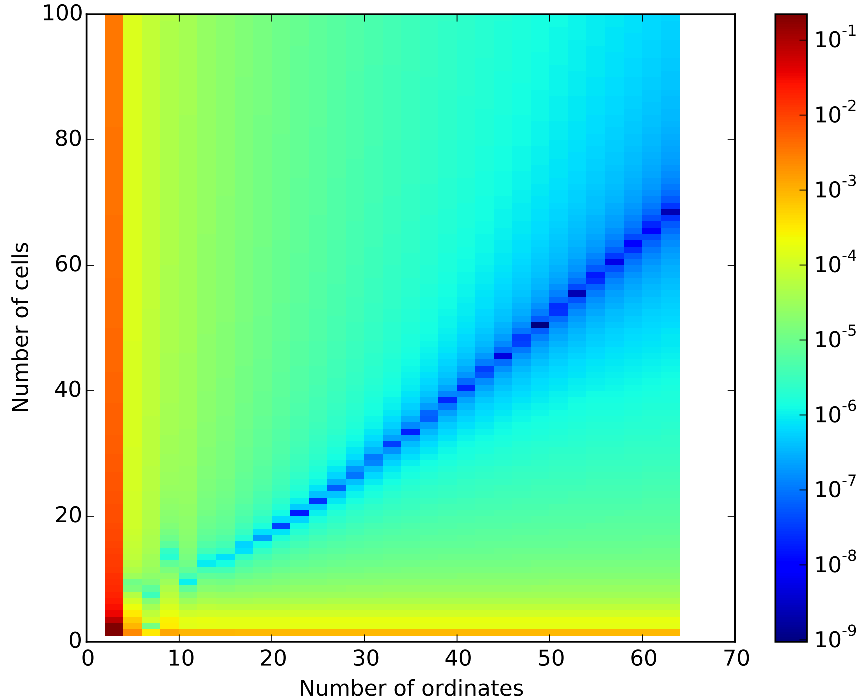

Figure 1: U-D_2O, absolute error in k

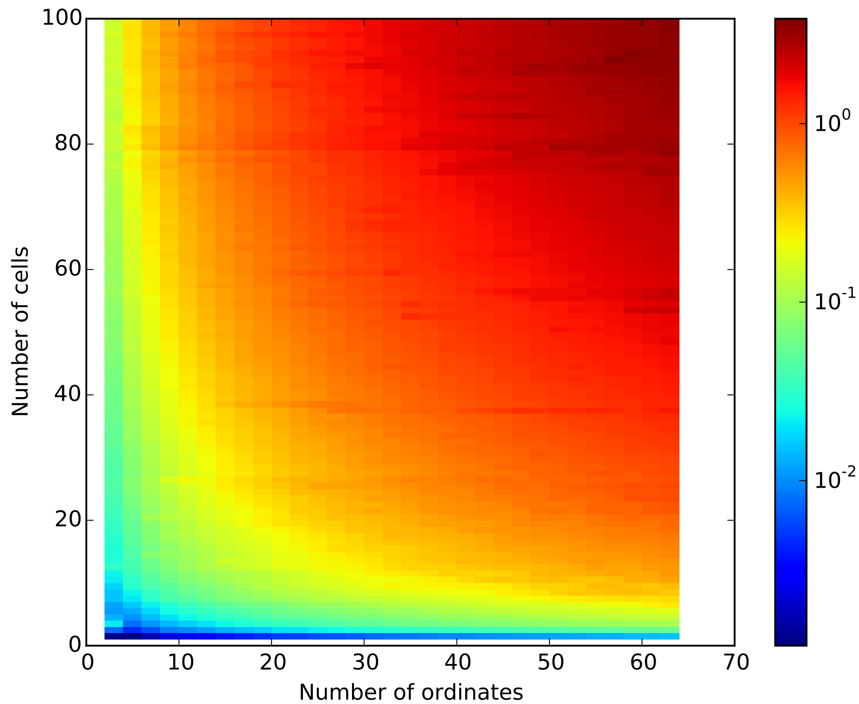

Figure 2: U-D_2O, solve time (sec)

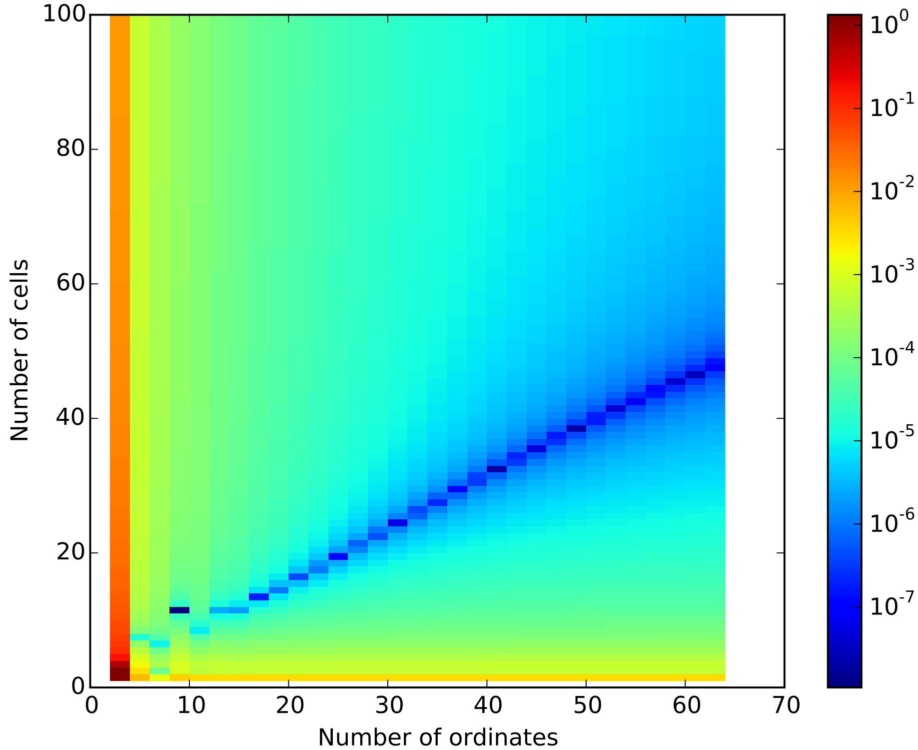

Figure 3: Uranium, absolute error in k

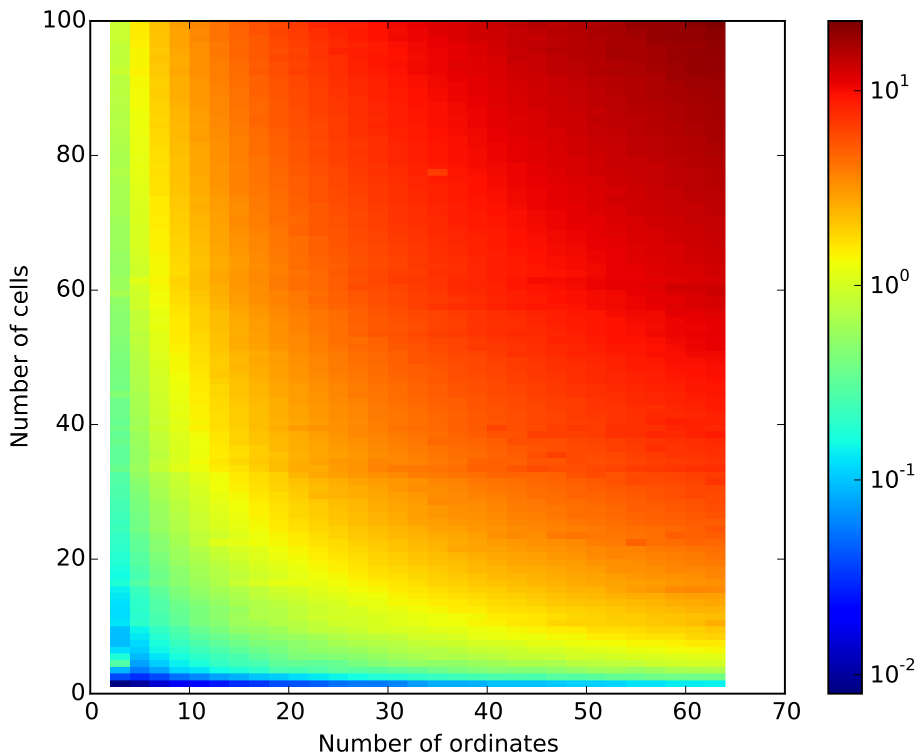

Figure 4: Uranium, solve time (sec)

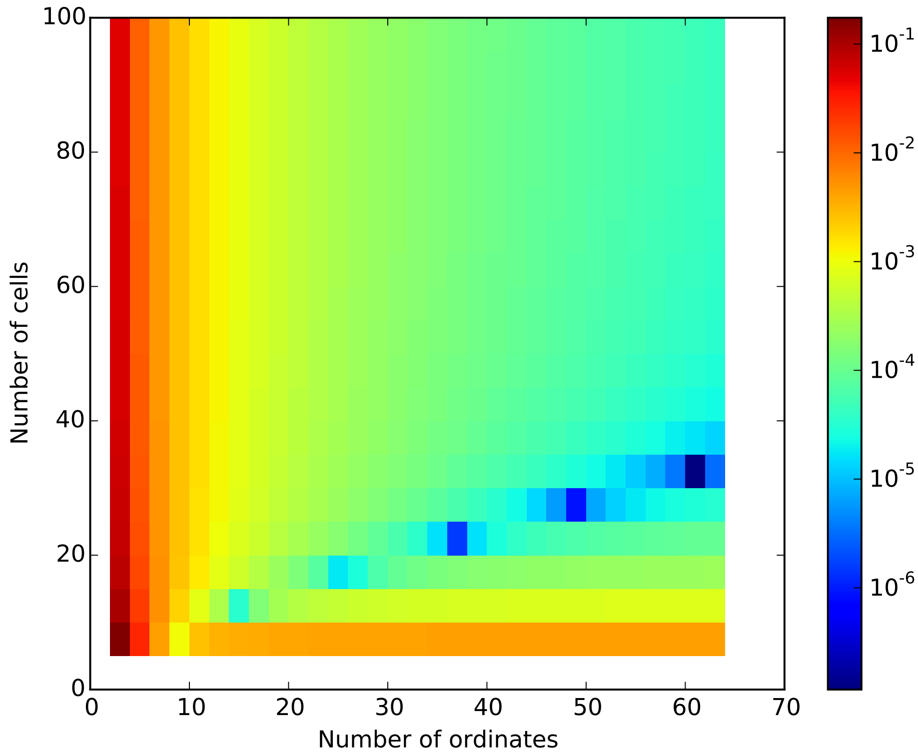

Figure 5: U-235, absolute error in k

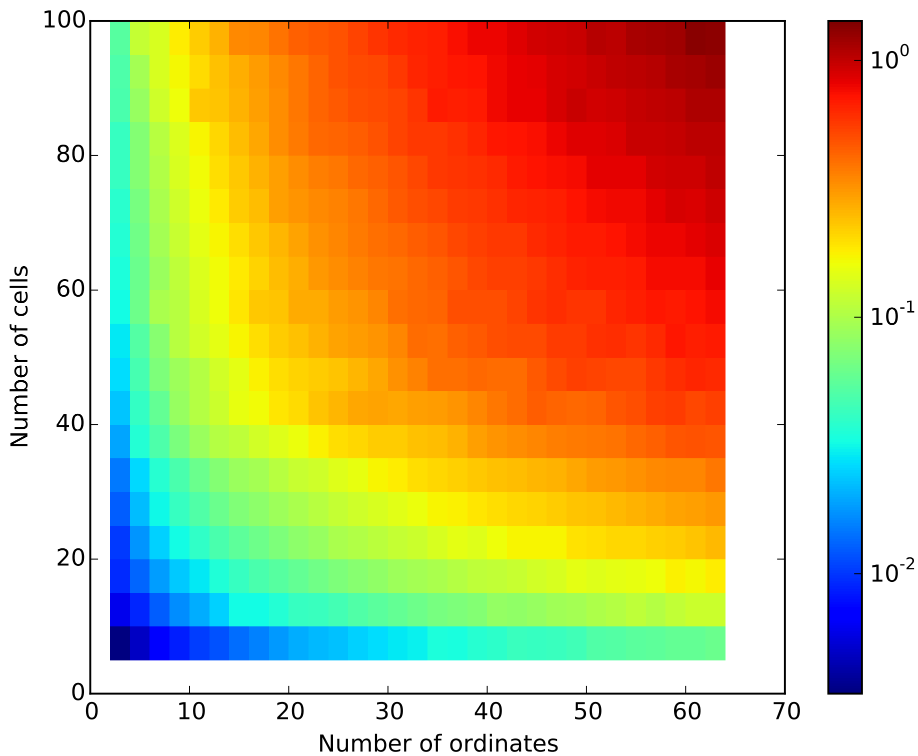

Figure 6: U-235, solve time (sec)

References

[1] Michael Allen Heroux and James M Willenbring. *Trilinos users guide*. Citeseer, 2003.

[2] Elmer Eugene Lewis and Warren F Miller. Computational methods of neutron transport. 1984.

[3] Mehmet Mercimek and H. Atilla Özgener. Discontinuous finite element formulations for neutron transport in spherical geometry. *Annals of Nuclear Energy*, 2014.

[4] Leonard Lorence William R. Martin, Carl E. Yehnert and James J. Duderstadt. Phase-space finite element methods applied to the first-order form of the transport equation. *Annals of Nuclear Energy*, 1981.