HW2 NE255 Lorenzo Vergari

1a **What are the major nuclear data libraries and which countries manage them?**

ENDF (latest version ENDF/B -VIII) produced by the Cross Section Evaluation Working Group (US & Canada)

JEFF (latest version JEFF3.3) from the Joint Evaluated Fission and Fusion File Organization, consisting of members of the NEA Data Bank participating countries (Argentina, Austria, Belgium, Czech Rep., Denmark, Finland, France, Germany, Greece, Hungary, Italy, Japan, Korea, Mexico, Netherlands, Norway, Poland, Portugal, Romania, Russia, Slovak Rep., Slovenia, Spain, Sweden, Switzerland, Turkey, UK)

JENDL (latest version JENDL-4.0) is handled by the Japanese Nuclear Data Committee (Japan)

BROND (latest version BROND-3.1) and RUSFOND (2010) compiled by Russian Federation

CENDL (latest version CENDL-3.1) by China

1b **At what energy is the lowest isolated resonance of 235U, 238U, 239Pu, 240Pu, 241Pu, and 242Pu?**

	U-235	U-238	Pu-239	Pu-240	Pu-241	Pu-242
ENDF	0.276 ev	6.674 ev	0.295 ev	1.056 ev	0.256 ev	2.676 ev
JEFF	0.275 ev	6.674 ev	0.301 ev	1.056 ev	0.257 ev	2.670 ev
JENDL	0.279 ev	6.673 ev	0.296 ev	1.055 ev	0.257 ev	2.680 ev

Source: https://www-nds.iaea.org/exfor/e4explorer.htm

1c **Why do we care about that?**

In correspondence of the resonance, we lose the typical 1/v behavior and typically absorption of a neutron is much more likely, therefore we observe a depression of the neutron flux at that energy. This is relevant because it represents the component of flux which is depressed in the first layers of a fuel rod (self-shielding) and the behavior of this resonance when T changes will be determinant for the Doppler Effect.

2a **Briefly compare the diffusion equation, deterministic methods, and Monte Carlo methods in terms of complexity, accuracy, run time, and range of applicability.**

	Diffusion Equation	Deterministic Method	MC method
Complexity	Least complex, solution by hand in some cases	Complex, multiple equations to be performed	Most complex: multiple generations of neutrons to be simulated
Accuracy	Least accurate, with discretized or homogeneous space, linearly anisotropic or isotropic direction and up to few energy groups	Discretized space, discretized direction and multiple energy groups	Most accurate, with continuous spatial, directional and energy distribution
Run Time	Fast running	Not fast running, but less time demanding than MC	Computationally expensive, parallelization often necessary
Range of Applicability	Simple geometries, not valid close to boundaries, sinks, sources	1D, 2D and 3D geometries. Not as limited as diffusion equation. Some approaches	All geometries, useful for studying physical objects such as reactors

		become unconvenient and difficult in multi-D problems (e.g. spher-harm)	

2b **Given what you've learned about deterministic methods so far, discuss their strengths and weaknesses**

Deterministic methods have some important strengths:

1) Relatively fast running, especially if compared to MC methods
2) They have a Global solution in output, therefore they have the same quality everywhere
3) Inputs of codes based on deterministic methods can be simple

However, they bear some weaknesses:

1) The quality of the solution is governed by the discretization of the variable
2) The are memory-intensive, especially in case of large problems.
3) Their accuracy suffers from truncation error
4) Angle discretization causes ray effect at angles different from the co-location points
5) They are constrained by their mesh
6) It is not simple to parallelize their execution

3a **What is the main challenge associated with the way that we derived the multigroup transport equation?**

The main challenge implied in the way we derived the multigroup transport equation stands in how we computed the group constants. As a matter of fact, we defined them by weighting the nuclear parameters on the angular flux energy distribution, which is an unknown variable of the transport equation.

$$\Sigma_g = \frac{\int_{E_g}^{E_{g-1}} dE\ \Sigma(\boldsymbol{r}, E)\psi(\boldsymbol{r}, \boldsymbol{\Omega}, E)}{\int_{E_g}^{E_{g-1}} dE\ \psi(\boldsymbol{r}, \boldsymbol{\Omega}, E)}$$

Therefore, we will have to use general guess fluxes for averaging the cross sections and building the group constants.

3b **Starting from the following general system of multigroup equations**

$$\hat{\Omega} \cdot \nabla\psi^g(\vec{r}, \hat{\Omega}) + \Sigma_t^g(\vec{r})\psi^g(\vec{r}, \hat{\Omega}) = \sum_{g'=0}^{G-1} \Sigma_s^{g' \to g}(\vec{r}, \hat{\Omega}' \cdot \hat{\Omega})\psi^{g'}(\vec{r}, \hat{\Omega}') + \frac{\chi_g}{4\pi} \sum_{g'=0}^{G-1} \nu_{g'} \Sigma_f^{g'}(\vec{r})\phi^{g'}(\vec{r}) + \frac{Q^g(\vec{r})}{4\pi},$$

where ϕ is scalar flux, write a set of five coupled equations for a five-group problem. Assume neutrons can only downscatter from fast groups (0 and 1) to thermal groups (2, 3, and 4). Assume that thermal groups can upscatter into other thermal groups and can downscatter. Assume both an external source and a fission source.

See attached document (page 1)

4. **Show that the Legendre polynomials below are orthonormal on the interval x ∈ [−1, 1]**

See attached (page 2)

5. **Consider the integral**

$$\int_{4\pi} d\hat{\Omega}\, |\hat{\Omega}|.$$

a. **Use the S4 LQN quadrature set to execute this integral. The LQN quadrature set is given below in Figure 1. Recall that μi = ηi = ξi for a given level i.**
b. **Repeat the integration with S6. What do you observe?**
c. **Write a short code to execute this integration (and higher orders if you'd like). Try a few different functions. Turn in the code and the evaluation of these functions. Include comments on what you observe.**

(a) See attached (page 3)
(b) See attached. (page 3)
We observe that the error has slightly risen when passing from s4 to s6. However, if we stick to the using the same number of significant figures of the weights (7), S4 and S6 integration lead to the same result (1.000000 * pi)
(c) See attached .m code

Evaluations:

1) **f=1; Exact value=12.56637 (**to the 7^{th} figure)

>> fun1 = @(mu,csi,nu) 1 ;

>> Sn_Quad(fun1,4)

ans = 12.566369357722113

>> Sn_Quad(fun1,6)

ans = 12.566373127633305

>> Sn_Quad(fun1,12)

ans = 12.566373127633312

>> Sn_Quad(fun1,16)

ans = 12.566361817899761

We see that the variability of the result is fairly reduced, as we had experienced in the hand-written calculation. Specifically, if we consider only the 7 significant numbers, the variability is around 5e-4 %

2) $\boldsymbol{f = \cos^2\theta \cos^2\phi \rightarrow \int f = 2 * \frac{\pi}{3} = 2.0943951023}$

>> fun2 = @(mu,csi,nu) (mu.^2)/(1+(nu/csi).^2) ;

>> Sn_Quad(fun2,4)

ans = 2.094394892953685

>> Sn_Quad(fun2,6)

ans =   2.094395521272217

>> Sn_Quad(fun2,8)

ans = 2.094394892953686

>> Sn_Quad(fun2,12)

ans = 2.094395521272217

>> Sn_Quad(fun2,16)

ans = 2.094393636316624

Even in this case, the variability is reduced to the 6th decimal figure

3) $\boldsymbol{f = \phi\theta^3 cos^2\theta\ sin^2\phi \rightarrow \int f = \frac{\pi^3}{9}\left(3\pi^2 - 14\right) = 53.774575647960752}$

>> fun3= @(mu,csi,eta)(atanshift(csi/eta))*(mu^2)*(eta^2)/((csi^2+eta^2))*((acos(mu))^3)

% note: here atanshift has been defined as the tan^-1 in [0,pi]. Code is attached

>> Sn_Quad(fun3,4)

ans =   52.426889309944102

>> Sn_Quad(fun3,6)

ans =   53.090445798743254

>> Sn_Quad(fun3,8)

```
ans =   53.472273271901173

>> Sn_Quad(fun3,12)

ans =   53.645431400223877

>> Sn_Quad(fun3,16)

ans =   53.702844259401964
```

With this function, the error is not negligible. However, we see that it drastically reduces as we increase the order.

1

$$
\begin{cases}
\hat{\Omega}\cdot\nabla\psi^0 + \Sigma_t^0\,\psi^0 = \Sigma_s^{0\to0}(\bar{r},\hat{\Omega}'\cdot\hat{\Omega})\,\psi^0(\bar{r},\hat{\Omega}') + \dfrac{\chi^0}{4\pi}\displaystyle\sum_{g'=0}^{4}\nu_{g'}\Sigma_f^{g'}(\bar{r})\,\phi^{g'}(\bar{r}) + \dfrac{Q^0}{4\pi} \\[2ex]
\hat{\Omega}\cdot\nabla\psi^1 + \Sigma_t^1\,\psi^1 = \cancel{\displaystyle\sum_{g'=0}^{4}}\,\Sigma_s^{g'\to1}(\bar{r},\hat{\Omega}'\cdot\hat{\Omega})\,\psi^{g'}(\bar{r},\hat{\Omega}') + \dfrac{\chi^1}{4\pi}\displaystyle\sum_{g'=0}^{4}\nu_{g'}\Sigma_f^{g'}(\bar{r})\,\phi^{g'}(\bar{r}) + \dfrac{Q_1}{4\pi} \\[2ex]
\hat{\Omega}\cdot\nabla\psi^2 + \Sigma_t^2\,\psi^2 = \displaystyle\sum_{g'=0}^{4}\Sigma_s^{g'\to2}(\bar{r},\hat{\Omega}'\cdot\hat{\Omega})\,\psi^{g'}(\bar{r},\hat{\Omega}') + \dfrac{\chi^2}{4\pi}\displaystyle\sum_{g'=0}^{4}\nu_{g'}\Sigma_f^{g'}(\bar{r})\,\phi^{g'}(\bar{r}) + \dfrac{Q_2}{4\pi} \\[2ex]
\hat{\Omega}\cdot\nabla\psi^3 + \Sigma_t^3\,\psi^3 = \displaystyle\sum_{g'=0}^{4}\Sigma_s^{g'\to3}(\bar{r},\hat{\Omega}'\cdot\hat{\Omega})\,\psi^{g'}(\bar{r},\hat{\Omega}') + \dfrac{\chi^3}{4\pi}\displaystyle\sum_{g'=0}^{4}\nu_{g'}\Sigma_f^{g'}\,\phi^{g'} + \dfrac{Q_3}{4\pi} \\[2ex]
\hat{\Omega}\cdot\nabla\psi^4 + \Sigma_t^4\,\psi^4 = \displaystyle\sum_{g'=0}^{4}\Sigma_s^{g'\to4}(\bar{r},\hat{\Omega}'\cdot\hat{\Omega})\,\psi^{g'}(\bar{r},\hat{\Omega}') + \dfrac{\chi^4}{4\pi}\displaystyle\sum_{g'=0}^{4}\nu_{g'}\Sigma_f^{g'}\,\phi^{g'} + \dfrac{Q_4}{4\pi}
\end{cases}
$$

NOTE:

$$\Sigma_t^0 = \Sigma_A^0 + \sum_{g'=0,\,g'\neq1}^{4}\Sigma_s^{0\to g'}(\bar{r},\hat{\Omega}\cdot\hat{\Omega}')$$

$$\Sigma_t^1 = \Sigma_A^1 + \sum_{g'=1}\Sigma_s^{1\to g'}(\bar{r},\hat{\Omega}\cdot\hat{\Omega}')$$

$$\Sigma_t^2 = \Sigma_A^2 + \sum_{g'=2}^{4}\Sigma_s^{2\to g'}(\bar{r},\hat{\Omega}\cdot\hat{\Omega}')$$

$$\Sigma_t^3 = \Sigma_A^3 + \sum_{g'=2}^{4}\Sigma_s^{3\to g'}(\bar{r},\hat{\Omega}\cdot\hat{\Omega}')$$

$$\Sigma_t^4 = \Sigma_A^4 + \sum_{g'=2}^{4}\Sigma_s^{4\to g'}(\bar{r},\hat{\Omega}\cdot\hat{\Omega}')$$

②

- $\langle P_0, P_0 \rangle = \int_{-1}^{1} \frac{1}{\sqrt{2}} \cdot \frac{1}{\sqrt{2}}\, dx = \frac{1}{2}\left[x\right]_{-1}^{1} = 1$ ✓

- $\langle P_0, P_1 \rangle = \int_{-1}^{1} \frac{1}{\sqrt{2}} \cdot \frac{\sqrt{3}}{\sqrt{2}}\, x\, dx = \frac{\sqrt{3}}{2}\left[\frac{x^2}{2}\right]_{-1}^{1} = 0$ ✓

- $\langle P_0, P_2 \rangle = \int_{-1}^{1} dx\, \frac{1}{\sqrt{2}} \sqrt{\frac{5}{2}} \left(\frac{3x^2-1}{2}\right) = \frac{\sqrt{5}}{4}\left[x^3 - x\right]_{-1}^{1} = 0$ ✓

- $\langle P_1, P_1 \rangle = \int_{-1}^{1} \sqrt{\frac{3}{2}}\, x\, \sqrt{\frac{3}{2}}\, x\, dx = \frac{3}{2}\left[\frac{x^3}{3}\right]_{-1}^{1} = \frac{1}{2} + \frac{1}{2} = 1$ ✓

- $\langle P_1, P_2 \rangle = \int_{-1}^{1} dx\, \sqrt{\frac{3}{2}}\, x \cdot \sqrt{\frac{5}{2}} \left(\frac{3x^2-1}{2}\right) = \frac{\sqrt{15}}{4}\int_{-1}^{1}(3x^3 - x)\,dx = \frac{\sqrt{15}}{4}\left[\frac{3x^4}{4} - \frac{x^2}{2}\right]_{-1}^{1} =$

$= \frac{\sqrt{15}}{4}\left[\cancel{\frac{3}{4}} - \cancel{\frac{1}{2}} - \cancel{\frac{3}{4}} + \cancel{\frac{1}{2}}\right] = 0$

- $\langle P_2, P_2 \rangle = \int_{-1}^{1} \sqrt{\frac{5}{2}} \sqrt{\frac{5}{2}} \left(\frac{3x^2-1}{2}\right)^2 dx = \frac{5}{8}\int_{-1}^{1}\left[9x^4 - 6x^2 + 1\right]dx =$

$= \frac{5}{8}\left[\frac{9}{5}x^5 - 2x^3 + x\right]_{-1}^{1} = \frac{5}{8}\left(\frac{9}{5} - 2 + 1 + \frac{9}{5} - 2 + 1\right) = \frac{5}{8} \cdot \left(\frac{18}{5} - 2\right) =$

$= \frac{5}{8} \cdot \frac{8}{5} = 1$ ✓

③

(a) $\int_{4\pi} d\hat{\Omega}\,|\hat{\Omega}| = \sum_{i=1}^{N} K|\Omega_i|\,w_i = \sum_{i=1}^{N} K\sqrt{\mu_i^2+\xi_i^2+\eta_i^2}\;w_i =$

Now, we can consider that the function $|\Omega_i|$, for how it's built (sum of squared values) is symmetric in each octant $\Rightarrow$ It's enough to compute the sum in one octant and multiply by 8

$$\Rightarrow \quad = 8\cdot \sum_{i=1}^{n} K\sqrt{\mu_i^2+\xi_i^2+\eta_i^2}\;w_i$$

K is a normalization constant for the whole solid angle, which leads to $\int_{4\pi} d\Omega = 4\pi$ despite $\sum_{i=1}^{N} w_i = 1$, i.e.

$$\int_{4\pi} d\Omega = 4\pi = K\sum_{i=1}^{N} w_i \overset{sym}{=} 8K\underbrace{\sum_{i=1}^{n} w_i}_{\text{1 for each octant}} = 8K\cdot 1 \Rightarrow K = \frac{\pi}{2}$$

- So we have, in the S4 quadrature:

$$\int d\Omega\,|\Omega| = 8\cdot\frac{\pi}{2}\cdot\sum_{i=1}^{4}\sqrt{\mu_i^2+\xi_i^2+\eta_i^2}\;w_i$$

Moreover, ~~from~~ Miller (4.3), we see that $\sqrt{\mu_i^2+\xi_i^2+\eta_i^2} = 1$, so it's enough to sum the weights

$$S4: \quad \int d\Omega\,|\Omega| = 8\,\frac{\pi}{2}\left[w(\mu_1,\eta_1,\xi_1) + w(\mu_1,\eta_2,\xi_1) + w(\mu_2,\eta_1,\xi_1)\right]$$

$$= \frac{\pi}{2}\,8\cdot\left[0.3333333\times 3\right] = 3.9999999\,\pi$$

(b)

$$S6 \quad \int d\Omega\,|\Omega| = 8\,\frac{\pi}{2}\sum_{i}^{6} w_i = 8\cdot\frac{\pi}{2}\cdot\left[w_{113} + w_{131} + w_{311} + w_{122} + w_{221} + w_{212}\right]$$

$$= 8\cdot\pi/2\cdot\left[3\times 0.1761263 + 3\times 0.1572701\right] = 4\pi\cdot 1.0000002$$