

## Problem 1<sup>1</sup>

The macroscopic cross section is given by  $\Sigma_s = (N_{UO_2})(\sigma_{UO_2})$ . This can be equivalently expressed as  $\Sigma_s = N_U\sigma_U + N_O\sigma_O$ . Stoichiometrically  $N_U = \frac{N_O}{2}$ , so we can say  $\Sigma_s = N_U\sigma_U + 2N_U\sigma_O = N_U(\sigma_U + 2\sigma_O)$ . Since  $N_U$  is composed of both  $^{235}\text{U}$  and  $^{238}\text{U}$ ,  $N_U = N_{U5} + N_{U8}$ . Additionally,  $\gamma = \frac{N_{U5}}{N_{U8}}$ , so  $N_U = N_{U8}(\gamma + 1)$  and in total  $\Sigma_s = N_{U8}(\gamma + 1)(\sigma_U + \sigma_O)$ . Given some material density  $\rho$ , enrichment factor (U5/U8 by weight)  $f$ , atomic weights  $m_i$  and Avogadro's number  $A$ ,  $N_{U8} = \rho(1 - f) \left( \frac{m_U}{m_{UO_2}} \right) \left( \frac{A}{m_{U8}} \right)$ . Further, we can say  $m_{UO_2} = m_U + m_{O_2}$  and  $m_U = fm_{U5} + (1 - f)m_{U8}$ . Altogether,

$$\Sigma_s = \rho(1 - f) \left( \frac{fm_{U5} + (1 - f)m_{U8}}{fm_{U5} + (1 - f)m_{U8} + 2m_O} \right) \left( \frac{A}{m_{U8}} \right) (\gamma + 1)(\sigma_U + \sigma_O)$$

Solving, when  $\rho = 10 \text{ g/cm}^3$ ,  $f = 5\%$ ,  $m_{U5} = 235.044 \text{ g/mol}$ ,  $m_{U8} = 238.051 \text{ g/mol}$ ,  $m_O = 15.999 \text{ g/mol}$ ,  $\gamma = \frac{f}{(1-f)} \left( \frac{m_{U8}}{m_{U5}} \right)$ ,  $\sigma_U = 8.9 \text{ b}$ , and  $\sigma_O = 3.75 \text{ b}$ , we get

$\Sigma_s = 0.3659 \text{ cm}^{-1}$

## Problem 2

a.)

Top 3 Supercomputers (per Top500.org)

1. **Sunway TaihuLight** (National Supercomputing Center; Wuxi, China): a 10,649,600 core CPU based machine using Sunway processors. Its performance peak was 93,014.6 TFlop/s and it has 1,310,720 GB memory.
2. **Tianhe-2** (National Super Computer Center; Guangzho, China): a 3,120,000 MIC machine - primarily Intel Xeon processors (Ivy Bridge/Xeon Phi). Its performance peak was 33,862.7 TFlop/s and it has 1,024,000 GB memory.
3. **Titan** (ORNL; Oak Ridge, TN, USA): a GPU/CPU hybrid with 560,640 cores (AMD Opteron CPUs/NVIDIA Tesla GPUs). Its performance peak was 17,590 TFlop/s and it has 710,144 GB memory.

Among the top 10 supercomputers, 5 are primarily CPUs, 3 incorporate MICs, and 2 utilize GPU acceleration.

b.)

The three types of processors: CPUs, GPUs and MICs all vary in their structure and characteristics. CPUs are the most well known processor type, and are designed to handle serial operations. MICs extend the ability of CPUs by including several cores together and thereby allowing parallelization. GPUs, on the other hand, consist of hundreds or thousands of cores which are optimized to handle parallel jobs. With this emphasis on parallelization, GPUs often sacrifice clock speed under the premise that with sufficient parallelization, individual losses will be compensated by the volume of work accomplished by the multitude of cores.

c.)

Where each architecture is optimized differently, it is challenging if not impossible to solve the neutron transport equation quickly and effectively on each machine. For example, Monte Carlo methods could be ideal on a GPU

system where parallelizability is one of the strongest points. Each of the GPUs many cores could handle a subset of the event scenarios, with results being aggregated after running. In this same way, CPUs might be a better choice for a deterministic method of solving the equation. The CPUs will be faster and likely have more memory, and will therefore not spend as much time as GPUs communicating results of each successive iteration through among necessary cores.

## Problem 3<sup>2</sup>

We have defined a sequence as converging if  $\|\vec{x}^{(k)} - \vec{x}\| < \varepsilon \quad \forall \quad k \geq N(\varepsilon)$  where  $\varepsilon > 0$ . Since we are considering a situation where the solution  $\vec{x}$  is unknown, we instead compare  $\vec{x}^n$  to  $\vec{x}^{n-1}$ .

**Norm 1:**  $\|\vec{x}\|_1 = \sum_{i=1}^5 |x_i|$

*Absolute:*

$$\begin{aligned}\epsilon &= \|\vec{x}^n - \vec{x}^{n-1}\|_1 \\ \epsilon &= 0.35\end{aligned}$$

*Relative:*

$$\begin{aligned}\eta &= \frac{\epsilon}{\|\vec{x}^{n-1}\|_1} \\ \eta &= 0.1556\end{aligned}$$

**Norm 2:**  $\|\vec{x}\|_2 = \left(\sum_{i=1}^5 x_i^2\right)^{1/2}$

*Absolute:*

$$\begin{aligned}\epsilon &= \|\vec{x}^n - \vec{x}^{n-1}\|_2 \\ \epsilon &= 0.1658\end{aligned}$$

*Relative:*

$$\begin{aligned}\eta &= \frac{\epsilon}{\|\vec{x}^{n-1}\|_2} \\ \eta &= 0.1351\end{aligned}$$

**Norm  $\infty$ :**  $\|\vec{x}\|_\infty = \max_{1 \leq i \leq 5} (x_i)$

*Absolute:*

$$\begin{aligned}\epsilon &= \|\vec{x}^n - \vec{x}^{n-1}\|_\infty \\ \epsilon &= 0.1\end{aligned}$$

*Relative:*

$$\begin{aligned}\eta &= \frac{\epsilon}{\|\vec{x}^{n-1}\|_\infty} \\ \eta &= 0.1053\end{aligned}$$

Of these 3 norms, the infinity norm seems to be the most restrictive as it has both the lowest absolute and relative error.

***Recalculating with the new  $\vec{x}^{n-1}$ :***

**Norm 1:**

*Absolute:*  $\epsilon = 0.15$

*Relative:*  $\eta = 0.0622$

**Norm 2:**

*Absolute:*  $\epsilon = 0.1034$

*Relative:*  $\eta = 0.0840$

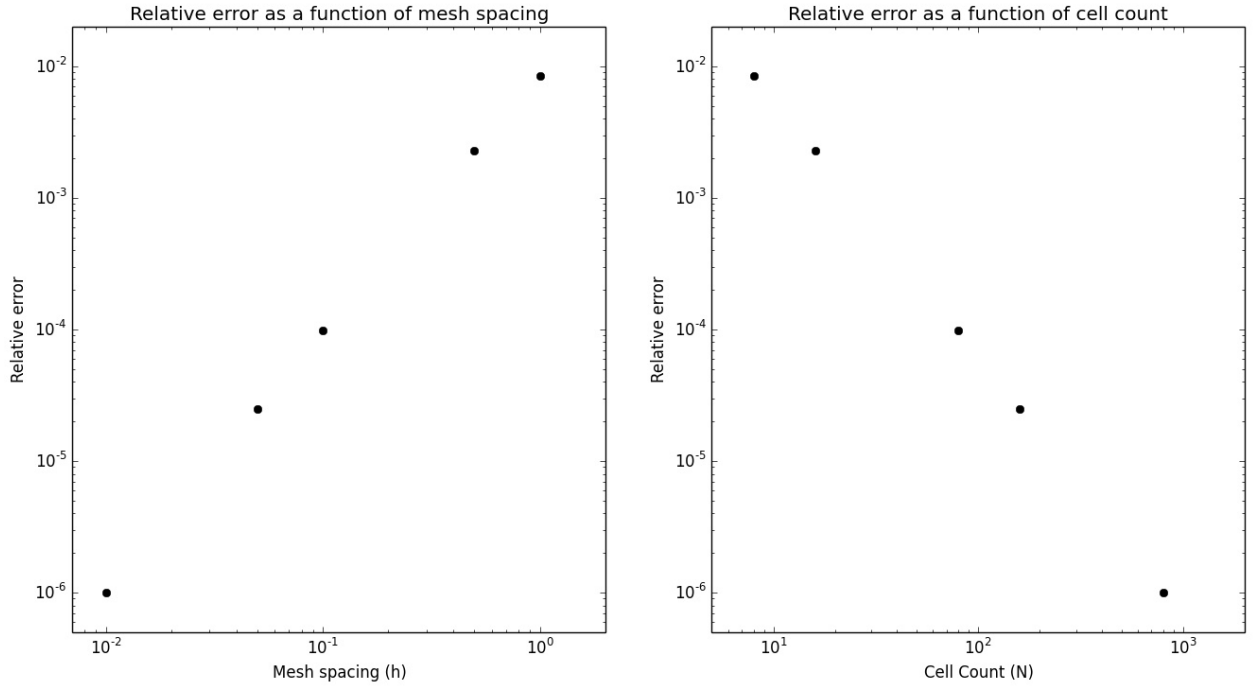
**Norm  $\infty$ :**

*Absolute:*  $\epsilon = 0.1$

*Relative:*  $\eta = 0.1087$

In this case, we see that the relative errors of norm 1 and norm 2 are significantly less than they were for the first  $(n - 1)$  vector, however the relative error for the infinity norm remains relatively constant. This suggests that depending on the chosen norm, we may want to be cognizant of our choice of convergence criteria. If we choose a criteria that is too small, it may take excessive amounts of time for our iteration to reach that value (or it may never reach it if it is out of the scope of our simulation's uncertainty).

## Problem 4



Since the data points tend to fall in relatively straight lines when plotted logarithmically on both axes, we know that the relative error is a power function of both mesh spacing and cell count. The degree of the power function is given by the slope of that line. We can determine that  $m \approx 2$  for relative error vs. mesh spacing so  $\Delta \propto h^2$  and  $m \approx -2$  for relative error vs. cell count so  $\Delta \propto \frac{1}{N^2}$ .

## Problem 5

### 6 Fundamental Assumptions of the Neutron Transport Equation:

1. *Particles are pointlike.* This means we do not need to consider rotation or quantum effects. Neglecting these allows us to write the transport equation as a function of energy while only being concerned with the particle's translational kinetic energy.
2. *Neutral particles travel in straight lines.* The particles' trajectories will not bend between collisions, and we can make the assumption that  $\frac{\partial \theta}{\partial t} = 0$  and  $\frac{\partial \varphi}{\partial t} = 0$ .
3. *Particle-particle collisions are negligible.* This allows us the freedom to neglect particle-particle interactions and express the transport equation as a linear differential equation.
4. *Material properties are isotropic.* This condition allows us to establish cross sections simply as functions of  $\vec{r}$  and  $E$ .
5. *Material composition is independent of time.* Similar to assumption 5, our cross sections become dependent only on  $\vec{r}$  and  $E$ .
6. *Quantities are expected values.* This is important to the transport equation as it means that we may be unable to properly predict fluctuations in our results for cases where we are dealing with low density media.

## Problem 6

a.)

- A. **Time rate of change:** The overall rate of change of the number of particles in the system.
- B. **Streaming loss rate:** The rate at which particles stream from the system (in each of three spatial directions, both angles  $\theta$  and  $\varphi$ , and energy).
- C. **Total interaction loss rate:** The rate at which interactions are quelled due to absorption.
- D. **External source rate:** The rate at which particles enter the system from an external source.
- E. **Inscattering source rate:** The rate at which particles scatter into a given location, direction and energy.
- F. **Fission source rate:** The rate at which particles are produced via fission.

b.)

For the time-independent form of the transport equation, we have  $\frac{\partial \psi}{\partial t} = 0$  so

$$\hat{\Omega} \cdot \nabla \psi(\vec{r}, \hat{\Omega}, E, t) + \Sigma(\vec{r}, E) \psi(\vec{r}, \hat{\Omega}, E, t) = S(\vec{r}, \hat{\Omega}, E, t) + \int_0^\infty dE' \int_{4\pi} d\hat{\Omega}' \Sigma_s(\vec{r}, E' \rightarrow E, \hat{\Omega}' \cdot \hat{\Omega}) \psi(\vec{r}, \hat{\Omega}', E', t) + \frac{\chi(E)}{4\pi} \int_0^\infty dE' \nu \Sigma_f(\vec{r}, E') \int_{4\pi} d\hat{\Omega} \psi(\vec{r}, \hat{\Omega}', E', t)$$

Including azimuthal symmetry, we can note that the scattering will only depend on the cosine of the scattering event, such that  $\mu = \hat{\Omega}' \cdot \hat{\Omega} = \cos(\theta)$ . Then,

$$\Sigma_s(\vec{r}, E' \rightarrow E, \hat{\Omega}' \cdot \hat{\Omega}) \longrightarrow \Sigma_s(\vec{r}, E' \rightarrow E, \mu)$$

$$\psi(\vec{r}, \hat{\Omega}, E, t) d\hat{\Omega} \longrightarrow \psi(\vec{r}, \mu, E, t) d\varphi d\mu$$

Combining these expressions into the transport equation and integrating over the symmetric angle  $\varphi$ , we end up with

$$\mu \nabla \psi(\vec{r}, \mu, E, t) + \Sigma(\vec{r}, E) \psi(\vec{r}, \mu, E, t) = S(\vec{r}, \mu, E, t) + 2\pi \int_0^\infty dE' \int_{-1}^1 d\mu' \Sigma_s(\vec{r}, E' \rightarrow E, \mu) \psi(\vec{r}, \mu', E', t) + \frac{\chi(E)}{2} \int_0^\infty dE' \nu \Sigma_f(\vec{r}, E') \int_{-1}^1 d\mu' \psi(\vec{r}, \mu', E', t)$$

## Problem 7

$$y'' + 3y = \sin(x)$$

The characteristic equation is  $r^2 + 3 = 0$ , so  $r = \pm i\sqrt{3}$ . The complementary equation then becomes

$$y_c = c_1 e^{i\sqrt{3}x} + c_2 e^{-i\sqrt{3}x}$$

Using Euler's formula, this can be re-expressed as

$$y_c = A \cos \sqrt{3}x + B \sin \sqrt{3}x.$$

The particular solution will also take the form

$$y_p = C \sin x + D \cos x,$$

which, when substituted into the original differential equation, gives

$$-C \sin x - D \cos x + 3C \sin x + 3D \cos x = \sin x$$

$$2C \sin x + 2D \cos x = \sin x$$

$$C = \frac{1}{2} \text{ and } D = 0.$$

The general solution is the combination of the complementary and particular solutions, then solved for the given initial conditions.

$$y = y_c + y_p = A \cos \sqrt{3}x + B \sin \sqrt{3}x + \frac{\sin x}{2}$$

$$y(0) = 1$$

$$A \cos 0 + B \sin 0 + \frac{\sin 0}{2} = 1$$

$$A = 1$$

$$y(1) = 3$$

$$\cos(\sqrt{3}) + B \sin(\sqrt{3}) + \frac{\sin(1)}{2} = 3$$

$$B = \frac{3 - \cos \sqrt{3} - \frac{1}{2} \sin 1}{\sin \sqrt{3}} \approx 2.776$$

Altogether, we find

$$y = \cos \sqrt{3}x + 2.776 \sin \sqrt{3}x + \frac{1}{2} \sin x$$

To simplify the transport equation to resemble this equation, we would need to first make the equation be 1-D and time independent. Furthermore, the source term,  $S$  ought to be oscillating in (1-D) space, with no fission or in-scattering.

This however would still only be a first order differential equation...

## Problem 8

Lowest Isolated Resonance (eV)	
U <sup>235</sup>	0.287
U <sup>238</sup>	6.63
Pu <sup>239</sup>	0.291
Pu <sup>240</sup>	1.07
Pu <sup>241</sup>	0.254
Pu <sup>242</sup>	2.63

The lowest isolated resonance energies are important as they represent the minimum energy that incident neutrons must have to generate substantial quantities of fission events. This is especially important to know in a reactor, where the objective is to maintain criticality. If neutrons are slowed to below this threshold, the reactor will be subcritical.

[1] Problem 1, collaborated w/ Caroline Hughes

[2] Problem 3, collaborated w/ Lakshay Seth