# Homework 2 - NE 255

## Information

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## Problem 1

Let $\gamma = N_{U-235}/N_{U-238}$ be a generic enrichment factor. We determine the macroscopic scattering cross section for $UO_2$ as a function of this parameter as follows:

$$\Sigma_s^{UO_2} = N_U \sigma_s^U + N_O \sigma_s^O$$
$$\Sigma_s^{UO_2} = \frac{\rho_{UO_2} N_A}{M_{UO_2}} \sigma_s^U + \frac{2\rho_{UO_2} N_A}{M_{UO_2}} \sigma_s^O.$$

Using the following relationship:

$$M_{UO_2} = \gamma M_{U_{235}} + (1-\gamma) M_{U_{238}} + 2M_O$$

we rewrite the the previous formula as

$$\Sigma_s^{UO_2} = \frac{\rho_{UO_2} N_A}{\gamma M_{U_{235}} + (1-\gamma) M_{U_{238}} + 2M_O} (\sigma_s^U + 2\sigma_s^O).$$

Consider the case $\rho_{UO_2} = 10g/cc, \sigma_s^U = 8.9b, \sigma_s^O = 3.75b$, and a weight enrichment of 5%. We convert weight percent to atomic percent as follows:

$$N_{U-235} = \frac{m_{U-235} N_A}{MW_{U-235}} = 1.281037e22$$
$$N_{U-238} = \frac{m_{U-238} N_A}{MW_{U-238}} = 2.403448e23$$
$$\gamma = N_{U-235}/N_{U-238} = 0.0533$$

Using the formula from Part 1, we obtain a macroscopic scattering cross section for $UO_2$

$$\Sigma_s^{UO_2} = 3.65b$$

## Problem 2

### (a)

The top three computers in the world currently are the Sunway TaihuLight, Tianhe-2, and the Titan. The Sunway TaihuLight

- The Sunway TaihuLight uses 40960 SW26010 manycore 64-bit RISC processors. These are based on the Sunway architecture but are of Chinese design. There are a total of 10649600 CPU cores on the system with the processing cores having 64 KB of scratch memory. The system runs on a custom Linux distro implementation of OpenACC 2.0.

- The Tianhe-2 is a 33.86 petaflop computer. It has 16000 nodes that each have two Intel Ivy Bridge Xeon processors and three Xeon Phi processors. Each node has 88 GB of memory. It ran on the Kylin Linux OS.
- The Titan uses AMD Opteron CPUs along with Nvidia Tesla GPUs. There are 18688 CPUs along with 18688 GPUs on the machine. The AMD Opteron 6274 CPU has 16 cores and 32 GB of DDR3 ECC memory. The Nvidia Tesla K20X GPU has 6 GB of GDD5R ECC memory. Titan uses Lustre storage. The Titan runs the Cray Linux Environment OS.
- Five computers have MICs, three computers are GPU-accelerated.

### (b)

- GPU - A GPU is characterized by hundreds of cores that handle thousands of threads simultaneously. GPUs are specifically designed to render 3D graphics. They can do texture mapping, polygon rendering, and are able to calculate coordinate transforms of vertices. GPUs have memory that is rapidly accessed and manipulated with average clock speeds on the 2-3 GHz range depending on the application.
- MIC - Combines multiple processor cores onto a single chip. They run on standard, existing programming tools making their use simple without the need for a chip specific language or programming. Can take advantage of a high degree of parallelism due to ease of communication.
- CPU - Central processing unit: the "brain" of a computer. Modern CPUs are microprocessors. They contain a control unit, an arithmetic logic unit, and a memory management. Capable of instruction-level and task-level parallelization. Modern CPUs have hyper-threading and clock rates are on the order of GHz.

### (c)

Some challenges of solving the NTE on all architectures involves the use of memory to store cross sections and the ability to parallelize sweeping algorithms on deterministic transport equations. GPU's can be used to accelerate Monte Carlo calculations but these algorithms must be rewritten to take advantage of the vector capabilities of GPU's.

## Problem 3

Consider the following vectors

$$x_{n-1} = \begin{pmatrix} 0.45 \\ 0.95 \\ 0.2 \\ -0.05 \\ 0.6 \end{pmatrix} \quad x_n = \begin{pmatrix} 0.5 \\ 0.9 \\ 0.3 \\ -0.1 \\ 0.5 \end{pmatrix}$$

we calculate the absolute and relative error using the following norms:

- 1-norm ( $||\mathbf{x}||_1 = \sum_{i=1}^{N} |x_i|$ )
  - Absolute Error: $||\mathbf{x}_{n-1} - \mathbf{x}_n||_1 = 0.35$
  - Relative Error: $\frac{||\mathbf{x}_{n-1} - \mathbf{x}_n||_1}{||\mathbf{x}_n||_1} = 0.1522$
- 2-norm ( $||\mathbf{x}||_2 = \sum_{i=1}^{N} |x_i^2|^{1/2}$ )
  - Absolute Error: $||\mathbf{x}_{n-1} - \mathbf{x}_n||_2 = 0.1658$
  - Relative Error: $\frac{||\mathbf{x}_{n-1} - \mathbf{x}_n||_2}{||\mathbf{x}_n||_2} = 0.1397$
- max-norm ( $||\mathbf{x}||_\infty = \max_i |x_i|$)
  - Absolute Error: $||\mathbf{x}_{n-1} - \mathbf{x}_n||_\infty = 0.1000$

- Relative Error: $\frac{||\mathbf{x}_{n-1}-\mathbf{x}_n||_\infty}{||\mathbf{x}_n||_\infty} = 0.1111$

The most restrictive norm is the infinity norm. For the vector

$$x_{n-1} = \begin{pmatrix} 0.49 & 0.92 & 0.4 & -0.09 & 0.51 \end{pmatrix}^T$$

we calculate the absolute and relative error norms:

- 1-norm ( $||\mathbf{x}||_1 = \sum_{i=1}^N |x_i|$ )
  - Absolute Error: $||\mathbf{x}_{n-1} - \mathbf{x}_n||_1 = 0.15$
  - Relative Error: $\frac{||\mathbf{x}_{n-1}-\mathbf{x}_n||_1}{||\mathbf{x}_n||_1} = 0.0652$
- 2-norm ( $||\mathbf{x}||_2 = \sum_{i=1}^N |x_i^2|^{1/2}$ )
  - Absolute Error: $||\mathbf{x}_{n-1} - \mathbf{x}_n||_2 = 0.1034$
  - Relative Error: $\frac{||\mathbf{x}_{n-1}-\mathbf{x}_n||_2}{||\mathbf{x}_n||_2} = 0.0871$
- max-norm ( $||\mathbf{x}||_\infty = \max_i |x_i|$)
  - Absolute Error: $||\mathbf{x}_{n-1} - \mathbf{x}_n||_\infty = 0.1000$
  - Relative Error: $\frac{||\mathbf{x}_{n-1}-\mathbf{x}_n||_\infty}{||\mathbf{x}_n||_\infty} = 0.1111$

We observe that different norms respond differently to differences in iteration vectors. We should select a norm depending on how tightly converged we want our solution to be. The max-norm shows the maximum difference in solution iterations and can be used to assure the absolute difference between iteration vector elements are below some tolerance. The other norms average out differences and can cause false convergence if one element is drastically different from the previous iterate element and all other values are only changed slightly.

# Problem 4

## a. Mesh Spacing

By calculating the slope of the line, we see order of convergence of approximately 2 ($O(h^2)$) when we consider mesh spacing.

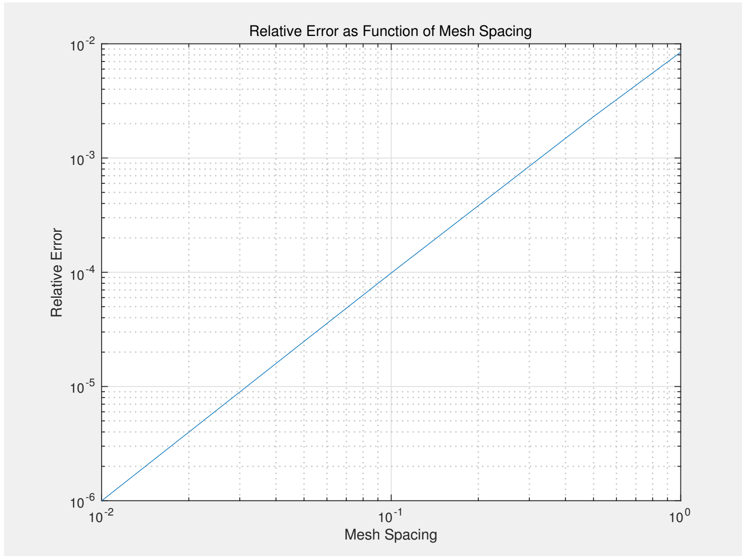
## b. Cell Count

By calculating the slope of the line, we see order of convergence of approximately 2 ($O(h^2)$) when we consider cell number.

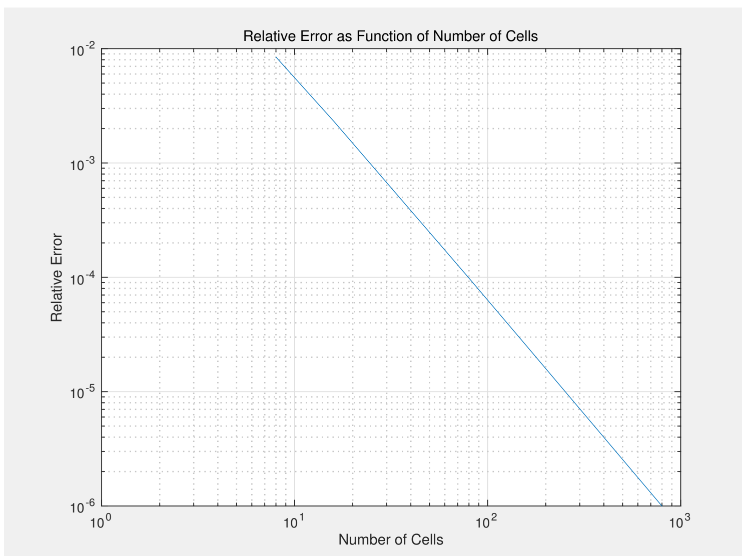
# Problem 5

Six assumptions in the neutron transport equation are:

- Neutrons (or photons) travel straight lines between collisions - neutral particle do not experience electromagnetic forces and therefore the interaction (scattering) term does not need to take into account these forces simplifying the scattering kinematics.
- Material properties are isotropic - this assumption is made to remove any sort of angular dependence of material properties which is usually valid except for low velocities.
- Particles are point object - the deBroglie wavelength of particles is small compared to the atomic diameter allowing neutrons and photons to be treated as point particles and neglecting quantum mechanical quantities such as spin.
- Particle-particle collisions are negligible - neglecting particle-particle interactions makes the transport equation linear.




Relative Error as Function of Mesh Spacing




Relative Error as Function of Cell Number

- Material compositions are time-independent - material properties change slowly compare to particle interaction time scales removing time-dependence of material cross sections.
- Quantities calculated are expected values - the neutral particle transport equation calculated mean values of quantities and neglects fluctuations of particle number in the system.

# Problem 6

$$\underbrace{\frac{1}{v}\frac{\partial\psi}{\partial t}}_{\text{A}} + \underbrace{\hat{\Omega}\cdot\nabla\psi(\vec{r},\hat{\Omega},E,t)}_{\text{B}} + \underbrace{\Sigma(\vec{r},E)\psi(\vec{r},\hat{\Omega},E,t)}_{\text{C}} = \underbrace{S(\vec{r},\hat{\Omega},E,t)}_{\text{D}}$$
$$+ \underbrace{\int_0^\infty dE' \int_{4\pi} d\hat{\Omega}'\Sigma_s(\vec{r},E'\to E,\hat{\Omega}'\cdot\hat{\Omega})\psi(\vec{r},\hat{\Omega}',E',t)}_{\text{E}}$$
$$+ \underbrace{\frac{\chi(E)}{4\pi}\int_0^\infty dE'\nu\Sigma_f(\vec{r},E')\int_{4\pi} d\Omega'\psi(\vec{r},\hat{\Omega}',E',t)}_{\text{F}}$$

## (a)

- A - time-dependence of angular flux.
- B - streaming term. Describes streaming of particles through space. The geometry of the system is expressed through the gradient term.
- C - collision reaction rate - expresses particle interaction of all types. The total cross section is the sum of the absorption and scattering cross sections.
- D - external source of particles into the system.
- E - scattering of particles into and out into a specific phase space volume element. This is a source and sink of particles when we look at a specific phase space volume.
- F - production of neutrons through fission. Fission is determined by the scalar flux reaction rate and emits particles with a certain distribution in energy and isotropically in angle.

## (b)

To include azimuthal symmetry, we recognize that scattering only depends on the angle of the scattering cosine. We can then simplify our integrals over the solid angle as follows:

$$\int_{4\pi} d\hat{\Omega}\psi(\vec{r},\hat{\Omega},E,t) = \int_0^{2\pi} d\varphi \int_{-1}^{1} d\mu\psi(\vec{r},\hat{\Omega},E,t) = 2\pi\int_{-1}^{1} d\mu\psi(\vec{r},\hat{\Omega},E,t).$$

We rewrite the streaming term as follows:

$$\hat{\Omega}\cdot\nabla\psi(\vec{r},\hat{\Omega},E,t) \to \mu\nabla\psi(\vec{r},\mu,E,t)$$

We rewrite the scattering cross section as:

$$\Sigma_s(\vec{r},\hat{\Omega}'\to\hat{\Omega}) \to \Sigma_s(\vec{r},\hat{\Omega}'\cdot\hat{\Omega}) = \Sigma_s(\vec{r},\mu).$$

We rewrite the fission term:

$$\frac{\chi(E)}{4\pi}\int_0^\infty dE' \int_{4\pi} d\hat{\Omega}'\nu(E')\Sigma_f(\vec{r},E',t)\psi(\vec{r},\hat{\Omega},E,t) =$$
$$\frac{\chi(E)}{4\pi}\int_0^\infty dE' \int_0^{2\pi} d\varphi' \int_{-1}^{1} d\mu'\nu(E')\Sigma_f(\vec{r},E',t)\psi(\vec{r},\hat{\Omega},E,t) =$$
$$\frac{\chi(E)}{2}\int_0^\infty dE'\nu(E')\Sigma_f(\vec{r},E',t)\phi(\vec{r},E,t).$$

# Problem 7

We solve

$$\frac{d^2y}{dx^2} + 3y(x) = \sin(x) \quad x \in [0,1]$$

where $y(0) = 1, y(1) = 3$ as follows: we consider the homogenous equation

$$\frac{d^2y}{dx^2} + 3y(x) = 0 \quad x \in [0,1]$$

and by inspection determine the solution of the homogenous equation to be

$$y(x) = C_1 \sin(\sqrt{3}x) + C_2 \cos(\sqrt{3}x).$$

We assume the particular solution has the form

$$y(x) = A\sin(x) + B\cos(x)$$

and plug this solution into our ODE

$$-A\sin(x) - B\cos(x) + 3A\sin(x) + 3B\cos(x) = \sin(x)$$

$$2A\sin(x) + 2B\cos(x) = \sin(x).$$

Comparing coefficients we obtain $A = \frac{1}{2}$ and $B = 2$. Our solution to the ODE is now

$$y(x) = C_1 \sin(\sqrt{3}x) + C_2 \cos(\sqrt{3}x) + \frac{1}{2}\sin(x).$$

We apply the boundary conditions and obtain two equations:

$$1 = C_2$$
$$3 = C_1 \sin(\sqrt{3}) + C_2 \cos(\sqrt{3}) + \frac{1}{2}\sin(1).$$

Solving for $C_1$ and $C_2$ we obtain

$$C_1 = \frac{3 - \cos(\sqrt{3}) - \frac{1}{2}\sin(1)}{\sin(\sqrt{3})}$$

$$C_2 = 1.$$

Our solution to the ODE is then

$$y(x) = \frac{3 - \cos(\sqrt{3}) - \frac{1}{2}\sin(1)}{\sin(\sqrt{3})}\sin(\sqrt{3}x) + \cos(\sqrt{3}x) + \frac{1}{2}\sin(x).$$

To reduce the transport equation, we assume a source that releases neutrons sinusoidally in space and we assume a total cross section of 3. We assume this is a one-speed group problem, no fission source present, and time-independence. We assume a one-dimensional problem and assume a diffusion approximation to the streaming term.

# Problem 8

Uranium-235 energy of lowest isolated resonance: 0.2 eV
Uranium-238 energy of lowest isolated resonance: 8 eV
Plutonium-239 energy of lowest isolated resonance: 0.4 eV
Plutonium-240 energy of lowest isolated resonance: 1 eV

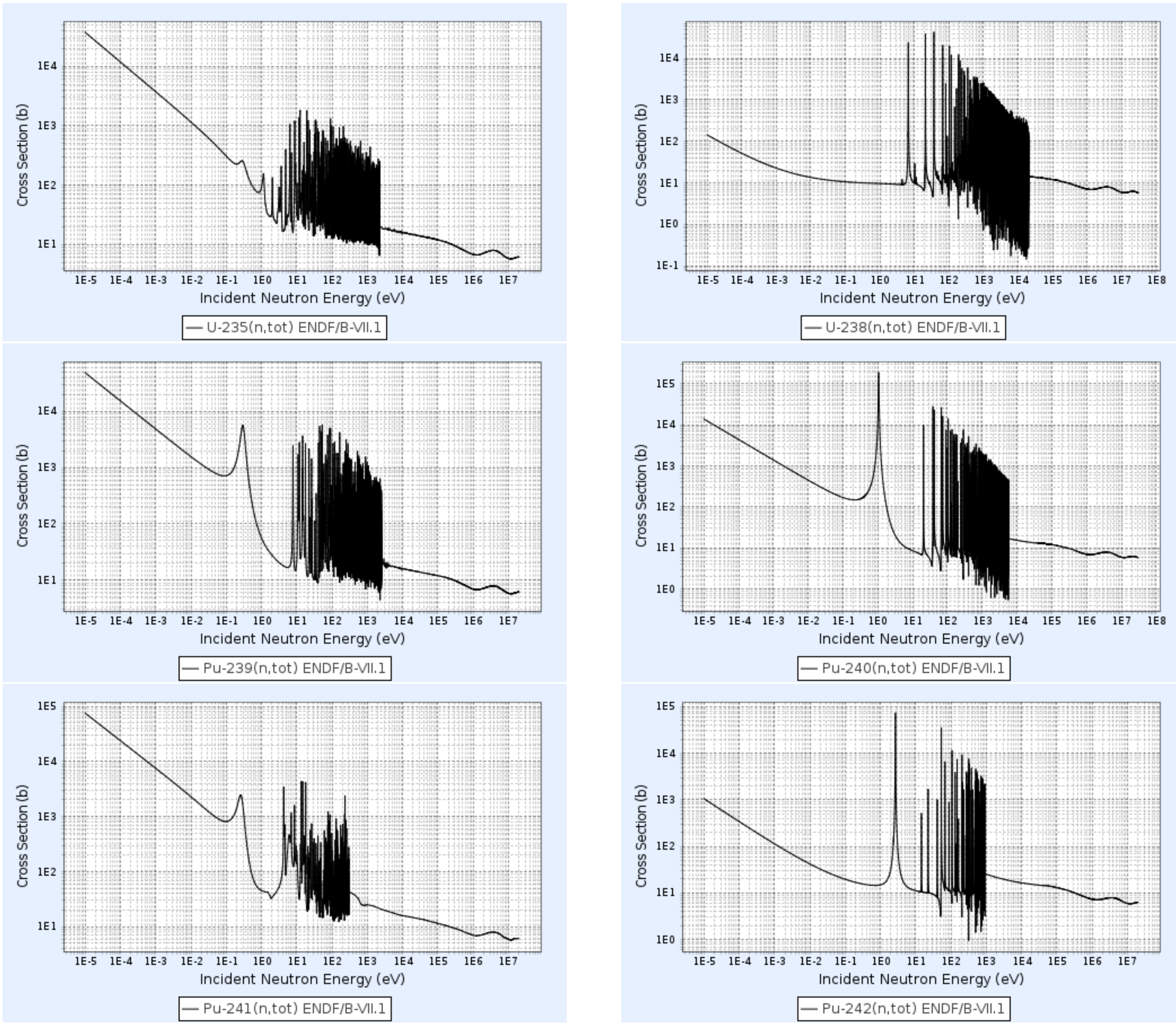



**Figure 0.3:** Total Cross Sections for U-235, U-238, Pu-239, Pu-240, Pu-241, and Pu-242

Plutonium-241 energy of lowest isolated resonance: 0.3 eV
Plutonium-242 energy of lowest isolated resonance: 5 eV

We care about the location of these resonances because in thermal systems, we must slow down neutrons to thermal energies and these resonances will remove neutrons from our system. These resonances also allow us to identify these materials in detection. We can use these resonances to determine what sort of fissile material is present.