Homework 2 - December 07, 2017. Due December 17, 2017.

SUBMISSION INSTRUCTIONS. Please pay attention to these as they will make grading your assignments less burdensome.

1. Put all of your code files in a folder called <your first name>_<your last name>_homework_3. For example I would call mine

andrew_osborne_homework_3

2. Compress your folder using the zip tool of your choice.

3. Send your homework to me via email (andrew.gs.osborne@gmail.com).

INTRODUCTION.

In this assignment you will develop a piece of code that will solve the coupled nuclear transmutation equations for a fast reactor by using the matrix exponential method you learned in class.

BACKGROUND. In class, you learned that for the transmutation chain from ^{238}U to ^{239}Pu, the coupled equations approximately describing the time evolution of the system are:

$$
\begin{aligned}
\frac{dN^{^{238}U}}{dt} &= -\left(\sigma_c^{^{238}U} + \sigma_f^{^{238}U}\right)\phi N^{^{238}U} \\
\frac{dN^{^{239}U}}{dt} &= \sigma_c^{^{238}U}\phi N^{^{238}U} - \left(\sigma_c^{^{239}U} + \sigma_f^{^{239}U}\right)\phi N^{^{239}U} - \lambda^{^{239}U} N^{^{239}U} \\
\frac{dN^{^{239}Np}}{dt} &= \lambda^{^{239}U} N^{^{239}U} - \left(\sigma_c^{^{239}Np} + \sigma_f^{^{239}Np}\right)\phi N^{^{239}Np} - \lambda^{^{239}Np} N^{^{239}Np} \\
\frac{dN^{^{239}Pu}}{dt} &= \lambda^{^{239}Np} N^{^{239}Np} - \left(\sigma_c^{^{239}Pu} + \sigma_f^{^{239}Pu}\right)\phi N^{^{239}Pu} - \lambda^{^{239}Pu} N^{^{239}Pu}
\end{aligned}
\tag{1}
$$

where N, λ, σ_c, σ_f refer to the concentration [atoms/barn-cm], decay constant [1/s], microscopic capture and fission cross sections of the superscripted nuclide [b], and ϕ refers to the neutron flux [neutrons/barn-second]. For simplicity, only the dominant reactions have been included in Eq. (1).

Question 1.

a) Fast reactor fuel rods are commonly composed of 10 w/o (percent by weight) Zirconium and 90 w/o actinides. For an actinide mix of 80 w/o ^{238}U and 20 w/o ^{239}Pu, and an overall rod density of 15 grams per cubic centimeter, compute the quantities of ^{238}U and ^{239}Pu, **in units of atoms per barn-centimeter**. Assume 10 w/o of the rod is composed of natural Zirconium.

b) Like you saw in class, Eq. (1) can be written as a matrix equation:

$$\dot{\vec{N}} = \left(A\phi + B\right)\vec{N} \tag{2}$$

write out the matrices *A* and *B*.

c) Create a Matlab function that takes as input **an array of fission and capture cross sections, and decay constants** for ^{238}U, ^{239}U, ^{239}Np, ^{239}Pu, and produces as outputs the **matrices *A* and *B***. E.g:

[A, B] = function create_transmutation_matrices(fission, capture, decay).

Be sure to fill out the comment header, describing inputs/outputs, etc. The file **data-Q1.mat** provided contains the cross sections and decay constants you need to create A, B.

c) Create a Matlab function that performs a burnup calculation with a matrix exponential algorithm. The function should take as input **an array of concentrations** of ^{238}U, ^{239}U, ^{239}Np, ^{239}Pu [atoms/barn-cm], **a one-group neutron flux value** (a scalar) [neutrons/barn-s], **the matrices *A*, *B***, and **a time in years**. The output should be **an array of nuclide concentrations** at the time specified by the input provided. E.g.:

[N] = function do_burnup(N0, A, B, flux, years);

d) Using the nuclide concentrations you computed in part a) and your functions, **compute N -vs- time** for 1 to 10 years of burnup at a flux of 3×10^{15} neutrons/cm^2-s (3×10^{-9} neutrons/barn-s). Plot your result for all 4 nuclides as a function of time. Do this in a main() function that calls your functions in the right order.

TIPS.
1) Use the expm() builtin Matlab function to compute the matrix exponential.
2) Pay attention to units.
3) You can cross check your answer to a) by converting it back to weight percentages.
4) The data file data-Q1.mat contains a variable named "zaids", to let you know which entries in the nuclear constants arrays correspond to which nuclide.

Question 2.

The data file **data-Q2.mat** contains a list of ZAID numbers for 1506 nuclides, as well as fission, capture and decay matrices of dimension 1506x1506.

a) In your main() function, **create a column vector** (matrix of dimension [1506x1]) of zeros. By looking at the "zaids" variable in data-Q2.mat, **insert the quantities of ^{238}U and ^{239}Pu** you found in Q1a) into the correct positions in the column vector.

b) Repeat Q1d) using your **new vector of nuclide concentrations, and the matrices in data-Q2.mat**. Compare with Q1d) and comment on the results.

Question 3.

Assume that you have a semi-infinite slab reactor with a thermal neutron flux of $\phi = 10^{14}$ n/cm^2•sec at $x = 0$ and vacuum boundary condition at $x = 1000\ cm$. Assume that the slab is made from a uniform 50/50 volume mixture of 5% enriched uranium metal and water at 20^{o}C and atmospheric pressure.

1) Use serpent to simulate the neutron flux in this system.
2) Use the tallies from your Serpent simulation to compute the one-group absorption and fission cross sections for the isotopes in the slab
3) Write a time independent finite difference model for the neutron diffusion equation for this system.
4) Compare the one group neutron flux from your diffusion simulation, and your Serpent simulation. Quantify how close they are.