Preparation and Application of Group Constants in Python

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INTRODUCTION

Repositories of statistical cross section data are integral to numerous nuclear engineering problems. The preparation of stored cross section data is often handled by various well established software such as NJOY. The goal of this project is the investigation of some techniques for converting point-wise cross section data into group constants. The group constants were also used to solve a simplified multigroup neutron diffusion problem for a pin cell modeled as a homogeneous material.

THEORY

Energy Group Structure

Oftentimes to simplify the problems encountered in the nuclear field the assumption is made that over a given energy range cross sections can accurately be represented by a constant value, in contrast to point-wise data. The choice of the energy bounds of each group are ideally rough, i.e. cover a large region reducing computation time, and fine enough to capture important features of the nuclides of interests. The group structures used throughout this project are Casmo 2 and Casmo 16.

Multigroup Neutron Diffusion

The content presented in this section is largely inspired by the heuristic derivation of the multigroup diffusion equations composed by Duderstadt and Hamilton [1]. The multigroup diffusion equations may be derived by balancing the neutron population in each energy group. The groupwise neutron balance equation may be written conceptually as:

$$\begin{bmatrix}\text{Time rate of}\\ \text{change of}\\ \text{neutrons in}\\ \text{group } g\end{bmatrix} = -\begin{bmatrix}\text{Change}\\ \text{due to}\\ \text{leakage}\end{bmatrix} - \begin{bmatrix}\text{Absorption}\\ \text{in}\\ \text{group } g\end{bmatrix} + \begin{bmatrix}\text{Source}\\ \text{neutrons}\\ \text{appearing}\\ \text{in group } g\end{bmatrix} - \begin{bmatrix}\text{Neutrons}\\ \text{scattering}\\ \text{out of}\\ \text{group } g\end{bmatrix} + \begin{bmatrix}\text{Neutrons}\\ \text{scattering}\\ \text{into}\\ \text{group } g\end{bmatrix}. \tag{1}$$

The mathematical representation of the neutron balance equation for a group structure with G energy groups is

$$\frac{1}{v_g}\frac{\partial \phi_g}{\partial t} = \nabla \cdot D_g \nabla \phi - \Sigma_{ag}\phi_g + S_g - \Sigma_{sg}\phi_g + \sum_{g'=1}^{G} \Sigma_{sg'g}\phi_{g'}, \quad g = 1, 2, 3, .., G. \tag{2}$$

Where v_g, D_g, Σ_g, ϕ_g, S_g, are neutron velocity, diffusion coefficient for flux, macroscopic cross section, flux, and source term respectively. The subscripts g and g' corresponds to the group that the parameter exists in. The source may be discretized into two terms, neutrons born from fission, and an external source,

$$S_g \equiv \chi_g \sum_{g'=1}^{G} \nu_{g'}\Sigma_{fg}\phi_{g'} + S_g^{ext}. \tag{3}$$

The scenario in which a scattering event causes a neutron to emigrate from group g' to a group g is accounted for by utilizing the group-transfer cross section, $\Sigma_{sg'g}$.

Equation 2. was simplified by assuming that the system is homogeneous meaning that there is no space dependence, the system is steady state so that there is no time dependence, and that there is no external source.

$$\Sigma_{tg}\phi_g = \chi_g \sum_{g'=1}^{G} \nu_{g'}\Sigma_{fg}\phi_{g'} + \sum_{g'=1}^{G} \Sigma_{sg'g}\phi_{g'}, \quad g = 1, 2, 3, .., G. \tag{4}$$

Which, written in matrix form is,

$$\boldsymbol{T\phi} = \boldsymbol{S\phi} + \frac{1}{k}\boldsymbol{F\phi}, \tag{5}$$

or

$$(\boldsymbol{T} - \boldsymbol{S})^{-1}\boldsymbol{F\phi} = k\boldsymbol{\phi}. \tag{6}$$

Note that this possesses the same form as the algebraic eigenvalue problem, $\boldsymbol{Ax} = \lambda\boldsymbol{x}$. Under the assumption of no upscattering the matrix $\boldsymbol{T} - \boldsymbol{S}$ is,

$$\boldsymbol{T} - \boldsymbol{S} = \begin{bmatrix} \Sigma_{R_1} & 0 & \cdots & 0 \\ \nu_1\chi_2\Sigma_{f_1} & \Sigma_{R_2} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ \nu_1\chi_G\Sigma_{f_1} & \nu_2\chi_G\Sigma_{f_2} & \cdots & \Sigma_{R_G} \end{bmatrix}. \tag{7}$$

While the fission matrix is,

$$\boldsymbol{F} = \begin{bmatrix} \nu_1\chi_1\Sigma_{f_1} & \nu_2\chi_1\Sigma_{f_2} & \cdots & \nu_n\chi_1\Sigma_{f_G} \\ \nu_1\chi_2\Sigma_{f_1} & \nu_2\chi_2\Sigma_{f_2} & \cdots & \nu_n\chi_2\Sigma_{f_G} \\ \vdots & \vdots & \ddots & \vdots \\ \nu_1\chi_G\Sigma_{f_1} & \nu_2\chi_G\Sigma_{f_2} & \cdots & \nu_G\chi_G\Sigma_{f_G}, \end{bmatrix}, \tag{8}$$

where the symbol Σ_{R_g} represents the removal cross section defined as,

$$\Sigma_{R_g} \equiv \Sigma_{tg} - \Sigma_{sgg}. \tag{9}$$

PYTHON PROGRAM

To solve Eq. 6 an algorithm was written using the programming language Python. The operation of this code can be neatly separated into two parts, firstly the conversion of pointwise cross section data into group constants, and secondly using the group constants from step one to evaluate Eq. 6. In it's current form a user may define the atomic density of each nuclide in the homogeneous mixture of interest to obtain the k value of Eq. 6. However, the group constants for each nuclide must already be evaluated, which is currently true for H_1, O_{16}, U_{335}, and U_{238}. The user may also define the temperature of the mixture, which will will later be shown to have a negligible impact on the magnitude of the group constants.

CROSS SECTION DATA

The point wise data used in this project was obtained directly from the Brookhaven National Labs website. To temperature adjust cross section data the method of exact Doppler broadening discussed by Cullen in [2] was incuded in the data generation portion of the algorithm. An example of the effects of temperature on cross sections is given in Fig. 1.

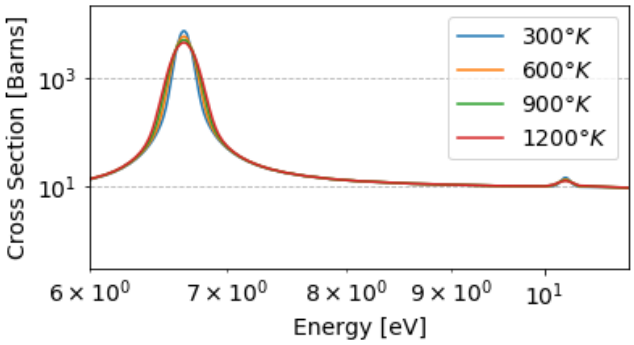

Fig. 1. Doppler-Broadening of total cross section of U_{238} for $E \in [6, 11]eV$ and temperatures: $300°K$, $600°K$, $900°K$, $1200°K$

GROUP VARIABLE CALCULATION

To convert point wise cross sections into group constants the averaging methods outlined by Duderstadt and Hamilton were used [1]. Most group constants are flux weighted averages, hence the need to calculate ϕ_g which is given by,

$$\phi_g \equiv \int_{E_g}^{E_{g-1}} dE\phi(E). \tag{10}$$

The fission and total cross sections are then,

$$\Sigma_{tg} \equiv \frac{1}{\phi_g} \int_{E_g}^{E_{g-1}} dE\Sigma_t(E), \tag{11}$$

and

$$\Sigma_{fg} \equiv \frac{1}{\phi_g} \int_{E_g}^{E_{g-1}} dE\Sigma_f(E). \tag{12}$$

The calculation of group constants for scattering are more complex, because a neutron may scatter from a group to numerous other groups. The phenomenon of scattering from one group to another is defined using the transfer-group cross section. When a neutron scatters and stays in the same group this is defined using the inter-group cross section Σ_{gg}. Both the inter-group and transfer-group cross sections are defined with,

$$\Sigma_{sg'g} \equiv \frac{1}{\phi_{g'}} \int_{E_g}^{E_{g-1}} dE \int_{E'_g}^{E_{g'-1}} dE'\Sigma_s(E')f(E' \to E)\phi(E') \tag{13}$$

where

$$f(E' \to E) = \begin{Bmatrix} \frac{1}{(1-\alpha)E'} & \alpha E' \le E \le E' \\ 0, & \text{otherwise} \end{Bmatrix} \tag{14}$$

and

$$\alpha = \left(\frac{A-1}{A+1}\right)^{1/2}. \tag{15}$$

The atomic mass number of the stationary nuclide is the variable A. Because the transfer group cross section is highly dependent on A a pattern may be observed where for heavy nuclides such as U_{235} and U_{238} the scattering matrix is functionally a diagonal matrix.

The probability, $P(E)$, that a fission neutron is born with energy E is represented by $\chi(E)$ and whose group wise form is,

$$\chi_g \equiv \int_{E_g}^{E_{g-1}} dE\chi(E) \tag{16}$$

The energy distribution of prompt neutrons is referred to as the fission, or Watt spectrum, which is an empirical formula given by

$$P(E) = 0.484e^{-E} \sinh \sqrt{2E}\ \text{MeV}^{-1}, \tag{17}$$

and is accurate in the energy range where practically all fission neutrons are born, 0.1 to 10 MeV [3]. The value of ν_g was approximated to be 2.5 for all groups.

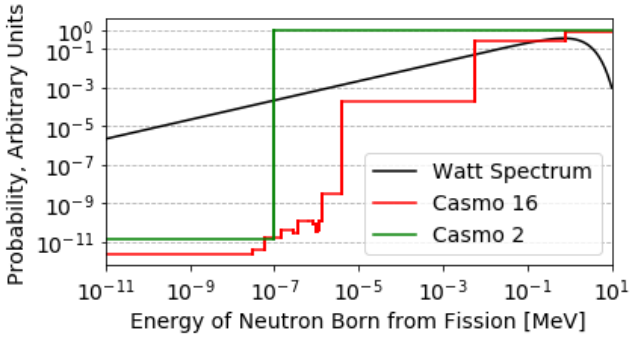

Fig. 2. Watt spectrum and χ_g values for the group structures Casmo-2 and Casmo-16.

Flux Approximation

An approximation of the flux shape must made because the diffusion equation must be solved for to obtain the flux, and the flux is necessary to calculate the group constants. A variation of the narrow resonance approximation was used as the flux shape,

$$\phi_{NR}(E) = \frac{1}{(\sigma_t(E) + \sigma_d)E} \tag{18}$$

where σ_d is the dilution or background cross section. The dilution cross section represents the number of barns of moderator per atom of the fuel atom.

Dilution Cross Section

The dilution cross section greatly impacts the values of the group constants, especially in resonance regions, as displayed in Fig. 3.

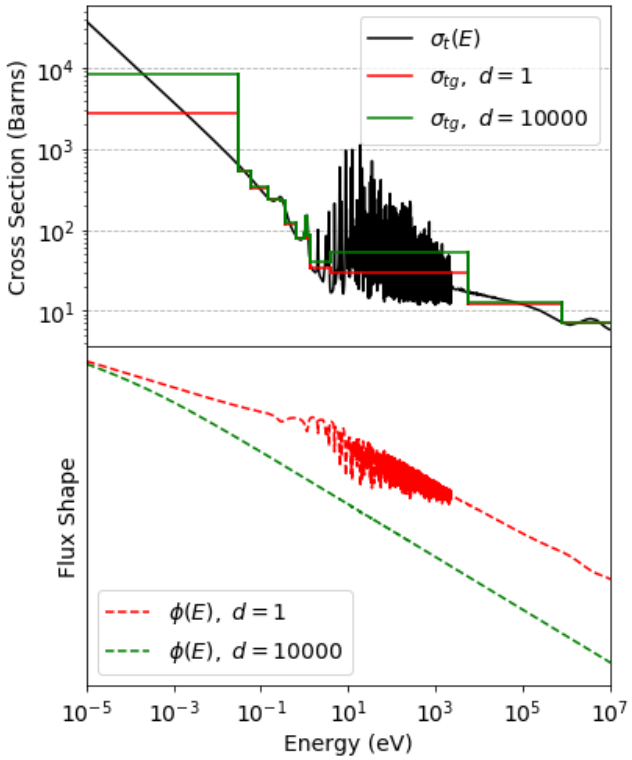

Fig. 3. Effects of increasing the dilution cross section on the flux shape and resultant group cross section of U_{235}

The dilution cross sections also impacts the degree to which Doppler broadening affects group constants. As the dilution cross section increases the dependence on the resonances decreases, reducing the impact that Doppler broadening has on the group constants, this contrast is exemplified by comparing Figs. 4 and 5.

Because the dilution cross section is itself dependent on the atomic densities of the nuclides in the homogeneous mixture, it would be computationally tedious to calculate the group constants for each specific case. Instead the group constants were calculated for the dilution cross section values of: 1, 10, 100, 1000, and 10000 barns, as shown in Tab. I.

Dilution	1	10	100	1000	10000
Fast	14.0	16.2	16.5	16.6	16.6
Thermal	80.0	118.9	202.6	247.5	254.7

TABLE I. Casmo-2 group constants of H_1 elastic scattering cross section values weighted with flux shapes derived from listed dilution cross sections, all values in barns.

With these tables for a given case the group constants can be interpolated for any given dilution cross section. The equation used to approximate the dilution cross section for the model of the homogeneous fuel pin as suggested during lecture is,

$$\sigma_d = \frac{N_{H_1}\sigma_{es,H_1} + N_{O_{16}}\sigma_{es,O_{16}} + N_{U_{235}}\sigma_{potential,U_{235}}}{N_{U_{238}}}. \tag{19}$$

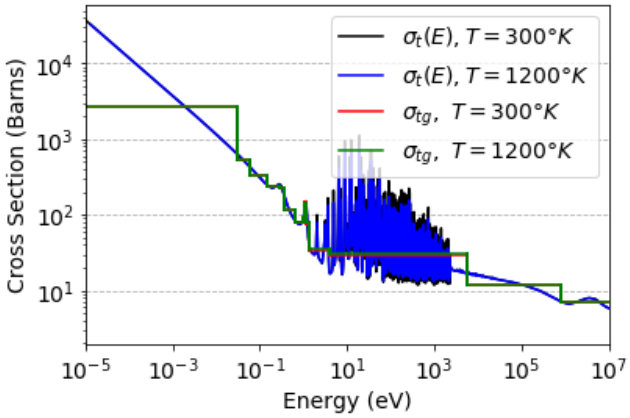

Fig. 4. Doppler-Broadening of total cross section of U_{235} for a dilution background of 1.

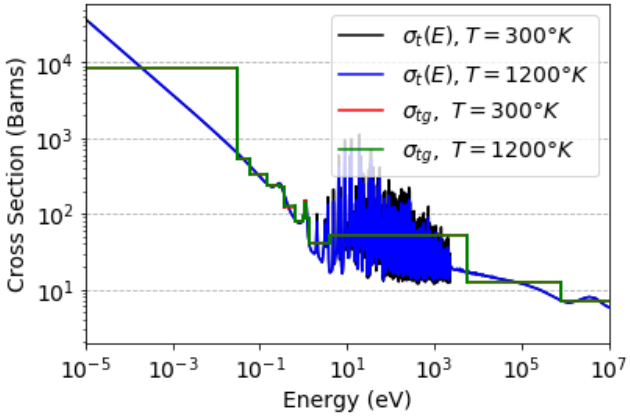

Fig. 5. Doppler-Broadening of total cross section of U_{235} for a dilution background of 10000.

RESULTS AND ANALYSIS

Group Constants Validity

Because cross section values are represented by point-wise data, The accuracy of the numerical integration of Eqs. 10 12 11 and 13 are highly dependent on the number of data points used to represent each group. To benchmark the group constants a unit test was performed where the group constants for U_{235} where calculated for a uniform flux of unity. The comparison of the group constants to tabulated thermal data verified that the group constants are indeed accurate. However,

Reaction	Casmo-2, d=1 ϕ_{Unity}	0.0253 eV	Casmo-2, d=1 ϕ_{NR}
Scattering	15.1 (b)	15.12 (b)	15.7 (b)
Fission	578 (b)	585.1 (b)	1369 (b)
Total	693 (b)	698.9 (b)	1637 (b)

TABLE II. Uniform flux unit test, comparison of the thermal group of Casmo-2 to the cross section of U_{235} at 0.0253 eV.

it should be noted that the group constants were accurate because 100000 data points were assigned to each group.

Pin Cell Simulation

As previously stated a pin cell was simulated as a homogeneous medium, for which the atomic densities were as shown in Tab. III. The results of solving the eigenvalue problem are

H_1	O_{16}	U_{235}	U_{238}
6	7	0.1	1.9

TABLE III. Atomic Density estimations for homogeneous pin cell.

displayed by Fig. **??**, and the concentration of U_{235} varied to ascertain that the results were physically accurate. As ex-

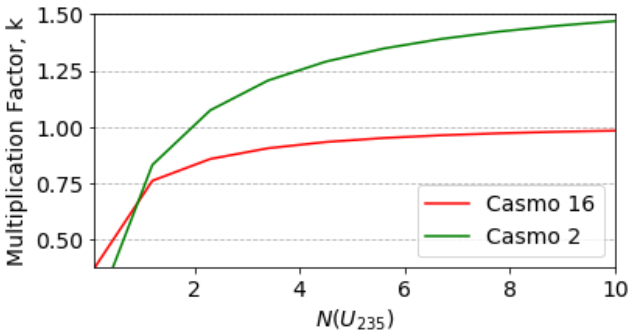

Fig. 6. Multiplication values for various atomic densities of U_{235}, for a temperature of $300K^{\circ}$

pected as the concentration of fissile material is increased the multiplication factor increased.

Unfortunately the section of code which handles the calculation of transfer cross sections is computationally intensive in its current form. As such only 10000 data points were assigned to each energy group. This was shown to have a great effect on the resultant multiplication factor, were for 200 points per group $k = 0.21$ and for 10000 points per group $k = 0.37$.

CONCLUSIONS AND FUTURE WORK

As of the writing of this document the Python code for calculating and employing group constants is in the late development stage. The calculation of group constants was benchmarked and shown to be accurate.

However, no tests specifically for the transfer cross sections have been performed. It is important to note that the number of data points used to represent each group was shown to significantly impact the resultant multiplication term obtained. There are two paths forward were by the transfer cross sections can be made to converge. First more data points can be added to each group at the cost of computation time, this method will only be advisable if the numerical integration function can be vectorized. Second if we are to assume that the point-wise data is linearly interprobable, then a linear equation can be used to represent both the flux and cross section data between points allowing for exact integration to be performed. The latter method was implemented originally to calculate the group constants but was found to be buggy and dropped for the more simplistic method of using the trapezoid rule for numerical integration.

The behavior of the multiplication factor behaved as one might expect, increasing with increasing fissile material concentration. Moving forward a unit test will be added that compares the results to the numerical solution of the diffusion equation for the same problem to answer obtained

Overall the basic mechanics of the algorithm have been established however unit tests to need to be written for the critical sections of code, namely the fission matrix, scatter matrix, and final calculation of the multiplication value. In addition temperature interpolation has yet to be added although it was shown that temperature does not have a significant affect on the group constants.

REFERENCES

1. J. DUDERSTADT and L. HAMILTON, *Nuclear Reactor Analysis*, New York: John Wiley and Sons, Inc., 1 ed. (1976).
2. D. E. CULLEN and C. R. WEISBIN, "Exact Doppler Broadening of Tabulated Cross Sections," *Nuclear Science and Engineering*, **60**, *3*, 199–229 (1976).
3. G. S. and E. M., *The Elements of Nuclear Reactor Theory*, D. Van Nostrand Company, Inc. (1952).