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Optimising the nuclear data energy group structure used for fusion systems

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The generation of reaction rates within Monte-Carlo (MC) transport codes can be accomplished via 1) the standard point-wise estimator approach of tallying the pointwise flux and pointwise partial cross sections and/or 2) the multigroup approach which convolves a pointwise neutron flux with pre-defined binned partial cross-sections. Even fine multigroup sampling is more efficient when compared to pointwise Monte-Carlo sampling due to the removal of the cross-section interpolation from the calculation. This paper describes the four stage optimization procedure used to find an energy binning format which enables an accurate enough and computationally efficient calculation of any reaction rate when applied to MC modeling of fusion devices. This optimum format, named FOMG (Fusion Optimised Multi-Group), was evaluated using a SINBAD (Shielding Integral Benchmark Archive Database) benchmark. Despite the number of multi-group bins exceeding the number of data elements for a significant number of the ENDF files the MCNP simulation took more than one hundred times longer to calculate reaction rates using the pointwise approach when compared to the multi-group method with FOMG structure.

KEYWORDS: Fusion Neutronics,Monte-Carlo,Multi-group,Unionised Energy-grid,MCNP, Reaction rate

I. Introduction

MC codes generate reaction rates mainly via two methods :[(1)] the "standard" pointwise estimator approach of tallying the reaction rates in the MC code and the "multigroup" approach. For every reaction that occurs in a MC code, the pointwise method requires that the cross-section be calculated at the exact energy of the reaction, which involves interpolation between finely spaced tabulated data. Models often comprise of hundreds/thousands of components, each of which are composed of tens/hundreds of isotopes. Thus, the calculation of reaction rates for every reaction and isotope is very computationally expensive.

The multi-group binning method (MGB) used by MC codes differs from deterministic energy grouping due to the intrinsic way in which the each method treats cross-section data. Deterministic methods access predefined, energy integrated cross-sections, whereas MC codes use point-wise data. Thus, a typical MC simulation using MC estimators (MCE) will need to compute 10's of reaction rates, each containing 100's to 100,000's of elements of point-wise data, for several materials in each simulation. In addition to this, the energy-cross-section element convolution requires a Legendre (or similar) interpolation in order convolve a neutron energy with a cross-section element at an exact energy location. Given that every energy structure has a different format and each reaction rate is calculated independently, this can be very computationally expensive. The multi-group method reduces the computational expense of calculating reaction rates within MC codes by storing neutron track-lengths at run time, after a reaction has taken place. When the MC simulation has ended, a script can be used to compute all the reaction rates using a unionsed energy grid, which is common to all cross-sections and all isotopes. This paper describes a method used to optimise the energy group structure and proposes an energy group structure to be used when modelling fusion devices.

II. Theory

Both the MGB and MCE methods are founded on the following definitions of particle flux. The average scalar particle flux, ϕ_V, within a cell of volume, V, given an angular vector flux, $\psi\left(\overrightarrow{r},\hat{\Omega},E,t\right)$ is given by

$$\phi_V = \frac{1}{V}\int\int\int\int \psi\left(\overrightarrow{r},\hat{\Omega},E,t\right) dE\, dt\, d\Omega\, dV \qquad (1)$$

Substituting the definition of the angular flux with its definition, $\psi = v\, n\left(\overrightarrow{r},\hat{\Omega},E,t\right)$, and integrating over the entire solid angle gives

$$\phi_V = \frac{1}{V}\int\int\int v\, N\left(\overrightarrow{r},E,t\right) dE\, dt\, dV \qquad (2)$$

The reaction rate, R, can then be calculated by substituting the microscopic cross-section into the reaction rate definition, giving $R = N_a\phi_V$, where N_a is the atomic number density.

The MGB method is based on the principle of substituting $N\left(\overrightarrow{r},E,t\right) = \int n\left(\overrightarrow{r},E,t\right) d\Omega$ into equation 1 and changing the integrating variable from velocity to position, $ds = vdt$. This allows the particle flux to be given in terms of the particle track length.

$$\phi_V = \frac{1}{V}\int\int\int N\left(\overrightarrow{r},E,s\right) dE\, ds\, dV$$

Thus, for every particle which travels through and reacts within a cell, c, the distance travelled between subsequent reactions (track length), ds, is recorded in an energy bin, i, defined by the interval [E, E + dE]. At the end of the particle simulation, the track lengths are calculated for each energy bin within each cell.

$$\phi_c^i = \sum \frac{W^c T_l^i}{V_c}$$

Where W is a particle weighting used for improving statistics. The objective of this work is to produce an energy binning structure which results in a multigroup reaction rate definition that is statistically indistinguishable from the pointwise reaction rate. Given that nuclear cross-sections may embed a 5% uncertainty, the chosen energy structure must ensure the following requirement is fulfilled:

$$\left| 1 - \frac{\overline{\sigma_{MG}}}{\overline{\sigma_{MCE}}} \right| < 0.05 \quad (3)$$

III. Modelling

The optimum group structure was found using three phases of modeling, with each of the phases of calculation improving the convergence of the optimum solution in the {N_{slow}, N_{mid}, N_{fast}} domain. In order to ensure the optimized structure to be found is capable of meeting the criterion set in equation 3 for all reactions, all three models focus on the reaction rates which require the most resolved energy structure. These correspond to reaction rates with the most challenging and large resonance regions within their associated cross-section such as Ni-58 (n,γ), Cr-52 (n,γ), W-186 (n,γ), Fe-56 (n, n') and O-16 (n,α).

The spherical model used to create a generic fusion neutron spectrum has been designed using fusion relevant materials. Conceptually, a sphere with a 14.1MeV neutron source is a good representation of a fusion reactor. The low-, mid-, high-energy contributions to the reaction rate will change from being dominated by mid-high energy regions in zone 2 to being dominated by low-mid energy regions in zone 8. Hence, many variations of spectra will be tested in order to ensure that the final optimised energy structure is suitable for all fusion applications.

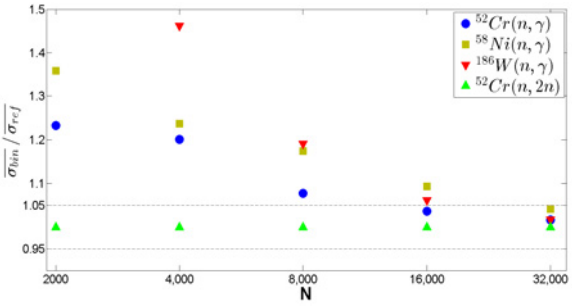

Figure 1: Phase 1 - The ratio of (n,γ) reaction rates calculated by the binning method, implementing an energy structure of 4000:N:4000, and the pointwise method for Cr-52, Ni-58 and W-186.

IV. Results

The error ratios of the phase 1 search for the optimum number of mid-energy groups, shown in figure 1, indicates that at least 20,000 bins are required in order to achieve the target of > 95% accuracy. Due to its larger average cross-section and finely structured resonance when compared to nickel and chromium, tungsten benefits the most from higher number of bins.

V. Conclusions

The optimal binning structure, named FOMG (Fusion Optimised Multi Group) is split into three distinct sections. The thermal energy region is defined in the range $10^{-5} eV \leq E_L < 1\ eV$ with 1,000 bins and an energy width of 1.0 meV. The mid energy group is defined in the range $1\ eV \leq E_L < 2\ MeV$ with 14,000 bins and a lethargy width of 1.036×10^{-3}. The high energy group is defined in the range $2\ MeV \leq E_H < 19.6\ MeV$ with 1,000 bins and an energy width of 17.6 keV.

A 16,000 bin structure has significantly more data points than most, but not all, of the directly accessed PENDF data files accessed by neutron transport codes, such as MCNP, during run time. For example, the number of some point-wise data components are Cr-52 (10,938), Fe-56 (10,097), H-1 (200), Ni-58 (15,962), O-16 (976) and W-186 (8,786). The significant decrease in computational expense is achieved by only accessing each of the PENDF files once at the end of the radiation transport simulation, as opposed to accessing and interpolating data from these files for every particle interaction that occurs. In addition to this, the FOMG structure is intended to be used as a unionised grid. Thus, the effective cross-section for each material can be calculated within the same loop of the code. An equivalent method, applied to a LWR system, led to an energy binning structure of 43,000 groups.

Examples of fission and fusion depletion calculations exist which use a low number of bins (VITAMIN-J [175 bins], WIMS [69 bins]). However, these often include an additional weighting parameter for each energy bin. These weighting parameters are optimised for a particlular reactor design, over a number of reaction cross-sections or for a set of important reactions. Thus, binning structures with a relatively low number of bins will undoubtedly suffer from self-shielding/dilution effects when calculating reaction rates which involve many cross-sections with significant resonances.

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